Electronic transport properties of liquid lanthanides

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ABSTRACT

The electronic transport properties like electrical resistivity (ρ), thermoelectric power (Q) and thermal conductivity (σ) of liquid lanthanides are calculated through Ziman's formulism. To describe electron-ion interaction we have used our newly constructed parameter free model potential alongwith Percus Yevick hard sphere (*PYHS*) reference system. To see the influence of exchange and correlation effect on the electronic transport properties, we have used five different local field correction functions like Hartree (*H*), Sarkar *et al* (*S*), Taylor (*T*), Ichimaru Utsumi (*IU*) and Farid *et al* (*F*). The obtained results have found good in agreement with available experimental data as well as other theoretical data. Lastly, we conclude that, our newly constructed model potential is capable to explain the electronic transport properties of liquid lanthanides. Copyright © 2011 VBRI press.

Keywords: Electronic transport properties; electrical resistivity; thermoelectric power; thermal conductivity; liquid lanthanides.

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Introduction

The electronic transport properties of liquid lanthanides near the melting point have not been studied experimentally up to date, although the unique character of the electronic structure and the wide application of these metals in engineering and technology attract permanent interest in

their transport properties [1]. Electronic transport properties of liquid metals play a vital role in metallurgy. The theoretical investigation of electronic transport properties of liquid metals has been of considerable interest [1-24] for several years within pseudopotential formalism. Investigation of electronic transport properties needs a model potential which is adequate for the concerned systems. Another essential ingredient to investigate the electronic transport properties is the static structure factor $S(q)$ which involves the interionic interaction through statistical mechanics [2]. In any case, the theoretical values of the electrical resistivity are very sensitive to the accuracy of the structure factor [3]. Thus the theory of electronic transport properties requires a correct profile of structure factor $S(q)$. The experimental data on the structure factors obtained by neutron and X-ray diffraction methods are available only for some liquid lanthanides near their melting points [4]. The most popular method for studying the electronic transport properties of liquid metals is the electrical conduction theory developed by Ziman [5-21] using the concept of model pseudopotential. This concept has been extremely useful over the last few decades for simple liquid metals and liquid transition metals [5-21].

Ziman's theory is widely used to investigate the electrical resistivity [5-21]. Its starting point rest on first order time dependent perturbation theory [5]. Here the scattering potential is assumed to be much weaker than the kinetic energy of electrons. So the Born approximation would be valid. Ziman's theory successfully takes into account all multi-phonon processes, Debye-Waller factors, Umklapp process, couplings to transverse phonons and anharmonic phonon effects without going through an intermediate description of the lattice oscillations in terms of phonons. It proves to be successful for liquid simple metals and their alloys [6, 7]. Ziman's theory was further extended for noble and transition metals [8, 9, 11-21]. 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 more computationally expensive than Ziman's original theory [5-21]. It is reported that when the t-matrix is expanded for multiple scattering the second and third terms increase the resistivity only by 7% and 1%, respectively [3]. The first term of the expansion (comprising the single-site scattering alone) corresponds to Ziman's original formula for the resistivity. In addition, the results obtained from the extended theory show a limited success [3] when compared with data. A relativistic correction to the Ziman theory may be needed for accurate prediction. In our calculations we have not considered this effect assuming that it would be very small relative to other effects for transition metals. On the other hand, the Ziman's theory has a very simple form which is easy to handle numerically. Since we intend to investigate electronic transport of liquid transition metals we assume that Ziman's original theory [5-21], notwithstanding its limitations, is adequate for the present purposes [11].

There are very few attempts [13, 14] have been made on some liquid lanthanides. In our literature survey [5-21], we have found that only one attempt to study the electronic transport properties of full liquid lanthanides series. So that present paper deals with the calculation of electronic transport properties like electrical resistivity (ρ), thermoelectric power (Q) and thermal conductivity (σ) of liquid lanthanides using our model potential [24, 25] alongwith Percus Yevick hard sphere (PYHS) [26] reference system.

