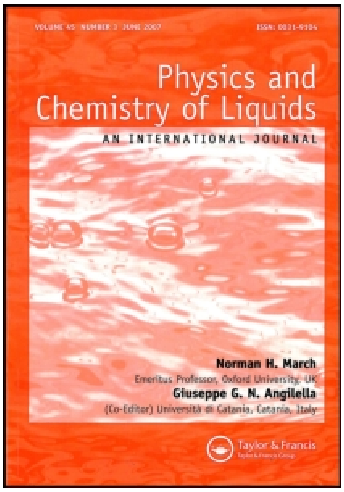

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Electrical transport properties of some liquid metals

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Electrical transport properties of some liquid metals

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In the present article, we report the electrical transport properties viz. the electrical resistivity (ρ), the thermoelectric power and thermal conductivity (σ) of several monovalent, divalent and polyvalent liquid metals of the different groups of the periodic table on the basis of model potential formalism. The well-known empty core model potential of Ashcroft is used for the first time with seven local field correction functions proposed by Hartree, Hubbard–Sham, Vashishta–Singwi, Taylor, Ichimaru–Utsumi, Farid *et al.* and Sarkar *et al.* in the present computation and found suitable for such study. In the calculation of these properties we have used the values of the theoretical structure factors due to hard core fluid theory. It is concluded that the comparisons of present and theoretical or experimental findings wherever exists are highly encouraging.

Keywords: Model potential; Electrical resistivity; Thermoelectric power; Thermal conductivity; Liquid metals

1. Introduction

During the last several years there has been an increasing interest in the properties of non-crystalline conductors such as liquid metals and liquid metallic alloys. Such a liquid exhibits metallic as well as fluid-like behaviour and hence can help to make a link between the theory of the liquid states and the theory of the electronic states in metals. And hence the study of electrical transport properties of liquid metals and their alloys remain one of the favourite quantities either experimentally or theoretically [1–24].

Despite the rich accumulation of experimental studies, the atomistic approach to the problem of the liquid metals had been very slow in progress, until Ziman [4,5] proposed the theory of electrical resistivity of liquid metals. Basically, there are three approaches for the theoretical investigations of transport properties of liquid metals. One is based on the nearly free electron picture [4,5], second one is the finite mean free path approach [6] and the third is based on tight-binding approximation [7]. The tight-binding approach usually involves either the average *t*-matrix approximation or the coherent

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potential approximation. A self-consisting approach corresponding to the finite mean free path is taking account of finite uncertainty in the electron momentum.

The Ziman's [4,5] nearly free electron (NFE) theory has been fairly successful in describing the quantitative behaviour of the electrical properties of simple liquid metals. This is because in these metals the mean free path is about 100 times the interatomic distance and the weak scattering picture should be valid. Even for the heavy polyvalent metals where the mean free path is only about two interatomic distances, the NFE model can yield results that are reasonable in agreement with the experiments. Calculations of electrical transport properties using structure factor from various experiments or different versions of bare ion potential and dielectric function, give correct order of magnitude but differ among themselves. In fact sometimes the theory is trusted sufficiently to use measured value of resistivity to determine the parameter of the potential. The Ziman's formula [4,5] is not expected to apply to d-state transition metals because the unfilled d-state cause strong resonant scattering which seems inappropriate for description by pseudopotential. Nevertheless, Evans *et al.* [8] put forward a version of equation of resistivity in which $|W(q)|^2$ was replaced by exact value of the squared matrix element for the scattering of a plane wave by a transition metal ion. The potential of the latter was taken to be Muffin–Tin potential as derived in solid state physics for band structure calculations and the exact scattering can be calculated by the phase shift method.

Kahjil and Tomak [17] have reported electrical resistivity of Sb, Bi, Sn and Pb liquid metals using Ziman's formula modified for finite mean free path. Daver *et al.* [18] have calculated resistivity and the mean free path using self-consistent method of about twenty liquid metals inclusive of noble metals. They have used the Ashcroft's empty core (EMC) pseudopotential [25], the parameter of the potential were chosen to yield the best agreement with the experimental structure factor. As they have fitted the potential parameter their results are very close to the experimental findings for simple metals while for Cu and Ag it deviates little. Very recently Geertsma *et al.* [19] have calculated density of states, resistivity and thermoelectric power (TEP) of liquid alkali metals and two liquid alloys Li–Na and Na–K. They have used linear response theory (LRT) to calculate the screened pseudopotential and the structure factor was obtained from the pair potential using modified hyper-netted chain (MHNC) theory of liquid. Their results of electrical resistivity for liquid alkali metals are very poor particularly for Li and Cs. Recently, Schnyders and Zytveld [20] have very carefully measured the electrical resistivity and thermoelectric power of liquid Ge and Si. They have also reported the electrical resistivity and thermoelectric power using the Ziman formalism, with a recent model pseudopotential and the experimental structure factor. They found that the thermoelectric power calculations are much more sensitive to the structure factor and evaluated this property using experimental structure factor but results were very poor while the resistivity deviates about 38% for Ge and 11% for Si, from the experimental data. Bose *et al.* [21] have reported the electrical transport properties of liquid Si and Ge semiconductors. Leavens *et al.* [22] have also calculated electrical resistivity using Ziman's formula and self-consistent approximation for liquid alkali metals Mg and Al. Their results of electrical resistivity using self-consistent approximation are better than Ziman's formula but could not avoid the reasonable deviation from the experimental findings. Ononiwu [23] has calculated the resistivity of all 3d, 4d and 5d transition metals using Ziman and *t*-matrix formula. Their *t*-matrix results are little close to the experimental findings for Ag, Au, Ni and Pd while Ziman's formula gives very high values for Au, Pt and Rh. Gorecki and Popielawski [24] have calculated the resistivity using self-consistent quasi-crystalline approximation. Their results are very poor. Recently, Baria [13,14] has reported electrical resistivities of some simple, non-simple as well as d- and f-shell metals. Also, Korkmaz and Korkmaz [15] have studied the temperature-dependent electrical resistivity of liquid alkali metals using Kubo formula [15]. Their temperature dependence results are found to be very close to the experimental data.

