Concept behind plasma and structural resistivities of liquid alkali metals

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The electrical resistivity of liquid alkali metals has been discussed on the basis of Ziman formulation with special emphasis to plasma and structural contributions. Two earlier relationship of Ascarelli et al., [Adv Phys, 16 (1967) 263, 717] [APH], (i) \( s(q)=(\{[(\phi(q))k_BT]+1\}^{1/2}) \) and (ii) \( \phi(q)=(4\pi^2/\Omega^2)u(q) \) have been improved and utilized in evaluating the plasma resistivity of alkali metals. The validity of modified form [Indian J Pure & Appl Phys, 28 (1990) 397] of structure factor-pair potential relationship \( s(q)=\{(\phi(0)U(q)/k_BT)+1\}^{1/2} \) has been tested herein evaluating plasma resistivity \( \rho_{PL}^{p} \). There appears an important role of total electronic band structural energy \( G(q) \) to the transport problems. This analogy has produced already satisfactory results of liquid phonon frequencies of alkali metals and here also the obtained results of resistivity are improved than \( \rho_{PH}^{P} \) values. The study confirms the validity of following formulae too: \( s(r)=(k_BT)/(2\pi^2\Omega r) \) and \( s(r)/u(r)^2=(2/3\pi^2\Omega r)k_BT=0.1 \) \( u_{r}^{2} \) where \( u_{r} \) is of the order of nearly 0.5 \( |U(r)| \).

1 Introduction

In the last three decades and a half the pioneer contribution of Ziman\(^1\) for the quantitative theory of electrical conductivity of metals in liquid phase based on the nearly-free-electron (NFE) model has given a new orientation to the area of liquid metals. He suggested to substitute a pseudopotential for the full atomic potential in the function \( U(q) \) of the form like; \( U(q) \approx -2/3E_F \) \( (1+q^2/q_s^2) \) for smaller values of momentum transfer, \( q \). The elementary notion behind \( U(q) \) is that the field of an ion, outside its core, is approximately a screened Coulomb potential of the Gerstenkorn\(^2\) form \( (-Ze^2/4\pi\epsilon_0 r) e^{-q^2/q_s^2} \); \( q_s \) is screening parameter. For the behaviour of \( U(q) \) over the range of integration from 0 to \( 2k_F \) limit he described that it depends sensitively upon atomic potential within the ion core.

Recently one of the author Srivastava\(^3\) has given full attention about the separation of plasma \( (\rho_{PL}^{p}) \) and structural \( (\rho_{PL}^{s}) \) contribution of the resistivities as desired in Ziman's ideology\(^1\). It is observed that the quantity \( s(q)/U(q) \) is almost the same at the both ends in the range of integration \( q=0 \) and \( q=2k_F \). Truly speaking, that in past all the quantitative calculations\(^4\), of electrical resistivity of liquid metals based on different pseudopotential modellings and structure factors deviate from above notion. It has been realized that the dominant part of the resistivity arises as one moves away from the cut off region \( q=1.4k_F \) of the potential \( U(q) \) towards highest integration limit \( q=2k_F \). Generally, before the cut off region \( q=1.4k_F \), \( U(q) \) is negative while after it is positive.

Ascarelli et al.\(^8\) have used an important relationship between the structure factor \( s(q) \) and the Fourier component of the interatomic potential \( \phi(r) \) in the region of smaller values of \( q \) in the estimation of plasma resistivity \( \rho_{PL}^{p} \) for alkali metals. Their estimated values of \( \rho_{PL}^{p} \) were not so closer to corresponding experimental values. However, the results were very good in case of Na and Rb. The main objectives of our present paper are the following:

(i) To give new insight to the plasma \( (\rho_{PL}^{p}) \) and structural \( (\rho_{PL}^{s}) \) resistivities by separation in the resistivity formula; (ii) To look again the Ascarelli et al.\(^8\) estimations of plasma \( (\rho_{PL}^{p}) \)-resistivity and their relationship between \( U(q) \) and \( \phi(q) \) quantities for smaller values of \( q \); (iii) To look again the present status of the electrical resistivity of liquid alkali metals.

