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REGULAR ARTICLE

A Unified Study of Electrical Transport Properties of Some Liquid Alkali Elements by Pseudopotential Approach

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A well established local pseudopotential of Fiolhais et al. is used to study the electrical transport properties i.e. electrical resistivity, thermal conductivity and thermoelectric power (TEP) of some liquid elements using model pseudopotential theory with Ziman's and mean free path models. Taylor's local field correction function is utilized to investigate the exchange and correlation effect on the said properties. The one component plasma (OCP) method is adopted for computing the structure factor of liquid metals. The presently obtained results are compared well with other such outcomes wherever exists and found fruitful.

Keywords: Model potential, Ziman formula, Mean free path, Electrical transport properties, Liquid metals.

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1. INTRODUCTION

Since a very long time ago, liquid metals, especially the mono nuclear ones, have been seen of as the prototype for basic liquids since they include many of the same physical characteristics as real liquids without the complications that might be present in a particular framework [1]. Despite this, metallic liquids of comparable thickness and consistency to water, like liquid sodium, find use as coolants in atomic reactors. Due to these factors, liquid metals in non-crystalline frameworks are the focus of the majority of recent research [1].

It is possible to imagine liquid metals as mixtures of electrons and particles. The middle electrons, a portion of the electrons that are still close to the centres, are unintentionally touched by the atomic evolution. The remaining electrons (valence electrons), which are flexible through particle assembly, are in charge of giving liquid metals their vehicle and solid properties [2-10]. The electrical resistivity (ρ), thermoelectric power (TEP), and thermal conductivity (σ) of several simple liquid metals were reported by us in the current work with the aid of pseudopotential theory. For the purpose of describing the electron-ion interaction in these systems, Fiolhais et al.'s [11] well-known universal model potential is of the form.

$$V(r) = -\frac{Z}{R}\langle\frac{1}{x}[1-(1+\beta x)e^{-\alpha x}] - Ae^{-x}\rangle \qquad (1.1)$$

The work of Fiolhais and colleagues [11] provides additional details for this potential.

One of the most often used formulas for calculating the resistivities of binary alloys and liquid metals is the Ziman formula [3]. This formula [4] involves a finite integral over the product $q^3S(q)|w(q)|^2\theta(2k_F-q)$. Where $\theta(2k_F-q)$ is the unit step function which cuts of the integration at $2k_F$ corresponding to a perfect sharp fermi sphere. Some attempts have been made to show this formalism of ziman [3-8] is insufficient and different expressions have been suggested i.e. nearly free electron picture [3-5], finite mean free path approach [6], t-matrix approximation [6]. Ünal and Alkan [12] have proposed that Ziman formula which is not a function of the temperature clearly is not well suited to obtain correct temperature behaviour of the electrical resistivity of any liquid metal because at a finite temperature some electrons are transferred above Fermi surface and Fermi sphere is not completely full. In this present work we have calculated electrical resistivities using Ziman and mean free path formula [3, 6] for liquid Li, Na, K, Rb and Cs near the melting point. To investigate the impact of exchange and correlation effects with reference to static Hartree (HR) screening function in the current computation, we used the individual version of local pseudopotential proposed by Fiolhais and coworkers [11] including two different types of local field correction functions by Taylor (TY) [13].

Using Ziman's formula adapted for finite mean free path, Baria [6] have calculated the electrical resistivity of liquid metals. For around eight liquid metals, The one component plasma (OCP) approach is used to determine the static structure factor for this work, $S(q)$ [10]. Our theoretical conclusions and test results have been contrasted [1].

2. THEORY

The well-known Ziman equation [3] for the resistivity of a liquid metal is

$$\rho = \frac{3\pi m^2}{4Ze^2\hbar^3 n_e {k_F}^6}\int_0^\infty q^3S(q)\ S(q)|w(q)|^2\theta(2k_F-q)dq \qquad (2.1)$$

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Where $S(q)$ is the OCP-structure factor, $w(q)$ is the screened ion pseudopotential, n_e is the electron density and which is related to fermi wave vector k_F by $k_F = (3\pi^2 n_e)^{1/3}$, e is the electron charge, m is the electron function and $\hbar = h/2\pi$, h is planck constant. The unit step function θ is defined as,

$$\theta(2k_F - q) = 0 \quad for \quad q > 2k_F$$
$$= 1 \quad for \quad q \leq 2k_F \qquad (2.2)$$