During the last several decades the concepts of pseudopotential have played an important role in the theory of liquid metals and their alloys [5–24]. Also, to the best of our knowledge after 1993, the electrical transport properties of such type of the liquid metals of the different groups of the periodic table have been reported by researchers very rare in the literature. Keeping in mind the cardinal features of these developments, in the present article we intend to report the electrical transport properties viz. electrical resistivity (ρ), TEP and thermal conductivity (σ) of several monovalent, divalent and polyvalent liquid metals of the different groups of the periodic table based on the well-known EMC potential of Ashcroft [25]. Hence, both the second and third approaches are beyond the confines of present objectives of the article as well as pseudopotential theory. So we will only be concerned with and concentrate on the first approach of nearly free electron theory of Faber [4,5]. In the present work, the theoretical structure factors are computed from the well-known Percus–Yevic (PY) hard sphere model with proper packing density [26]. Seven different types of the local field correction functions proposed by Hubbard–Sham (HS) [27, 28], Vashishta–Singwi (VS) [29], Taylor (T) [30], Ichimaru–Utsumi (IU) [31], Farid *et al.* (F) [32] and Sarkar *et al.* (S) [33] are employed for the first time to investigate the influence of exchange and correlation effects with reference to the static Hartree (H) [34] screening function in the present computations.

2. Theoretical methodology

The Faber [4,5] approach of investigating electrical resistivity of liquid metals assumes the model of a gas of conduction electrons that interact with and are scattered by irregularly placed metal ions. As an external electric field drives the electron through the disordered medium, the scattering determines the electrical resistance that can be calculated using perturbation theory: the transition rate from an initial state $|\mathbf{k}\rangle$ to the final state $|\mathbf{k}+\mathbf{q}\rangle$ on the Fermi level with the density of state is given by

$$P(\theta) = \frac{2\pi}{\hbar}\left|\langle \boldsymbol{k}+\boldsymbol{q}\right| W |\boldsymbol{k}\rangle\big|^{2}\frac{1}{2}N_{\mathrm{FE}}(E_{\mathrm{F}}), \tag{1}$$

where θ is the angle between k and $k+q$, the factor 1/2 arises from the fact that electron spin does not change on scattering. Now the conductivity in the relaxation time approximation is given by

$$\sigma = \frac{1}{3}e^{2}v_{\mathrm{F}}^{2}\tau N_{\mathrm{FE}}(E_{\mathrm{F}}). \tag{2}$$

Here e is electronic charge, v_F velocity of the electrons at the Fermi level and the relaxation time τ. The relaxation time τ is given by

$$\frac{1}{\tau} = \int (1 - \cos\theta) P(\theta) \mathrm{d}\Omega, \tag{3}$$

where θ is scattering angle, Ω is solid angle and $P(\theta)$ is probability for scattering through the angle θ.

Now assuming the free-electron distribution, an expression for the electrical resistivity of liquid metal in terms of the average of the product of the structure factor and pseudopotential matrix element can be written as [1–24]

$$\rho = \frac{3\pi m^2}{4e^2\hbar^3 n k_F^6} \int_0^\infty S(q) \left| V(q) \right|^2 q^3 \mathrm{d}q \theta(2k_F - q). \tag{4}$$

where n the electron density is related to Fermi wave number and θ is the unit step function that cuts of the q-integration at $2k_F$ corresponding to a perfectly sharp Fermi surface. Also, $S(q)$ is the PY-structure factor and $V(q)$ the screened ion pseudopotential form factor.

The expression of the TEP is given by [3,4]

$$\mathrm{TEP} = -\left(\frac{\pi^2 k_B^2 T}{3|e|E} \chi \right)_{E=E_F}, \tag{5}$$

with

$$\chi = 3 - \frac{2S(2k_F) V^2(2k_F)}{\left\langle S(q) \left| V(q) \right|^2 \right\rangle}, \tag{6}$$

It is well known that if a temperature gradient is applied to a metal the conduction electrons will carry a heat current along it even though an electric current is prevented from flowing and that indeed they are responsible for the major part of the thermal conductivity. The expression of σ for the liquid metal can be written as [3,4]

$$\sigma = \left(\frac{\pi^2 k_B^2 T}{3|e|^2 \rho} \right). \tag{7}$$

Here, e, E, E_F, T, k_B and χ are the electronic charge, energy, Fermi energy, temperature (in K), the Boltzmann's constants and the term of dimensionless thermoelectric power.

