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Electrical conductivity and Knight shift of some non-trivalent metals at molten state

R. R. THAPA

Department of Mathematics, Tribhuvan University, Post-Graduate Campus, Biratnagar, Nepal

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Abstract. Electrical conductivity is one of the important physical properties of a metal. It is a matter of interest to study the electrical conductivity of a metal at its molten state. In the present theoretical work we have considered the monovalent liquid metals sodium and potassium and bivalent ones magnesium and zinc near the melting point and used Harrison's first principal pseudopotential technique which is basically an orthogonalised plane wave method. A study of the existing literature reveals that the work with the magnetic property like Knight shift of metals is scarce. This has encouraged us to apply the said HFP technique to study the Knight shift of the present metals. Our results for electrical conductivity corroborate well the observed values. For Knight shift also the computed values are in reasonable agreement with the experimental results.

Keywords. Liquid metal, Electrical conductivity, Knight shift, Pseudopotential.

1. Introduction

The electrical conductivity is an important physical property of a metal. In the present work we have studied theoretically the electrical conductivity of some non-trivalent metals at molten stage near their melting point. A method to study the electrical conductivity of a liquid metal is Faber-Ziman's electrical conduction theory based on the concept of model pseudopotential. In this approach a liquid metal is assumed to consist of a system of ions and electrons [1]. Besides metals the electrical conductivity of some binary liquid alloys has also been studied in details by Faber and Ziman through such pseudopotential. However, a problem of model pseudopotential is its transferability because sometimes with the change of environment the change of parameters is also required to get a good agreement with the experimental results.

In this work Harrison's first principle pseudopotential technique, based on the concept of orthogonalised plane waves, has been applied to compute various electronic and core interactions in order to obtain the Fourier transform of the crystal potentials [2] termed as the form factor, $w(k, q)$. The computed form

factors have been consequently used to calculate the desired physical properties through formulae developed by various authors in the past few decades.

Here for the computation of conductivity we have used Ziman's formula. Knight shift has been computed by Knight's formula. And for this purpose monovalent metals like sodium and potassium and bivalent metals like magnesium and zinc have been considered.

2. Basic formalism

Ziman's formula for resistivity is [3]

$$\rho = \frac{3\pi Z\Omega_0}{4h^2e^2v_F^2}\int_0^1 a(q)\left|w(k,\,q)\right|^2 \eta^3 d\eta, \tag{i}$$

where Ω_o is the atomic volume of the metal, Z its valency, v_F the velocity of electron and

$$\eta = \frac{q}{k_F}. \tag{ii}$$

Hence, electrical conductivity is given by

$$\gamma = \frac{1}{\rho}. \tag{iii}$$

The Knight shift has been computed through Knight's formula [4]:

$$\frac{K_1}{K_0} = \frac{P_F^{'}}{P_F^0} = \frac{-3Z}{4E_Fk_F^2}\int_0^\infty a(q)\,w(k,\,q)\,q\ln\left|\frac{q+2k_F}{q-2k_F}\right| dq, \tag{iv}$$

where P_F denotes the Cauchy principal value and E_F the Fermi energy.

3. Results and discussion

We have computed the form factors of the monovalent metals like sodium and potassium and bivalent metals like magnesium and zinc by using various sets of eigenvalues and corresponding eigen functions of Herman-Skillman and Clementi and also the $X\alpha$-exchange parameters as suggested by different authors viz. Slater, Kohn-Sham and Schwarz [5–9].

Further, the experimental and theoretical structure factors [$a(q)$] measured by various authors have also been considered during the evaluation of the electrical conductivity and Knight shift of the above-mentioned metals [10, 11]. The results thus obtained have been presented in the Table below.

Table. Electrical conductivity and Knight shift

Metal	**Eigenvalues due to**	**Electrical conductivity (MS/m)**		**Knight shift (%)**	
		Theoretical	**Experimental**	**Theoretical**	**Experimental**
Na	Herman-Skillman	10.91	10.36	0.075	0.116
K	Herman-Skillman	7.61	7.58	0.301	0.253
Mg	Herman-Skillman	3.37	3.65	0.091	0.112
Zn	Clementi	3.13	2.67	0.386	0.336

It is observed that for sodium the eigenvalues of Herman-Skillman give better result than those of Clementi. In case of potassium also it is found that instead of the eigenvalues of Clementi those of Herman-Skillman present better picture. The form factors so obtained are furnished in Figure 1 and Figure 2. The form factors of magnesium and zinc are depicted in Figure 3 and Figure 4 respectively.