An important application of pseudopotentials is the calculation of electronic transport properties of disordered materials such as liquid, amorphous and their alloys. The problem with model pseudopotentials is that of their transferability, because still there is no accurate method to obtain the form factor by which all the properties of liquid metals may be successfully investigated. It is found that a particular pseudopotential may be suitable for some properties of some metals and unsuitable for other properties of other metals. The usefulness of any model potential depends on how many number of parameters it involves. Generally, the potential involving less number of parameters is considered to be, comparatively a better one than that involving more number of parameters because it avoids more complexities in the calculation. It has been observed that a unique method of determination of the potential parameter has not been pointed out so far. A number of investigators have used fitting procedure in which the potential parameters are fitted in such a way that a good agreement with experimental findings to be obtained. Such a procedure will generally give good results for a certain property, but the same set of parameters will not give good results for other properties. Hence, we thought it worthwhile to construct a parameter free model potential which, by employing, explains the physical as well as chemical properties of condensed matter.

A pseudopotential method employing a simple model of a solid composed of atomic cores and valence electrons can predict the existence and properties of new solids and their properties [27]. By implementing this idea we have constructed a new model potential which is splitted into three regions [24, 25],

$$
\begin{aligned}
W_B(r) &= 0; & r < r_i, \\
&= -\left(\frac{Ze^2}{r_a}\right)\left\{2 - exp\left(\frac{r}{r_a} - 1\right)\right\}; & r_i \le r \le r_a \\
&= -\left(\frac{Ze^2}{r}\right); & r > r_a
\end{aligned}
$$

---------------- (1)

Basically, this form of the pseudopotential is the modified version of the Ashcroft's empty core model [28]. Here we have considered actual core of an ion as an empty core rather than pseudizing it. The whole effective region is splitted into three parts. The effective weak potential felt by an electron is sandwiched between empty core and long range coulomb potential which is continuous at $r = r_a$ and is considered between the ionic radius (r_i) and atomic radius (r_a). Here we have included both the features of the

pseudopotential – cancellation as well as weak remaining interaction around the ion. Another important part of the model potential is that it is parameter free. In the reciprocal space, the corresponding bare-ion form factor is given by [**24, 25**],

$$W_B(q) = \frac{-4\pi Z e^2}{q^3 r_a \Omega (1 + q^2 r_a^2)^2} \begin{bmatrix} 2(1 + 2 q^2 r_a^2) \sin(q\ r_a) - q r_a (1 + 3 q^2 r_a^2) \cos(q\ r_a) + \\[4pt] 2(1 + q^2 r_a^2)^2 \{q\ r_i \cos(q\ r_i) - \sin(q\ r_i)\} \cdot \exp\left(\frac{r_i}{r_a} - 1\right) \\[4pt] \left\{ \left(-2q^3 r_a^3 + q^3 r_a^2 r_i + q^5 r_a^4 r_i\right) \cos(q\ r_i) - \right. \\[4pt] \left. \left(-q^2 r_a^2 + q^4 r_a^4 + q^4 r_a^3 r_i + q^2 r_a r_i\right) \sin(q\ r_i) \right\} \end{bmatrix} \quad \text{---------------- (2)}$$

Here *Z, e, Ω, q, r_i* and *r_a* are the valency, electronic charge, atomic volume, wave vector, ionic radius and atomic radius respectively. To see the influence of exchange and correlation effects on electronic transport properties, we have incorporated various local-field correction functions, viz; Hartree (H) [29], Sarkar *et al* (S) [**30**], Taylor (T) [**31**], Ichimaru Utsumi (IU) [**32**] and Farid *et al* (F) [**33**].

Theory

Within the pseudopotential formalism, the widely used Ziman's formula [**5-21**] for the electrical resistivity *(ρ)* of a nearly free electron liquid metal is,

$$\rho = \frac{3\pi m^2}{4 e^2 \hbar^3 n\, k_F^6} \int_0^{\infty} dq\, q^3\, S(q) |W(q)|^2 \theta(2k_F - q)$$

---------------- (3)

The thermoelectric power *(Q)* and thermal conductivity *(σ)* of liquid metals are respectively given by,

$$Q = -\frac{\pi^2 k_B^2 T}{3e\ E_F} \left[3 - \frac{2 S(2k_F)\ |W(2k_F)|^2}{\langle S(q)\rangle |W(q)|^2} \right]$$

---------------- (4)

And,

$$\sigma = \left(\frac{\pi^2 k_B^2 T}{3|e|^2 \rho} \right) \quad \text{---------------- (5)}$$

In equations (3)-(5) *m, e, n, k_F, S(q), W(q), θ(2k_F - q), k_B, T* and *E_F* are the electron mass, electronic charge, electron density, Fermi wave number, structure factor, screened electron ion pseudopotential form factor, unit step function, Boltzmann's constant, temperature and Fermi energy respectively.