In the present work, we have used Ashcroft's well known EMC model potential [25] including seven different types of the local field correlation functions [27–34]. The form factor explored in the present investigation is of the form [25],

$$W(q) = \frac{-4\pi Z e^2}{\Omega_O q^2 \varepsilon(q)} \cos(q r_C), \tag{8}$$

where, Z is the valence, Ω_o the atomic volume, r_c the parameter of the potential and $\varepsilon(q)$ the modified Hartree dielectric function [34]. The parameter of the potential r_c may be set from appropriate experimental information (e.g. the Fermi surface or ionisation energy). In this instance, it was determined by the known electrical resistivities of the liquid metals at the melting points.

3. Results and discussion

The input parameters and constants used in the present computations are narrated in table 1. The input parameters are taken from the literature [2,17,18,34]. The presently computed results of electrical transport properties viz. ρ, TEP and σ of several liquid

Table 1. The input parameters and constants.

Metals	Z	Ω_O (au)	T (K)	η	r_C (au)
Li	1	146.46	453	0.46	0.97
Na	1	266.08	378	0.46	1.60
K	1	480.84	343	0.46	2.00
Rb	1	627.15	313	0.43	2.05
Cs	1	775.73	323	0.43	2.07
Rh	1.5	95.60	2236	0.45	0.71
Ir	1.5	99.80	2720	0.45	0.72
Cu	1.5	119.6	1423	0.46	0.69
Ag	1.5	173.06	1273	0.45	0.94
Ni	1.5	85.21	1773	0.45	0.59
Pd	1.5	113.87	1853	0.47	0.68
Pt	1.5	120.31	2053	0.47	0.68
Ti	1.5	129.3	2073	0.44	0.84
V	1.5	106.47	2273	0.44	0.78
Cr	1.5	92.90	2273	0.45	0.73
Mn	1.5	103.09	1633	0.45	0.69
Fe	1.5	89.25	1933	0.44	0.65
Co	1.5	85.74	1923	0.45	0.62
Zr	1.5	172.32	2273	0.44	0.92
Be	2	54.78	1562	0.45	0.75
Mg	2	157.68	1053	0.46	1.36
Ca	2	292.93	1223	0.46	1.61
Sr	2	381.17	1153	0.46	1.87
Ba	2	427.80	1103	0.46	2.38
Zn	2	103.27	823	0.46	1.28
Cd	2	145.55	723	0.45	1.01
Hg	2	157.68	393	0.45	1.57
Au	2	228.46	1423	0.46	0.74
La	2	216.63	1243	0.43	0.84
Yb	2	312.75	1123	0.43	0.8
Ce	2	265.24	1143	0.42	0.81
Th	2	222.98	2031	0.42	0.88
Eu	2	369.26	1203	0.42	0.95
Al	3	111.46	1043	0.45	1.12
Ga	3	131.99	423	0.43	1.17
In	3	175.90	533	0.45	1.28
Tl	3	194.00	688	0.45	1.45
Gd	3	254.93	1703	0.43	0.79
Si	4	121.48	1733	0.38	0.97
Ge	4	146.25	1253	0.38	1.007
Sn	4	180.85	623	0.43	1.04
Pb	4	203.86	713	0.46	1.41
Sb	5	205.26	903.9	0.4	1.33
Bi	5	238.56	544.6	0.4	1.4

metals are narrated in tables 2–4 with available experimental [2,4,16,17,20] or theoretical [2–4, 13–21] data whenever exists in the literature.

The comparisons for the presently calculated ρ of some liquid metals with available experimental [2,4,16,17,20] or theoretical [2–4,13–21] yielding are narrated in table 2. From table 2 it is noticed that the present results of ρ of the liquid metals are found in qualitative agreement with the experimental [2,4,16,17,20] or theoretical [2–4,13–21] findings. Also, it is noted that among the seven employed local field correction functions, the local filed correction function due to H (without exchange and correlation)

Table 2. Electrical resistivity (ρ) (in μΩ cm) of liquid metals.

	Present results								
Metals	H	HS	VS	T	IU	F	S	Expt. [2,4,16,17,20]	Others [2–4,13–21]
Li	21.87	27.09	33.09	38.76	41.37	42.33	30.57	24.7	4.58, 5.48, 7, 7.3, 13.76, 18.91, 20.95, 21.15, 23.2, 23.8, 24.7, 24.86, 25, 26.80
Na	8.42	10.96	13.79	15.51	17.11	17.31	12.53	9.6	5.3, 7.9, 8.44, 9.48, 9.82, 10.11, 10.25, 10.38, 13.58, 13.91, 15.8, 16.3, 18.50, 17.24, 37.7
K	10.28	13.80	18.21	20.58	23.07	23.33	16.19	13	11.1, 11.48, 11.61, 13.31, 13.60, 13.67, 14.06, 14.87, 15.38, 18.29, 18.5, 19.6, 20.27, 26.11
Rb	22.66	30.74	42.48	50.05	56.00	57.16	37.27	22.5	10, 14.70, 18.62, 19.8, 20.8, 20.97, 22, 23.09, 23.38, 23.55, 23.62, 26.85, 26.67, 30.66, 36.74
Cs	37.05	50.65	72.83	89.23	99.11	102.11	63.22	36	10, 13.8, 14.9, 15.44, 19.81, 20.71, 22.73, 31.29, 31.47, 32.25, 34.67, 39.73, 45.86, 50.44, 54.9, 62.71
Rh	51.28	60.69	70.12	81.07	84.88	86.88	64.90	–	50.10, 72.47, 94.74, 96, 196
Ir	53.15	63.01	72.99	84.52	88.54	90.64	67.60	–	70.17, 90, 95, 96.64, 105.85
Cu	79.13	94.16	110.33	129.16	135.08	138.62	102.39	20	10, 19, 19.85, 20.05, 21, 26.7, 30.78
Ag	62.72	76.37	91.90	108.15	114.52	117.41	85.16	19	9.96, 17.55, 20, 21.7, 26.97, 28.5, 40
Ni	65.83	77.30	88.68	102.52	106.84	109.43	81.96	85	27, 41.02, 41.4, 54.9, 55.36, 81.78, 87
Pd	75.46	89.49	104.49	122.25	127.58	130.96	96.96	83	16, 36, 41.07, 58.1, 65.99, 79, 84.30
Pt	82.11	97.58	114.34	134.11	140.00	143.76	106.15	90	22, 44.83, 62, 60.62, 90, 94.6, 99.75
Ti	53.30	64.12	75.55	87.87	92.73	94.90	70.05	400	–
V	47.17	56.25	65.44	75.64	79.57	81.37	60.62	200	–
Cr	44.77	52.99	61.12	70.49	73.87	75.55	56.55	80	–
Mn	62.85	74.50	86.48	100.43	105.11	107.67	80.13	180	–
Fe	57.84	68.24	78.52	90.63	94.78	96.99	72.61	140	–
Co	60.08	70.62	81.05	93.63	97.67	100.01	74.92	100	–
Zr	67.86	82.65	99.44	116.93	123.90	127.00	92.14	400	–
Be	11.75	13.80	15.30	16.83	17.79	17.98	13.84	–	17, 17.23, 19.19, 31.47, 54.9
Mg	23.79	28.02	32.46	37.93	38.98	40.12	30.28	26	16.42, 17.3, 23.7, 27.02, 29.13, 29.75, 59.08