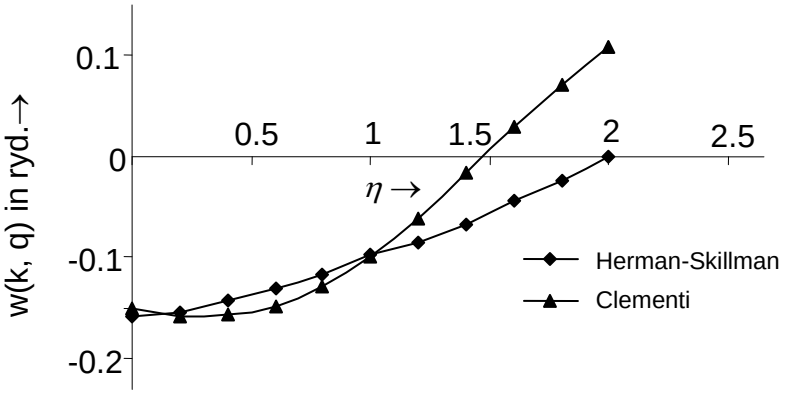

Fig. 1: Form factor of Na

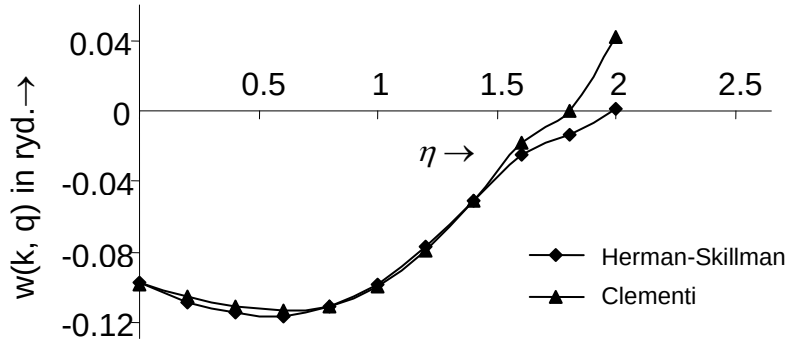

Fig. 2: Form factor of K

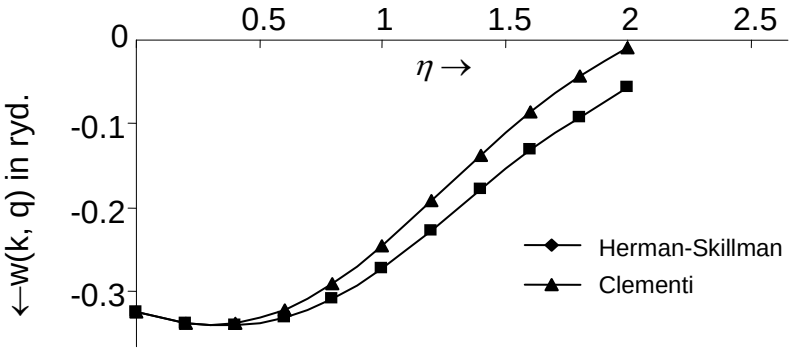

Fig. 3: Form factor of Mg

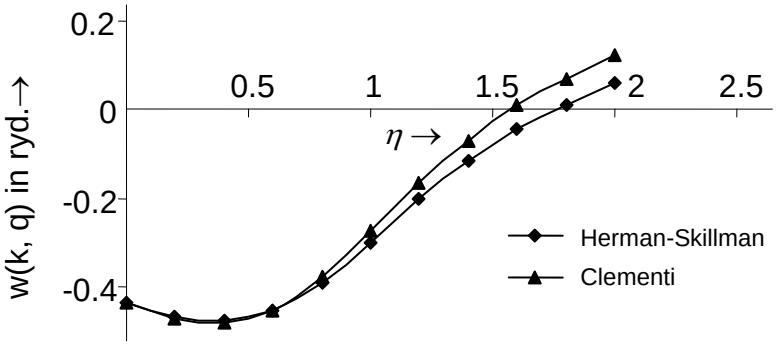

Fig. 4: Form factor of Zn

It is found that in case of magnesium the form factor as computed by using the eigenvalues of Herman-Skillman improves the result and gives almost the same value with the structure factor of Worner *et al* [12]. In case of Zn the form factor obtained through the eigenvalues of Clementi with α=2/3 gives better agreement with the structure factor of Waseda [10].

Hence, further investigation of Knight shift has been carried out with these form factors using $X\alpha$-parameters as proposed by Schwarz [9]. The computed values of Knight shift are in reasonable agreement for the metals under investigation.

4. Summary and conclusion

HFP pseudopotential technique has been applied to compute the electrical conductivity of the monovalent metals sodium and potassium and the bivalent ones magnesium and zinc in liquid phase around melting point with the help of Ziman's formula. Side by side the Knight shift of them has also been calculated on using Knight's formula. In all the cases a reasonable agreement with the experimental results has been noticed.

During our investigation it has been observed that unlike other properties such as resistivity, thermo-electric power, Fermi energy, density of states etc., which involve square of the form factor, the Knight shift depends linearly upon $w(k, q)$. Hence, through the computation of Knight shift one can assess the correctness of the magnitude as well as the sign of the form factor. The electrical conductivity depending upon the square of the form factor can be used to test the correctness of its magnitude only. However, it has been observed that the electrical conductivity having lower magnitude and more sensitiveness to the nature and magnitude of the form factor can serve the purpose quite satisfactorily.

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