2 Mathematical Analysis

The Fourier transform of interatomic potential \( \phi(r) \) (a quantity of bond structure) is given by\(^5\):

\[
\phi(q) = (4\pi^2Z^2/\Omega^2q^2)[1-G(q)]
\]

where

\[
G(q) = (4\pi Z^2/\Omega^2q^2)^2 \frac{U(q)}{v(q)} \{v(q)-1\}
\]
where \( G(q) \) is total electronic-band structure energy function (called as Cochran Function), \( U(q) \) is screened pseudopotential and \( \varepsilon(q) \) is dielectric screening constant. Substituting the value of \( G(q) \) from Eq.(2) in Eq. (1), we get:

\[
\phi(q) = [4\pi^2e^2\Omega q^2]^{-1} U^2(q) \varepsilon(q) + [4\pi^2e^2\Omega q^2]^{-1} U(q) \varepsilon(q)
\]  

\( \ldots (3) \)

Ascarelli \textit{et al.} \textsuperscript{8} have applied the second-term of Eq.(3) only for the relationship between the quantities \( \phi(q) \) and \( U(q) \) for smaller values of \( q \) in the following relationship:

\[
s(q) = [(\phi(q) / k_B T) + 1]^{-1}
\]  

\( \ldots (4) \)

and described \( \rho_{PL} \) as:

\[
\rho_{PL} = 3 \pi n q^2 / 4 E_F^2
\]  

\( \ldots (5) \)

It has been observed earlier \textsuperscript{9} that Eq.(4) is failure in describing phonon spectrum of liquid metals. Finally two important formulae \textsuperscript{3,5}:

\[
s(q) = [(\phi(0) G(q) / k_B T + 1)]^{-1}
\]  

\( \ldots (6) \)

\[
s(q) \phi(q) = q k_B T
\]  

\( \ldots (7) \)

describe the resistivity integrand as:

\[
<s(q) U^2(q)>
\]  

\( \ldots (8) \)

\[
= \frac{4\pi^2 e^2 \Omega q^2}{1 - s(q)} \frac{1}{\varepsilon(q)} \left[ \frac{1}{\varepsilon(q)} \left[ 1 - s(q) - 1 \right] \right]\]

\( \ldots (9) \)

which is different than Ascarelli \textit{et al.} \textsuperscript{8}, consideration:

\[
<s(q) U^2(q)>
\]  

\( \ldots (10) \)

In deriving Eq. (8) here we have given full respect to Eq.(3).

3 Numerical Computation and Results

We have computed plasma resistivity \( \rho_{PL} \) by using Fig. (8) in the well-known electrical resistivity formula\textsuperscript{1}. In such calculations we have employed the same experimental and theoretical structure factors data as above. In order to see the role of dielectric screening, we have used two different forms of \( \varepsilon(q) \). (i) Static Hartree dielectric screening and (ii) Singwi \textit{et al.} \textsuperscript{12}, dielectric screening\textsuperscript{12}. The obtained results are presented in Table I together with theoretical values of \( \rho_{APH} \) (Ascarelli \textit{et al.} \textsuperscript{8} values) and experimental \( \rho_{exp} \) values. The results obtained from experimental and theoretical \( s(q) \) data are differentiated by putting symbol \( E \) and \( T \), respectively on top of \( \rho \) values similarly symbol Static and Singwi written in suffix positions of \( \rho \) values differentiate results obtained from two different dielectric screenings.