(*Continued*)

Table 2. Continued.

	Present results								
Metals	H	HS	VS	T	IU	F	S	Expt. [2,4,16,17,20]	Others [2–4,13–21]
Ca	26.27	31.96	38.53	45.52	47.09	48.52	35.84	33	16, 26.4, 32.61, 33, 35.12, 52.45, 64
Sr	61.89	75.64	94.16	115.46	119.41	123.91	87.21	85	7, 61.1, 79.39, 82, 85, 87.12, 102.63
Ba	324.11	400.38	510.09	634.34	666.95	692.06	469.64	306	15, 290, 300.91, 306, 307.23, 449.22
Zn	36.22	41.82	47.49	55.29	56.77	58.40	43.94	37	11.64, 27.17, 35.6, 37, 37.83, 38.74,
Cd	30.44	37.09	43.35	49.06	52.80	53.56	40.02	34	11.08, 19.44, 23, 30.4, 37.83, 38.74, 53.04
Hg	83.32	97.92	114.43	135.81	140.46	144.81	106.43	91	30, 88.93, 90.93, 91.12, 102
Au	251.61	306.55	371.01	439.93	469.39	481.29	343.22	31	21.4, 27, 32.24, 34.95, 36.2, 41.26, 108
La	171.26	209.09	251.83	295.77	316.45	323.73	232.87	140	74.37,147.58,165, 332.07
Yb	325.78	403.61	501.01	599.53	643.63	660.63	461.72	110	90.17, 118.56, 137, 177.02
Ce	251.33	309.37	378.56	448.73	481.01	492.88	349.57	125	89.13, 127.17, 134, 267.33
Th	157.25	192.56	232.33	272.36	291.93	298.47	214.77	–	108.23, 137.21, 186.47
Eu	292.05	365.74	460.59	552.58	596.44	612.12	422.91	244	–
Al	20.76	24.02	26.77	30.23	31.24	31.90	24.58	24	12.17, 20.8, 21.65, 22.21, 25.58, 27, 34.12
Ga	21.87	27.09	33.09	38.76	41.37	42.33	30.57	26	23, 26, 29.63, 26.49, 81.18
In	8.42	10.96	13.79	15.51	17.11	17.31	12.53	33	30. 65, 31.94, 24, 33, 35.6, 40.75
Tl	10.28	13.80	18.21	20.58	23.07	23.33	16.19	73	60.7, 73.1
Gd	22.66	30.74	42.48	50.05	56.00	57.16	37.27	195	–
Si	37.05	50.65	72.83	89.23	99.11	102.11	63.22	66.8, 80	41.2, 45.5, 55, 57.4, 66.2, 75.9
Ge	51.28	60.69	70.12	81.07	84.88	86.88	64.90	60, 75.2	46.3, 57, 66.6, 57, 67.3, 69, 180
Sn	53.15	63.01	72.99	84.52	88.54	90.64	67.60	48	39.5, 42.6, 48, 52
Pb	79.13	94.16	110.33	129.16	135.08	138.62	102.39	95	57.46, 64, 68.9, 90.59, 94.57, 96.64, 121, 135.24
Sb	62.72	76.37	91.90	108.15	114.52	117.41	85.16	115	78, 83.5, 113.5, 113.5
Bi	65.83	77.30	88.68	102.52	106.84	109.43	81.96	128	86.4, 88.6, 128.1, 130

gives the minimum numerical value of the electrical resistivity, while the local field correction function due to F gives the maximum value. The present results of the ρ obtained from H-local field correction function for Li, Na, Rb, Cs, Mg, Ba, Zn, Hg and Sn, those obtained from HS-function for K, Pd, Pt, Ca, Cd, Al, Ga, Ge and Pb, those obtained from VS-function for Ni, those obtained from IU-function for Sb as well as Bi and those obtained from S-function for Sr and Si liquid metals are found very close to the experimental [2,4,16,17,20] or theoretical [2–4,13–21] data. The computed data of the ρ for Cu, Ag, Au, La, Yb, Ce and Eu are found higher while those for Ti, V, Cr, Mn, Fe, Co, Zr, In, Tl and Gd are found lower than available experimental [2,4,16,17,20] results. Hence, the resistivity calculations using well-known Ziman's formula are very inferior for all d- and f-shell metals. The experimental data for Rh, Ir, Be and Th are not available so our present results are predictive in nature.