Results and discussion

The input parameters [**1, 4**] used to perform present computations is tabulated in **Table 1**. The electrical resistivity *(ρ)*, thermoelectric power *(Q)* and thermal conductivity *(σ)* of liquid lanthanides are presented in tables 2-4, respectively along with the available experimental data [**4**] as well as other theoretical data [**1, 12, 13, 34-37**]. Here we take valency *(Z)* equal to 3 for all liquid lanthanides.

(3)

Table 1. The input parameters used in the present computations.

Metal	T (K) [1-2]	Density *n* (gm/cm³) [1, 4]	η [1, 4]	r_i (Å)	r_a (Å)
La	1243	5.95	0.43	1.06	1.87
Ce	1143	6.67	0.42	1.03	1.82
Pr	1233	6.61	0.43	0.90	1.82
Nd	1323	6.92	0.40	1.00	1.81
Pm	1353	6.92	0.48	0.98	1.63
Sm	1346	7.069	0.48	0.96	1.62
Eu	1103	4.61	0.42	0.95	2.00
Gd	1603	6.91	0.43	0.94	1.79
Tb	1653	7.24	0.43	0.92	1.76
Dy	1703	8.14	0.43	0.91	1.75
Ho	1753	8.25	0.43	0.89	1.74
Er	1793	8.37	0.44	0.88	1.73
Tm	1817	8.56	0.48	0.87	1.56
Yb	1123	6.2	0.43	0.86	1.94
Lu	1953	9.18	0.44	0.85	1.72

From **Table 2**, the present results for Gd, Tb, Ho and Yb are found in excellent agreements with the experimental data [**4**] and available theoretical data [**1, 12, 13, 34-37**] due to the Hartree (H) [**29**] local field correction function, whereas for Eu, Er, Tm and Lu, it is due to Taylor (T) [**31**] local field correction function. But for La, Ce, Pr, Nd, Pm and Sm, poor agreements have been achieved due to Hartree [**29**] local field correction function.

From **Fig. 1**, it is seen that the electrical resistivity (ρ) has minimum numerical values due to the Hartree (H) local field correction function while maximum due to the Farid *et al* (F) for all the liquid lanthanides. Another important noticeable point is that the different forms of the exchange and correlation functions have much sensible effect on the numerical values of the electrical resistivity (ρ). The Hartree local field correction function gives lower deviation from experimental data for liquid lanthanides compare to other local field correction function.

From **Table 3**, it is found that the effect of the local filed correction function on the numerical values of thermoelectric power (Q) is not much sensible as compare to the electrical resistivity. The thermoelectric power (Q) has minimum numerical values due to the Hartree (H) local field correction function while maximum due to the Ichimaru Utsumi (IU) [**32**] local field correction function.

Table 2. Electrical resistivity ($\mu \Omega$ cm) of liquid lanthanides.

| Metal	H [29]	S [30]	T [31]	IU [32]	F [33]	Others [1, 12, 13, 34-37]	Expt. [4]
La	354	498	599	644	652	171.26, 209.09, 251.83, 295.77, 316.45, 323.73, 232.87, 332.07	140
Ce	332	461	552	592	599	251.33, 309.37, 378.56, 448.73, 481.01, 492.88, 349.57, 267.63	125
Pr	201	279	335	358	362	139	-
Nd	301	416	498	533	539	157	-
Pm	271	377	451	485	490	164	-
Sm	245	342	409	440	445	182	-
Eu	184	264	326	350	355	292.05, 365.74, 460.59, 552.58, 596.44, 612.12	244
Gd	227	317	382	409	414	22.66, 30.74, 42.48, 50.05, 56.00, 57.16, 37.27	195
Tb	212	295	354	379	383	192	-
Dy	216	298	357	381	385	210	-
Ho	197	271	325	347	350	221	-
Er	187	258	308	329	333	226	-
Tm	164	226	270	289	292	237	-
Yb	134	189	230	246	250	325.78, 403.61, 501.01, 599.53, 643.63, 660.63, 461.72, 177.02, 114	110
Lu	167	229	273	291	294	230	-
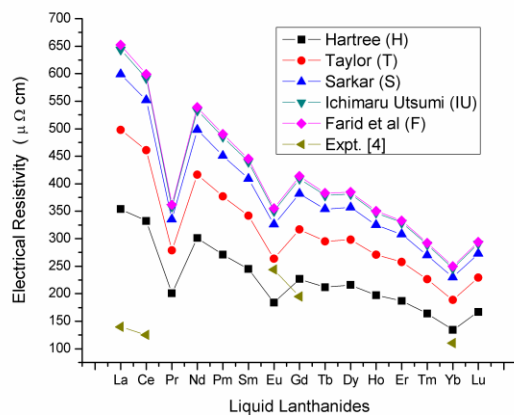
Fig. 1. Graph of calculated electrical resistivity versus liquid lanthanides.