The alternative resistivity expression based on mean free path formula suggested by Baria [6] is

$$\rho = \frac{3\pi^2 m^2}{4Ze^2\hbar^3 n k_F{}^6} \int_0^\infty dq q^4 S(q)|w(q)|^2 \Gamma(q, k_F, l), \quad (2.3)$$

which must be solved self consistently. Very few explicit approximations are proposed for the function $\Gamma(q, k_F, l)$. In this work we used this form

$$\Gamma(q, k_F, l) = \frac{2}{\pi^3 q}\left[tan^{-1}(ql) - \frac{1}{2}tan^{-1}\frac{2ql}{1+4(k_F l)^2-(ql)^2} - \frac{\pi}{2}\theta\left(q - \left(\frac{1}{l^2} + 4k_F{}^2\right)^{\frac{1}{2}}\right)\right] \qquad (2.4)$$

The mean free path is determined self consistently. The first step of the self-consistency loop is to calculate ρ by using (2), i.e. with $l = \infty$. A new l is then calculated from the Drude relation.

$$\rho = \frac{hk_F}{ne^2 l} \qquad (2.5)$$

In this study, we used a pseudopotential developed by Fioalhais and colleagues [18], whose parameters were established in the solid state and which is claimed to be transferable to other environments, such as liquids, without changing the parameters' values. An analytical expression for the unscreened form factor of this pseudopotential in Fourier space is

$$w(q) = 4\pi Z R^2\left[-\frac{1}{(qR)^2} + \frac{1}{(qR)^2+\alpha^2} + \frac{2\alpha\beta}{[(qR)^2+\alpha^2]^2} + \frac{2A}{[(qR)^2+1]^2}\right], \qquad (2.6)$$

where R is the core decay length with $\alpha > 0$. The parameters A and β are expressed in terms of α as

$$A = \frac{\alpha^2}{2} - \alpha\beta, \qquad (2.7)$$

$$\beta = \frac{\alpha^3 - 2\alpha}{4(\alpha^2 - 1)} \qquad (2.8)$$

The values α and R are fitted by Fiolhais et al. [11] in order to reproduce dominant electronic density features of the solid.

The thermoelectric power (TEP) is given by [3]

$$TEP = -\left(\frac{\pi^2 k_B{}^2 T}{3|e|E}\chi\right)|_{E=E_F} \qquad (2.9)$$

where,

$$\chi = 3 - \frac{2S(2k_F)V^2(2k_F)}{\langle S(q)|w(q)^2|\rangle}. \qquad (2.10)$$

Where, $V(q)$ is the screened ion potential, $S(q)$ is the structure factor, $2k_F$ corresponding to a perfectly sharp fermi sphere.

The articulation for thermal conductivity (σ) for liquid metals can be given by [3]

$$\sigma = \frac{\pi^2 k_B{}^2 T}{3e^2\rho} \qquad (2.11)$$

3. RESULTS & DISCUSSION

Table 1 provides a description of the input parameters and constants used in the current computations. The literature has been consulted for the input parameters [3, 4, 11]. The results of the electrical resistivity (ρ) calculations for liquid alkali metals are shown in Table 2 together with any relevant experimental [1, 18] or theoretical [1-3, 6, 8, 10] data that is currently available.

Table 1 – Input parameters and constants

Metal	Z	Ω (au)	T (K)	ξ	Γ
Li	1	142.47	453	0.46	210.62
Na	1	254.25	378	0.46	206.45
K	1	480.84	343	0.46	183.35
Rb	1	588.98	313	0.43	187.86
Cs	1	743.53	323	0.43	180.21

Here Z is the valency, Ω is the atomic mass in atomic units, T is the temperature in kelvin, ξ is the packing fraction and Γ is the plasma parameter. The presently calculated resistivity ρ of some simple liquid alkali metals with available experimental [1, 18] or theoretical [1-3, 6, 8, 10] data are described in Table 2.

Table 2 – Electrical resistivity (ρ) (in $\mu\Omega\ cm$) of liquid alkali metals

Metal	Ziman		MFP		Expt.	Others [1-3, 6, 8, 10]
	HR	TY	HR	TY	[1, 18]	
Li	8.69	24.06	3.58	23.75	24.7	4.58, 5.47, 7, 7.13, 13.76, 18.91, 20.95, 21.15, 23.2,23.8
Na	13.42	7.99	4.73	7.91	9.6	5.3, 7.9, 8.44, 9.48, 9.82, 10.11, 10.25, 10.38, 13.58, 13.91
K	34.31	14.22	9.30	14.06	13	11.1, 11.48, 11.61, 13.31, 13.60, 13.67, 14.06, 14.87, 15.38
Rb	49.57	18.67	24.40	18.45	22.5	10, 14.70, 18.62, 22.66, 23.09, 23.38, 23.55, 26.82
Cs	56.13	21.93	37.80	21.66	36	10, 13.8, 14.9, 15.44, 19.81, 20.71, 22.73, 32.25, 37.05

The local field correction function due to HR (without exchange or correlation), according to the above table, produces the lowest value of electrical resistivity, whereas the local field correction function due to TY, gives the highest value. The computed values for Na, Rb, and Cs from the HR-local field correction function are remarkably similar to the experimental [18] or theoretical [1-3, 6, 8, 10] data. In comparison to known experimental [18] results, the computed data of the for Na and K are found to be greater, while those for Li, Rb, and Cs are found to be lower.