In comparison with the presently computed results of ρ from static H-function, the percentile influences for Li, Na, K, Rb, Cs, Rh, Ir, Cu, Ag, Ni, Pd, Pt, Ti, V, Cr, Mn, Fe, Co, Zr, Be, Mg, Ca, Sr, Ba, Zn, Cd, Hg, Au, La, Yb, Ce, Th, Eu, Al, Ga, In, Tl, Gd, Si, Ge, Sn, Pb, Sb and Bi liquid metals of HS, VS, T, IU, F and S-functions are

Table 3. Thermoelectric power (TEP) (in μV K) of liquid metals.

	Present results								
Metals	H	HS	VS	T	IU	F	S	Expt. [2–4,20]	Others [3,16,20,21]
Li	−5.46	−5.56	−5.60	−5.54	−5.70	−5.67	−5.57	21.50	11.14, 13.5
Na	−8.75	−8.75	−8.75	−8.75	−8.76	−8.75	−8.75	−9.90	−8.67, −8.93
K	−11.84	−11.84	−11.84	−11.84	−11.84	−11.84	−11.84	−15.50	−11.69, −11.84
Rb	−12.45	−12.49	−12.48	−12.42	−12.51	−12.49	−12.47	−7.70	−12.53, −12.67
Cs	−13.82	−13.93	−13.94	−13.76	−14.06	−13.99	−13.89	6.40	25.23, 30.88
Rh	−15.00	−15.25	−15.37	−15.29	−15.67	−15.59	−15.29	–	–
Ir	−18.76	−19.06	−19.22	−19.12	−19.60	−19.50	−19.13	–	–
Cu	−10.32	−10.52	−10.64	−10.58	−10.92	−10.85	−10.57	−3.5	−4.44
Ag	−13.11	−13.32	−13.43	−13.33	−13.68	−13.61	−13.36	−1.9	−3.60
Ni	−10.44	−10.63	−10.73	−10.68	−10.97	−10.92	−10.66	7.8	2.25
Pd	−12.71	−12.98	−13.12	−13.06	−13.49	−13.41	−13.04	5.5	−2.53
Pt	−14.49	−14.79	−14.97	−14.89	−15.41	−15.31	−14.87		−2.03
Ti	−17.83	−18.09	−18.22	−18.11	−18.52	−18.44	−18.14	–	−4.07
V	−17.16	−17.40	−17.52	−17.43	−17.81	−17.73	−17.45	–	−4.71
Cr	−15.27	−15.50	−15.62	−15.54	−15.89	−15.82	−15.55	–	−5.29
Mn	−11.22	−11.42	−11.52	−11.46	−11.77	−11.71	−11.46	–	0.02
Fe	−12.29	−12.49	−12.60	−12.53	−12.84	−12.78	−12.53	–	7.60
Co	−11.54	−11.75	−11.85	−11.80	−12.11	−12.05	−11.79	0.6	1.91
Zr	−23.44	−23.81	−23.99	−23.83	−24.44	−24.32	−23.88	–	−6.16
Be	−7.97	−7.97	−7.97	−7.97	−7.97	−7.97	−7.97	–	–
Mg	−6.35	−6.52	−6.59	−6.52	−6.80	−6.74	−6.54	–	4.93, 5.28
Ca	−10.78	−11.14	−11.25	−10.97	−11.61	−11.47	−11.14	−1.6	−3.3
Sr	−12.30	−12.64	−12.85	−12.76	−13.48	−13.36	−12.73	0.06	−1.0
Ba	−15.53	−15.81	−16.04	−16.02	−16.63	−16.55	−15.93	0.03	0.8
Zn	−4.11	−4.18	−4.23	−4.22	−4.35	−4.33	−4.20	0.10	2.60, 3.05
Cd	−7.01	−7.02	−7.02	−7.01	−7.02	−7.02	−7.02	0.5	1.98, 2.32
Hg	−2.69	−2.74	−2.77	−2.77	−2.86	−2.85	−2.75	4.6	2.7
Au	−16.42	−16.55	−16.64	−16.60	−16.83	−16.79	−16.59	−0.6	−5.32
La	−14.07	−14.18	−14.24	−14.20	−14.37	−14.34	−14.21	1.1	0.34
Yb	−15.73	−15.88	−15.97	−15.92	−16.19	−16.14	−15.92	–	0.16
Ce	−14.48	−14.62	−14.69	−14.64	−14.86	−14.82	−14.65	0.7	0.96
Th	−23.60	−23.77	−23.87	−23.79	−24.08	−24.02	−23.81	–	–
Eu	−19.08	−19.25	−19.35	−19.27	−19.59	−19.54	−19.29	–	0.30
Al	−4.75	−4.83	−4.85	−4.82	−4.93	−4.90	−4.83	−2.10	−0.40, −0.87
Ga	−5.46	−5.56	−5.60	−5.54	−5.70	−5.67	−5.57	–	–
In	−8.75	−8.75	−8.75	−8.75	−8.76	−8.75	−8.75	0.82	1.20
Tl	−11.84	−11.84	−11.84	−11.84	−11.84	−11.84	−11.84	–	–
Gd	−12.45	−12.49	−12.48	−12.42	−12.51	−12.49	−12.47	–	–
Si	−13.82	−13.93	−13.94	−13.76	−14.06	−13.99	−13.89	−0.3	−1.4, −2.2, −3.5, −3.3, −6.4
Ge	−15.00	−15.25	−15.37	−15.29	−15.67	−15.59	−15.29	−2.1	−1.1, −3.6, −10.1
Sn	−18.76	−19.06	−19.22	−19.12	−19.60	−19.50	−19.13	0.6	1.30
Pb	−10.32	−10.52	−10.64	−10.58	−10.92	−10.85	−10.57	0.71	−4.86, −4.86, 2.6
Sb	−13.11	−13.32	−13.43	−13.33	−13.68	−13.61	−13.36	−0.3	1.60
Bi	−10.44	−10.63	−10.73	−10.68	−10.97	−10.92	−10.66	0.9	1.92