Table 3. Thermoelectric power (μ V K) of liquid lanthanides.

Metal	H [29]	S [30]	T [31]	IU [32]	F [33]	Others [12]	Expt [4]
La	-11.98	-12.13	-12.12	-12.29	-12.27	-14.07,-14.18,-14.24,-14.20,-14.37,-14.34,-14.21	1.1
Ce	-10.25	-10.38	-10.37	-10.51	-10.50	-14.48,-14.62,-14.69,-14.64,-14.86,-14.82,-14.65	0.7
Pr	-10.84	-11.00	-10.99	-11.17	-11.15	-	-
Nd	-11.59	-11.75	-11.74	-11.92	-11.90	-	-
Pm	-12.22	-12.36	-12.35	-12.51	-12.50	-	-
Sm	-12.18	-12.33	-12.32	-12.49	-12.47	-	-
Eu	-12.31	-12.55	-12.54	-12.83	-12.80	-19.08,-19.25,-19.35,-19.27,-19.59,-19.54,-19.29	-
Gd	-14.68	-14.91	-14.89	-15.14	-15.11	-	-
Tb	-14.75	-14.97	-14.96	-15.21	-15.18	-	-
Dy	-14.42	-14.63	-14.61	-14.84	-14.82	-	-
Ho	-14.76	-14.97	-14.96	-15.20	-15.18	-	-
Er	-15.13	-15.34	-15.33	-15.58	-15.55	-	-
Tm	-15.29	-15.51	-15.50	-15.73	-15.71	-	-
Yb	-11.27	-11.48	-11.47	-11.72	-11.69	-15.73,-15.88,-15.97,-15.92,-16.19,-16.14,-15.92	-
Lu	-15.92	-16.15	-16.14	-16.39	-16.36	-	-

The improvements in the present results have been observed than others theoretical data [**12**] if it compares with the available experimental data [**4**]. As we have seen from the equation (4), the thermoelectric power (Q) is very sensitive to the size of the Fermi surface and hence depends on the behaviour of the scattering as k_F increases. It also depends on the magnitude of the pseudopotential $W_B(q)$ and structure factor $S(q)$. The value around three has been calculated for a free electron i.e. where the plasma potential is dominant so that most of the weightage comes from values of the structure factor $S(q)$ where q is not too close to $2k_F$. This gives the positive sign to the thermoelectric power (Q). But when the psudopotential is large, the resistance is determined by scattering vectors near $2k_F$ and the structure factor $S(q)$ is rising quickly in this region. At that time the negative values of the thermoelectric power (Q) is shown easily, simply by the great increase of scattering that is occurred when q is increased slightly. In liquid, the structure factor $S(q)$ increases more sharply near $q=2k_F$. This makes no difference where only small values of q are effective but clearly makes the thermoelectric power (Q) more negative when the effect of the ion core is large. Due to this all values of the thermoelectric power (Q) becomes negative.

From **Table 4**, it is noticed that the influence of the local field correction function is much effective on the numerical values of thermal conductivity (σ). Hartree (H) [**29**] produces maximum numerical value of thermal conductivity (σ) while Farid et al (F) [**33**] produces minimum to it. The present results are in good agreement with experimental data [**4**] for Gd and Yb due to the Hartree (H) [**29**] local field correction function whereas for Eu, it is due to Sarkar *et al* (S) [**31**] local field correction function.