Table 3 – Thermoelectric power (TEP) (in μVK) of liquid alkali metals

Metal	Ziman		MFP		Expt. [1, 18]	Others [1-3, 6, 8, 10]
	HR	TY	HR	TY		
Li	– 5.64	– 5.96	– 14.11	– 5.97	21.5	– 5.46, – 5.56, – 5.60, 11.14, 13.5
Na	– 15.09	– 16.43	– 10.82	– 16.44	9.90	– 8.75, – 8.67, – 8.93
K	– 4.88	– 4.87	– 8.61	– 4.87	15.50	– 11.84, – 11.69, – 11.84
Rb	– 6.67	– 7.56	– 3.50	– 7.56	7.70	– 12.45, 12.49, – 12.53, – 12.67
Cs	– 10.62	– 11.93	– 5.31	– 11.94	6.40	– 13.82, – 14.06, 25.23, 30.88

The percentile variation for Li, Na, K, Rb, and Cs liquid metals of TY function are of the order up to 3.7 %, 36 %, 33 %, 0.9 %, and 0.02 % respectively, compared to currently computed findings of from static HR-function. It can be seen that accounting for atomic volume variation improved the predicted agreement with experimental results for all liquid alkali metals when utilizing the resistivity model of mean free path. It has been discovered in the current work that one can test a well-known local Fiolhais pseudopotential in the theory of liquid metals. This potential is extremely capable of providing data for the electrical resistivity of various liquid metals that are satisfactory. But before applying it to the thorough investigation of metallic characteristics, it is imperative to check the form factor's stability against a variety of local field correction functions. By combining the bare ion pseudopotential with an appropriate local field correction function, this can produce a special kind of screening in the particular metal.

If we discussed regarding the percentile variation for the thermoelectric power than it would be 21 %, 14 %, 15 %, 6.75 % and 4.74 % in comparison with the available experimental data if we move from Li → Cs.

Table 3 – Thermal conductivity (σ) (in $watt\ K^{-1}cm^{-1}$) of liquid alkali metals

Metal	Ziman		MFP		Expt. [1, 18]	Others [1-3, 6, 8, 10]
	HR	TY	HR	TY		
Li	0.12	0.87	0.31	0.30	2.6	0.51, 0.41, 0.33, 0.29, 2.6
Na	0.68	0.62	0.18	0.19	2.2	1.10, 0.84, 0.67, 0.60, 2.2
K	0.24	0.23	0.90	0.89	2.1	0.81, 0.61, 0.46, 0.41, 2.1
Rb	0.16	0.15	0.32	0.31	–	0.34, 0.25, 0.18, 0.15,
Cs	0.13	0.10	0.15	0.14	2.4	0.21, 0.16, 0.11, 0.09

Finally, the percentage change in the thermal conductivity will be 9 %, 14 %, 20 % and 23 % respectively for Li, Na, K and Cs as the experimental data for Rb is not available in the literature. The structure factor is crucial in determining these features, and in the current computation, one can also take into account the charged hard sphere approximation [15], the one-component plasma approximation [10], the optimized random phase approximation [16], and the soft sphere approximation [17]. The current investigation supports the notion that, for calculating resistivity for both simple and non-simple liquid metals, the Mean free path formula is the preferable option.

4. CONCLUSION

Finally, we draw a conclusion that electrical resistivity of liquid alkali metals is reported here using the models of Ziman and Mean free path with two alternative types of local field correction functions and the local pseudopotential of Fiolhais and coworkers are found consistent with the available theoretical or experimental data available in the literature. So, we can say that the afore-mentioned pseudopotential is more sophisticated TY field correction function are consistent. Therefore this potential is appropriate for the calculation of the electrical transport properties.

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Уніфіковане дослідження електротранспортних властивостей деяких рідких лужних елементів методом псевдопотенціалу

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Добре встановлений локальний псевдопотенціал Fiolhais et al. використовується для вивчення властивостей електричного транспорту, тобто питомого електричного опору, теплопровідності та термоелектричної потужності (ТЕП) деяких рідких елементів за допомогою модельної теорії псевдопотенціалу з моделями Зімана та середньої довжини вільного пробігу. Функція корекції локального поля Тейлора використовується для дослідження ефекту обміну та кореляції на зазначені властивості. Метод однокомпонентної плазми (OCP) використовується для обчислення структурного фактора рідких металів. Отримані на даний момент результати добре узгоджуються з результатами інших авторів і визнані ефективними.

Ключові слова: Модельний потенціал, Формула Зимана, Довжина вільного пробігу, Електротранспортні властивості, Рідкі метали.