of the order of 23.87–93.55%, 30.17–105.58%, 34.24–126.95%, 35.66–152.25%, 36.71–175.60%, 18.35–69.42%, 18.55–70.54%, 18.99–75.18%, 21.76–87.20%, 17.42–66.23%, 18.59–73.55%, 18.84–75.08%, 20.30–78.05%, 19.25–72.50%, 18.36–68.75%, 18.54–71.31%, 17.98–67.69%, 17.54–66.46%, 21.79–87.15%, 17.45–53.02%, 17.78–68.64%, 21.66–84.70%, 22.22–100.21%, 23.53–113.53%, 15.46–61.24%, 21.85–75.95%, 17.52–73.80%, 21.84–91.28%, 22.09–89.03%, 23.89–102.78%, 23.09–96.11%, 22.45–89.81%, 25.23–109.59%, 15.70–53.66%, 23.87–93.55%, 30.17–105.58%, 34.24–126.95%, 35.66–152.25%, 36.71–175.60%, 18.35–69.42%, 18.55–70.54%, 18.99–75.18%, 21.76–87.20% and 17.42–66.23%, respectively.

Table 4. Thermal conductivity σ (in watt $K^{-1}cm^{-1}$) of liquid metals.

	Present results							
Metals	H	HS	VS	T	IU	F	S	Others [4]
Li	0.51	0.41	0.33	0.29	0.27	0.26	0.36	2.6
Na	1.10	0.84	0.67	0.60	0.54	0.53	0.74	2.2
K	0.81	0.61	0.46	0.41	0.36	0.36	0.52	2.1
Rb	0.34	0.25	0.18	0.15	0.14	0.13	0.21	–
Cs	0.21	0.16	0.11	0.09	0.08	0.08	0.12	2.4
Rh	1.06	0.90	0.78	0.67	0.64	0.63	0.84	–
Ir	1.25	1.05	0.91	0.79	0.75	0.73	0.98	–
Cu	0.44	0.37	0.31	0.27	0.26	0.25	0.34	–
Ag	0.50	0.41	0.34	0.29	0.27	0.26	0.36	–
Ni	0.66	0.56	0.49	0.42	0.41	0.40	0.53	–
Pd	0.60	0.51	0.43	0.37	0.35	0.35	0.47	–
Pt	0.61	0.51	0.44	0.37	0.36	0.35	0.47	–
Ti	0.95	0.79	0.67	0.58	0.55	0.53	0.72	–
V	1.18	0.99	0.85	0.73	0.70	0.68	0.92	–
Cr	1.24	1.05	0.91	0.79	0.75	0.73	0.98	–
Mn	0.63	0.54	0.46	0.40	0.38	0.37	0.50	–
Fe	0.82	0.69	0.60	0.52	0.50	0.49	0.65	–
Co	0.78	0.66	0.58	0.50	0.48	0.47	0.63	–
Zr	0.82	0.67	0.56	0.47	0.45	0.44	0.60	–
Be	3.25	2.76	2.49	2.27	2.14	2.12	2.76	–
Mg	1.08	0.92	0.79	0.68	0.66	0.64	0.85	–
Ca	1.14	0.93	0.77	0.66	0.63	0.62	0.83	–
Sr	0.45	0.37	0.30	0.24	0.24	0.23	0.32	–
Ba	0.08	0.07	0.05	0.04	0.04	0.04	0.06	–
Zn	0.55	0.48	0.42	0.36	0.35	0.34	0.46	3.2
Cd	0.58	0.48	0.41	0.36	0.33	0.33	0.44	2.5
Hg	0.12	0.10	0.08	0.07	0.07	0.07	0.09	2.75
Au	0.14	0.11	0.09	0.08	0.07	0.07	0.10	–
La	0.18	0.15	0.12	0.10	0.10	0.09	0.13	–
Yb	0.08	0.07	0.05	0.05	0.04	0.04	0.06	–
Ce	0.11	0.09	0.07	0.06	0.06	0.06	0.08	–
Th	0.32	0.26	0.21	0.18	0.17	0.17	0.23	–
Eu	0.10	0.08	0.06	0.05	0.05	0.05	0.07	–
Al	1.23	1.06	0.95	0.84	0.82	0.80	1.04	2.4
Ga	0.51	0.41	0.33	0.29	0.27	0.26	0.36	2.07
In	1.10	0.84	0.67	0.60	0.54	0.53	0.74	–
Tl	0.81	0.61	0.46	0.41	0.36	0.36	0.52	3.2
Gd	0.34	0.25	0.18	0.15	0.14	0.13	0.21	–
Si	0.21	0.16	0.11	0.09	0.08	0.08	0.12	–
Ge	1.06	0.90	0.78	0.67	0.64	0.63	0.84	–
Sn	1.25	1.05	0.91	0.79	0.75	0.73	0.98	2.9
Pb	0.44	0.37	0.31	0.27	0.26	0.25	0.34	2.4
Sb	0.50	0.41	0.34	0.29	0.27	0.26	0.36	2.6
Bi	0.66	0.56	0.49	0.42	0.41	0.40	0.53	2.5