From equation (3)-(5), it is found that electronic transport properties are mainly depend upon the structure factor $S(q)$ and model potential $W(q)$. From present results, it is observed that the discrepancy between present results and experimental data [**4**] goes on decreasing as the atomic number increases from La to Lu. These behaviours must be

related to the partial f shell of liquid lanthanides because the structural information experimentally obtained seems to be affected more or less by the electronic structure of outer shell for these elements which is clearly seen from **Fig. 1**. These results give qualitative support for the suggestion that a partial overlapping of one atom with another for the elements having a nearly empty f shell (i.e. La) is larger than that for the elements having a nearly filled f shell (i.e. Lu). Due to this phenomenon, present results for electronic transport properties gives poor results for La to Sm while better results for Eu to Lu.

Table 4. Thermal conductivity (watt K^{-1} cm^{-1}) of liquid lanthanides.

Metal	Thermal conductivity (watt K^{-1} cm^{-1})						
	H [29]	S [30]	T [31]	IU [32]	F [33]	Others [12]	Expt. [4]
La	0.09	0.06	0.05	0.05	0.05	0.18,0.15,0.12,0.10,0.10,0.09, 0.13	0.217
Ce	0.08	0.06	0.05	0.05	0.05	0.18,0.15,0.12,0.10,0.10,0.09, 0.13	0.223
Pr	0.15	0.11	0.09	0.08	0.08	-	-
Nd	0.11	0.08	0.06	0.06	0.06	-	-
Pm	0.12	0.09	0.07	0.07	0.07	-	-
Sm	0.13	0.10	0.08	0.07	0.07	-	-
Eu	0.15	0.10	0.08	0.08	0.08	0.10,0.08,0.06,0.05,0.05,0.05, 0.07	0.110
Gd	0.17	0.12	0.10	0.10	0.09	0.34,0.25,0.18,0.15,0.14,0.13, 0.21	0.201
Tb	0.19	0.14	0.11	0.11	0.11	-	-
Dy	0.19	0.14	0.12	0.11	0.11	-	-
Ho	0.22	0.16	0.13	0.12	0.12	-	-
Er	0.23	0.17	0.14	0.13	0.13	-	-
Tm	0.27	0.20	0.16	0.15	0.15	-	-
Yb	0.21	0.15	0.12	0.11	0.11	0.08,0.07,0.05,0.05,0.04,0.04, 0.06	0.245
Lu	0.29	0.21	0.17	0.16	0.16	-	-

Vora [**12**] and Baria [**14**] have calculated electrical resistivity of f shell liquid metal like La, Ce, Eu, Gd, Yb and Lu using the Ziman's formalism. They have fitted valency *(Z)* or potential parameter *(r_c)* in such a way that their results are found in good agreement with the experimental data. But the present study is free from any such type of fitting procedure. We have taken actual oxidation states (valancies Z) rather than fitting. Our potential is also parameter free model potential. Even though we have not taken any fitting procedure, our results are in quite good agreements with available experimental data [**4**] and available theoretical data [**1, 12, 14, 34-37**]. There are significant improvements in the present results are found in the case of electrical resistivity *(ρ)* (except La, Ce, Pr, Nd, Pm & Sm) and thermoelectric power *(Q)* than the others' results obtained by Vora [**12**] using the Ashcroft's empty core model potential [**28**]. This confirms the validity of our model potential to explain the electronic transport properties of liquid lanthanides.

Conclusion

The electronic transport properties of liquid lanthanides have been successfully investigated by Ziman's [**5-21**] formula along with our newly constructed parameter free model potential. The electronic transport properties are much sensitive to the choice of different form of local field correction functions and structure factor *S(q)*. The structure factor *S(q)* due to the Percus-Yevick hard sphere (PYHS) [**26**] reference system is also capable to explain the electronic transport properties of liquid lanthanides. So application of our newly constructed model potential in the present study definitely adds new contribution to understand the electronic transport properties of liquid lanthanides. Thus the proper choice of the model potential along with the local field correction function and structure factor *S(q)* plays a vital role in the study of the electronic transport properties of liquid lanthanides.

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