BIBECHANA
A Multidisciplinary Journal of Science, Technology and Mathematics
ISSN 2091-0762 (online)
Journal homepage: http://nepjol.info/index.php/BIBECHANA

Electrical conductivity and Knight shift of liquid alkali metals

S. K. Chakrabarti[1*], I. S. Jha[1], R. N. Yadav[2], B. P. Singh[3]
[1]Department of Physics, Tribhuvan University, M. M. A. M. Campus, Biratnagar, Nepal
[2]Department of Mathematics, Tribhuvan University, M. M. A. M. Campus, Biratnagar, Nepal
[3]Department of Physics, Tilka Manjhi Bhagalpur University, Bhagalpur, Bihar, India
*Corresponding author: skc_2007@yahoo.com
Article history: Received 22 October, 2012; Accepted 12 November, 2012

Abstract

In the present work we have considered two alkali metals—sodium and potassium—at their molten stage near the melting point. For the purpose of this theoretical investigation we have used Harrison's first principle (HFP) pseudopotential technique which is basically an orthogonalised plane wave method. The electrical resistivity has been computed through Ziman's formula. Then the electrical conductivity of the present metals is found out just by taking the reciprocal of the values so obtained. Our computed results have been compared with the experimental data and a good agreement is obtained. 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 alkali metals. For this purpose we have used Knight's formula. Our computed values of Knight shift are in reasonable agreement for the metals under investigation.

Keywords: Electrical conductivity; Knight shift; Pseudopotential; Alkali metals.

1. Introduction

One of the important physical properties of a metal is its electrical conductivity. This electrical conductivity is found to vary gradually with the increase in temperature. It is really a matter of interest to study the electrical conductivity of a metal at its molten stage. 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 the present work Harrison's first principle (HFP) pseudopotential technique, based on the concept of orthogonalised plane waves (OPW), has been applied to compute various electronic and core interactions in order to obtain the Fourier transform of the crystal potentials termed as the form factor [2], w(k, q). The computed form factors have been consequently used to calculate the physical properties through formulas developed by various authors in the past few decades.

Here for the computation of resistivity we have used Ziman's formula. Knight shift has been computed by Knight's formula. And for this purpose the liquid alkali metals sodium and potassium have been considered near their melting points.

2. Basic Formalism

Ziman's formula for resistivity is [3]

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

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

$$\eta = \frac{q}{k_F}. \qquad \text{(ii)}$$

Hence, electrical conductivity is given by

$$\gamma = \frac{1}{\rho}. \qquad \text{(iii)}$$

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

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

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 alkali metals sodium and potassium using various sets of eigenvalues and corresponding eigen functions of Herman-Skillman and Clementi and also the Xα-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 monovalent metals [10, 11]. The results thus obtained have been presented in the Table. The form factors are furnished in Fig. 1 and Fig. 2.

Table: Electrical conductivity and Knight shift

Metal	Eigenvalues due to	Electrical conductivity (MS/m)		Knight shift (%)	
		Theoretical	Experimental	Theoretical	Experimental
Na	Herman-Skillman	10.7	10.36	0.075	0.116
K	Herman-Skillman	7.6	7.58	0.301	0.253

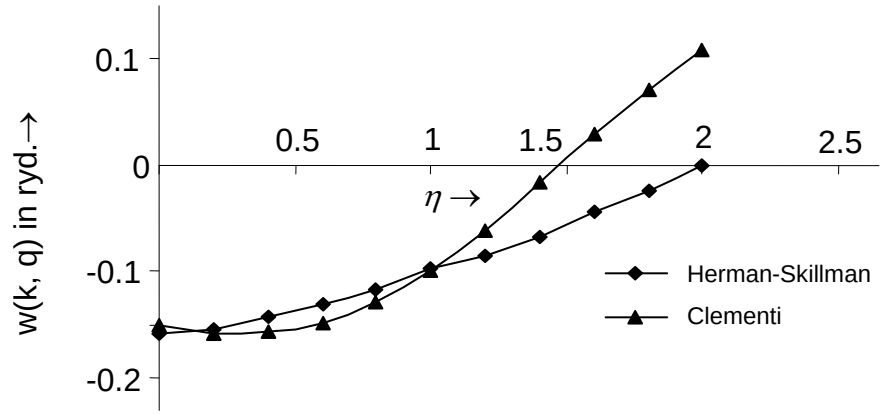

Fig. 1: Form factor of Na

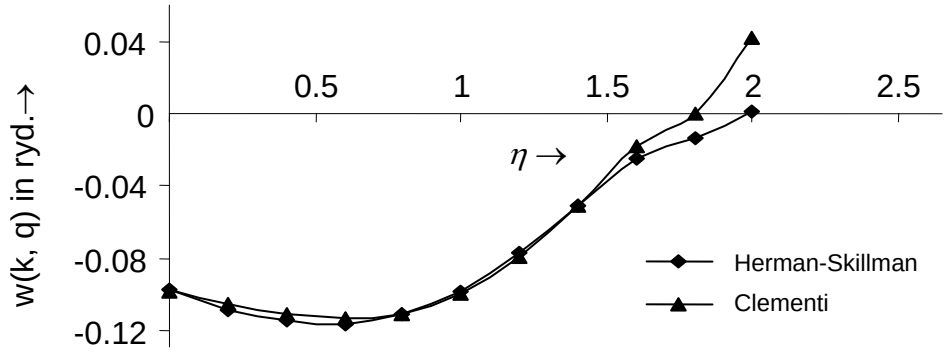

Fig.2 : Form factor of K

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.

So, further investigation of Knight shift has been carried with these form factors using Xα-parameters as proposed by Schwarz. 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 alkali metals sodium and potassium 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 both 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, vide equation (iv), 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 serves the purpose quite satisfactorily.

References

[1] C. R. Dasgupta, Physics, Book Syndicate, Kolkata (1972).
[2] W. A. Harrison, Pseudopotential in the Theory of Metals, Benjamin, New York (1966).
[3] J. M. Ziman, Adv. Phys., 16 (1967) 551.
[4] W. D. Knight, A. G. Berger and V. Heine, Ann. Phys., 8 (1959) 173.
[5] F. Herman and J. Skillman, Atomic Structure Calculation, Prentice Hall, New Jersey (1963).
[6] E. Clementi, IBM J. Res. and Dev., 9 (1965) 2.
[7] J. C. Slater, Phys. Rev., 81 (1951) 385.
[8] W. Kohn and L. J. Sham, Phys. Rev., A140 (1965) 1133.
[9] K. Schwarz, Phys. Rev., B5 (1972) 2466.
[10] Y. Waseda, The Structure of Non-Crystalline Materials, McGraw Hill Book Co., New York (1980).
[11] G. E. Pake, Solid State Physics, Academic Press, New York (1966).