The calculated results of ρ for Li, Na, K, Rb, Cs, Cu, Ag, Ni, Pd, Pt, Ti, V, Cr, Mn, Fe, Co, Zr, Mg, Ca, Sr, Ba, Zn, Cd, Hg, Au, La, Yb, Ce, Eu, Al, Ga, In, Tl, Gd, Si, Ge, Sn, Pb, Sb and Bi liquid metals deviate in the range of 9.68–71.38%, 12.29–80.31%, 6.15–79.46%, 0.71–154.04%, 2.92–183.64%, 295.65–593.10%, 230.11–517.95%, 3.58–28.74%, 9.08–57.78%, 8.42–59.73%, 76.28–86.68%, 59.32–76.42%, 5.56–44.04%, 40.18–65.08%, 30.72–58.69%, 0.01–39.92%, 68.25–83.04%, 7.77–54.31%, 3.15–47.03%, 2.60–45.78%, 5.92–126.16%, 2.11–57.84%, 10.47–57.53%, 8.44–59.13%, 711.65–1452.55%, 22.33–131.24%, 196.16–500.57%, 101.06–294.30%, 19.69–150.87%, 0.08–32.92%, 4.19–62.81%, 47.55–74.48%, 68.04–85.92%, 70.69–88.38%, 5.36–52.86%, 1.15–44.80%, 10.73–88.83%, 0.88–45.92%, 0.42–45.46% and 14.51–48.57% from the experimental data [2,4,16,17,20], respectively.

The comparisons for the presently calculated TEP of some liquid metals with available experimental [2–4,20] or theoretical [3,16,20,21] yielding are narrated in table 3. From table 3, it is noticed that the present results of the TEP of liquid metals are found in qualitative agreement with the experimental [2–4,20] or theoretical [3,16,20,21] findings. Also, it is noted that among the seven employed local field correction functions, the local field correction function due to H (without exchange and correlation) gives the minimum numerical value of the TEP, while the local field correction function due to IU gives the maximum value. The computed data of the TEP for Rb, Cu, Ag, Al, Si, Ge and Sb are found higher while those for Li, K, Cs, Ni, Pd, Co, Ca, Sr, Ba, Zn, Cd, Hg, Au, La, Ce, In, Sn, Pb and Bi are found lower than available experimental [2,4,16,17,20] results.

The percentile influences from static H-function on the TEP for Li, Rb, Cs, Rh, Ir, Cu, Ag, Ni, Pd, Pt, Ti, V, Cr, Mn, Fe, Co, Zr, Mg, Ca, Sr, Ba, Zn, Cd, Hg, Au, La, Yb, Ce, Th, Eu, Al, Ga, In, Gd, Si, Ge, Sn, Pb, Sb and Bi liquid metals of various local field correction functions are found of the order of 1.47–4.40%, 0.16–0.48%, 0.43–1.74%, 1.67–4.47%, 1.60–4.48%, 1.94–5.81%, 1.60–4.35%, 1.82–5.08%, 2.12–6.14%, 2.07–6.35%, 1.46–3.87%, 1.40–3.79%, 1.51–4.06%, 1.78–4.90%, 1.63–4.48%, 1.82–4.94%, 1.58–4.27%, 2.68–7.09%, 1.76–7.70%, 2.76–9.59%, 1.80–7.08%, 1.70–5.84%, 0.00–0.14%, 1.86–6.32%, 0.79–2.50%, 0.78–2.13%, 0.95–2.92%, 0.97–2.62%, 0.72–2.03%, 0.89–2.67%, 1.68–3.79%, 1.47–4.40%, 0.00–0.11%, 0.16–0.48%, 0.43–1.74%, 1.67–4.47%, 1.60–4.48%, 1.94–5.81%, 1.60–4.35% and 1.82–5.08%, respectively. Out of 44 liquid metals the experimental data of only 27 metals are available in the literature for comparisons. Large percentile deviation are found from the experimental data [2,4,16,17,20] in the computed results of the TEP for Li, Na, K, Rb, Cs, Cu, Ag, Ni, Pd, Co, Ca, Zn, Cd, Hg, Au, La, Ce, Al, In, Si, Ge, Sn, Pb, Sb and Bi liquid metals. But for liquid Li, Rb and Cs such calculations may be less reliable in view of the accuracies involved in the structure factor and pseudopotential results used. The negative sign of computed TEP for Li seems impossible to be predicted in terms of the usual pseudopotential formalism for simple metals, since the effect of the d-resonance above the Fermi level appears to give rise to the significant increase in the scattering amplitude in this metal.