The results \( \rho_{Static} \) of metals given in forth column of Table I are more closer to the experimental value \( \rho_{exp} \).
except for Na, while the results $\rho_{\text{Static}}$ of column seventh are quite satisfactory in case of Li and for remaining metals the results are almost similar. The results of $\rho_{\text{Singew}}$ are more closer to experimental values as compared to $\rho_{\text{Singew}}^E$. It is observed that the values $\rho_{\text{Singew}}^T$ for Na and K are excellent as compared to other metals and $\rho_{\text{Singew}}^E$ values. The results of Li and Cs are much improved in case of $\rho_{\text{Static}}^E$ and $\rho_{\text{Static}}^T$ as compared to $\rho_{\text{APH}}^E$ values of Ascarelli et al. (APH). Also in results in case of Na and K for $\rho_{\text{Singew}}^T$ values are excellent as compared to $\rho_{\text{APH}}^E$ values.

The discrepancy in resistivity values in case of Li has been removed by using two different types of other dielectric screenings (i) Sham$^{13}$ (ii) Srivastava$^{14,15}$. The results obtained by using experimental $s(q)$ data for these dielectric screenings in case of Li are $\rho_{\text{Sham}}^E = 24.3$ $\mu\Omega$ cm, $\rho_{\text{Srivastava}}^E = 25.5$ $\mu\Omega$ cm. which are excellent than other existing results of the literature.
In the third phase of our investigation when we look at the lowest limit \( q = 0 \) in electrical resistivity formula, where \( U^2(q) \rightarrow |U(0)|^2 = (2/3 \, ZE_F)^2 \) and \( s(q) \rightarrow s(0) = (2/3 \, ZE_F/k_BT)^{-1} \); \( s(0) \phi(0) = k_BT \) and \( \phi(0) = 2/3 \, ZE_F \), for Static Hartree dielectric constant, \( s(q) \); we find \( s(0) |U(0)|^2 = (2/3 \, ZE_F) k_BT \). According to Ziman, \[ s(0) |U(0)|^2 = 0.1 \, u_g^2 \] ...(13)

where \( u_g \) is the energy band gap. A combined form is described as:

\[ s(0) |U(0)|^2 = (2/3 \, ZE_F) k_BT = 0.1 \, u_g^2 \] ...(14)

When we evaluate the values of \( u_g \) for alkali metals, we find the values from Li to Cs as 1.7, 1.3, 1.0, 0.9 and 0.8 eV, respectively which are lower than the corresponding theoretical values of electronic band structure energy \( E_{\text{H}} \) of liquid alkali metals as 2.4, 1.4, 1.6, 1.9 and 2.1 eV. Actually the measured values of energy band gap, \( u_g \) for liquid alkali metals are unknown. We present here only a theoretical estimation. When we use \( s(0) \) values of Waseda for liquid alkali metals we find that \( u_g \) from Li to Cs comes out here nearly of the order of 0.5 \( |U(0)| \). This is all about the presentation of the concept of energy band gap, \( u_g \) of Ziman on the basis of present study.

4 Conclusion

The following important conclusions have been drawn from the present study;

(i) For the first time the findings reported in this paper fulfill completely the proposed concepts of Ziman regarding the separation of electrical resistivity, \( \rho_1 \) into \( \rho_p \) and \( \rho_{\text{el}} \) parts and the inclusion of idea of energy bands of liquid metals. (ii) The structural contribution is more dominant than plasma contribution in case of liquid Li as compared to other group members. (iii) The present estimation of plasma resistivity \( \rho_p \) from the concept of structure and pair potential relationship has given good results of alkali metals, except for the case of Rb metal which were also not found in Ascarelli et al.'s concept. Over all the present concept has given good results of plasma resistivity of alkali metals. (iv) The present consideration of structure-pair potential relationship as described by Eqs (6) and (7) is valid and may be considered as modification of APIH relationship [Eq. (4)]. This has been already confirmed in the investigation of liquid phonon spectrum. (v) Dielectric screening plays an important role in the estimation of resistivity. (vi) For \( q = 0 \) value, following two important formulae are valid:

\[ s(0) |U(0)|^2 = (2/3 \, ZE_F) k_BT = 0.1 \, u_g^2 \]

where \( u_g \) is of the order of nearly 0.5 \( |U(0)| \) and \( s(0) \phi(0) = k_BT \).

References

2. Gerstenkorn H, Ann Phys, 10 (1952) 49.