The comparisons for the computed σ of some liquid metals with available theoretical [4] yielding are reported in table 4. From table 4 it is noticed that the present results of the σ of liquid metals are found in qualitative agreement with the theoretical [4] findings. Out of 44 liquid metals the theoretical data of only 14 metals are available in the literature for comparisons. Also, it is noted that, among the seven employed local field correction functions, the local field correction function due to F gives the minimum numerical value of σ, while the local field correction function due to H (without exchange and correlation) gives the maximum value. The computed data of the σ for Li, Na, K, Cs, Zn, Cd, Hg, Al, Ga, Sn, Pb, Sb and Bi metals are found lower than available theoretical results [4].

In comparison with the presently computed results of the σ from static H-function, the percentile influences for Li, Na, K, Rb, Cs, Rh, Ir, Cu, Ag, Ni, Pd, Pt, Ti, V, Cr, Mn, Fe, Co, Zr, Be, Mg, Ca, Sr, Ba, Zn, Cd, Hg, Au, La, Yb, Ce, Th, Eu, Al, Ga, In, Tl, Gd, Si, Ge, Sn, Pb, Sb and Bi liquid metals of various local field correction functions are of the order of 19.61–49.02%, 23.64–51.82%, 24.69–55.56%, 26.47–61.76%, 23.81–61.90%, 15.09–40.57%, 16.00–41.60%, 15.91–43.18%, 18.00–48.00%, 15.15–39.39%, 15.00–41.67%, 16.39–42.62%, 16.84–44.21%, 16.10–42.37%, 15.32–41.13%, 14.29–41.27%, 15.85–40.24%, 15.38–39.74%, 18.29–46.34%, 15.08–34.77%, 14.81–40.74%, 18.42–45.61%, 17.78–48.89%, 12.50–50.00%, 12.73–38.18%, 17.24–43.10%, 16.67–41.67%, 21.43–50.00%, 16.67–50.00%, 12.50–50.00%, 18.18–45.45%, 18.75–46.88%, 20.00–50.00%, 13.82–34.96%, 19.61–49.02%, 23.64–51.82%, 24.69–55.56%, 26.47–61.76%, 23.81–61.90%, 15.09–40.57%, 16.00–41.60%, 15.91–43.18%, 18.00–48.00% and 15.15–39.39%, respectively. The calculated results of the σ for Li, Na, K, Cs, Zn, Cd, Hg, Al, Ga, Tl, Sn, Pb, Sb and Bi liquid metals deviate in the range of 80.38–90.00%, 50.00–75.91%, 61.43–82.86%, 91.25–96.67%, 82.81–89.38%, 76.80–86.80%, 95.64–97.45%, 48.75–66.67%, 75.36–87.44%, 74.69–88.75%, 56.90–74.83%, 81.67–89.58%, 80.77–90.00% and 73.60– 84.00% from the theoretical data [4], respectively.

The numerical values of the electrical transport properties viz. ρ, TEP and σ are found to be quite sensitive to the selection of the local field correction function and showing a significant variation with the change in the function. Thus, the calculations of the electrical transport properties viz. ρ, TEP and σ are one of the sensitive tests for the proper assessment of the form factor of the model potential and in the absence of experimental information such calculations may be considered as one of the guidelines for further investigations either theoretical or experimental. In contrast with the reported studies, the present study spans the metallic elements of the different groups of the periodic table on a common platform of the model potential and common criteria for evaluating parameter of the model potential. This is very much essential for obtaining concrete conclusions.

It is apparent that for all liquid metals, using the resistivity model of Ziman [5], better calculated agreement with experimental values was obtained by allowing variation in atomic volume. One could conclude from this information that structure information in resistivity models seems to be required. In the present work, it has been found that one can try a well-known local EMC pseudopotential in the theory of the liquid metals. This EMC model potential is capable of giving satisfactory results for electrical transport properties of some liquid metals. But, it is absolutely necessary to examine the stability of the form factor against various local field correction functions before its application for the comprehensive study of metallic properties. This can give a unique combination of the bare ion pseudopotential with a proper local field correction function and hence one can also decide the nature of screening in the particular metal.

The improvement in the present findings may be achieved either by incorporating other forms of exchange and correlation effects or by suggesting the modification in determining the parameter of the potential. As the structure factor plays an important role in determining these properties, one can also include one-component plasma approximation [35], charge hard sphere approximation [36], soft sphere approximation [36] in the present calculations.

It is strongly emphasised previously by Esposito *et al.* [37] that the Ziman's formula describes electrical transport correctly for simple liquid metals while self-consistent results of resistivity are over estimates if mean free paths are comparable or smaller than interatomic distances, which happens in the d- and f-shell metals. In the present investigations, we have reported the electrical resistivity of simple and non-simple liquid metals using Ziman's formula. The present investigations confirm that the

Ziman's approach is the better choice for the resistivity calculations of simple and non-simple liquid metals.

4. Conclusions

Lastly we concluded that the electrical transport properties viz. ρ, TEP and σ of monovalent, divalent and polyvalent liquid metals of the different groups of the periodic table using EMC model potential and PY hard sphere model with seven different types of local field correction functions are reported for the first time. The EMC model potential with more advanced IU, F and S-local field correction functions generate consistent results regarding the electrical transport properties. Hence, the EMC model potential is found suitable for studying the electrical transport properties of liquid metals. Also, the present investigation predicts that the present study of the electrical transport properties is sensitive to the selection of the proper local field correction function.

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