Mathematical determination of electrical resistivity and Knight shift of liquid metals

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Abstract: In the present work Harrison's first principle technique, based on the concept of orthogonalised plane waves, has been successfully applied to compute various electronic and core interactions in order to obtain the Fourier transform of the crystal potential, termed as the form factor. The computed form factors have been consequently used to compute the physical properties through formulae developed by various authors in the past few decades.

Keywords : Liquid metals, Pseudopotential, Electron transport properties, Electrical resistivity, Knight shift.

1. Introduction

One of the important physical properties of a metal is its electrical resistivity. It is found to vary gradually with the increase in temperature. It is really a matter of interest to determine the resistivity of a metal when it melts. A method to study the electrical resistivity of liquid metals is the electrical conduction theory developed by Faber and Ziman using the concept of model pseudopotential. In this approach a liquid metal is assumed to consist of a system of ions and electrons. This concept of pseudopotential for calculating various dynamic properties of metals has been in vogue for the last four decades. An important application of pseudopotential is the calculation of transport properties of disordered materials such as liquid or amorphous metals. Resistivity of some binary liquid alloys has also been explained in details by Faber and Ziman through such pseudopotential. However, a problem with model pseudopotential is its transferability because sometimes with change of environment the change of parameters are also required to get good agreement with the experimental results. The present work is based on Harrison's first principle (HFP) pseudopotential technique which is basically an orthogonalised plane wave (OPW) method. Through this technique the electrical resistivity of monovalent liquid metals has been computed near melting point using well-known Ziman's formula. The concept is then extended for divalent and trivalent metals. The computed results for monovalent metals like sodium and potassium, divalent metals like magnesium and zinc and trivalent metals like aluminium and gallium have been compared with the experimental data and an overall reasonable agreement is obtained. In this course impact of various input parameters too has been studied viz. core energy eigenvalues, exchange parameter, OPW parameter, as provided by different authors.

A study of the literature reveals that although different physical properties of metals have been studied by various authors, the study of magnetic properties such as Knight shift is scarce. Hence, it deserves investigation on using Knight's formula through the HFP technique.

2. Basic Formalism

2.1 *Electrical Resistivity :*

The electrical resistivity has been computed through Ziman's formula given by [1]

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

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

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

2.2 *Knight Shift :*

The Knight shift has been computed through the equation given by [2]

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

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

3. Results and Discussion

We have computed the form factor, $w(k, q)$, of some metals viz. monovalent metals (Na, K), divalent metals (Mg, Zn) and trivalent metals (Al, Ga), using various sets of eigenvalues and corresponding eigen functions of Herman-Skillman [3] and Clementi [4] and also the $X\alpha$-exchange parameters as suggested by different authors viz. Slater [5], Kohn-Sham [6] and Schwartz [7]. Further, the experimental and theoretical structure factors [$a(q)$] measured by various authors have also been taken into consideration during the evaluation of the electrical resistivity and Knight shift of the metals under investigation. The results thus obtained have been presented in the Table and the form factors are depicted in Figures 1 to 6.

Table
Electrical Resistivity and Knight Shift

Metal	Eigenvalues due to	Electrical resistivity (μΩ-cm.)		Knight shift (%)	
		Theoretical	Experimental	Theoretical	Experimental
Na	Herman-Skillman	9.17	9.65	0.071	0.116
K	Herman-Skillman	13.15	13.2	0.307	0.253
Mg	Herman-Skillman	29.7	27.4	0.089	0.112
Zn	Clementi	31.9	37.4	0.388	0.336
Al	Clementi	37.1	37.1	0.112	0.164
Ga	Clementi	24.9	25.8	0.426	0.449

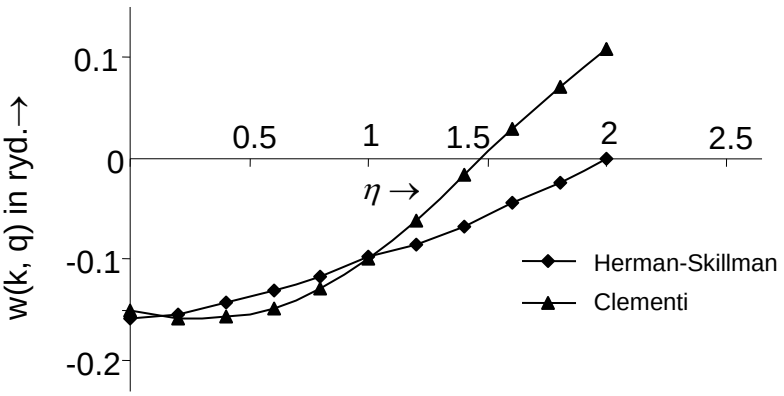

Fig.1: Form factor of Na

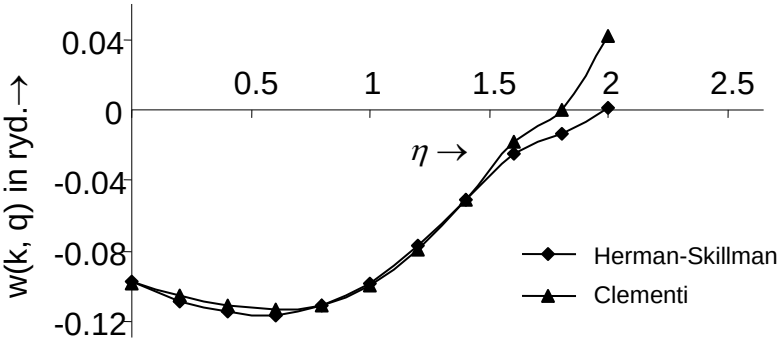

Fig.2 : Form factor of K

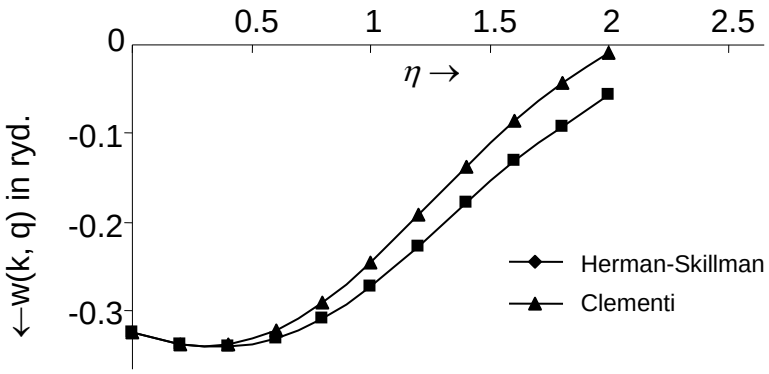

Fig.3 : Form factor of Mg

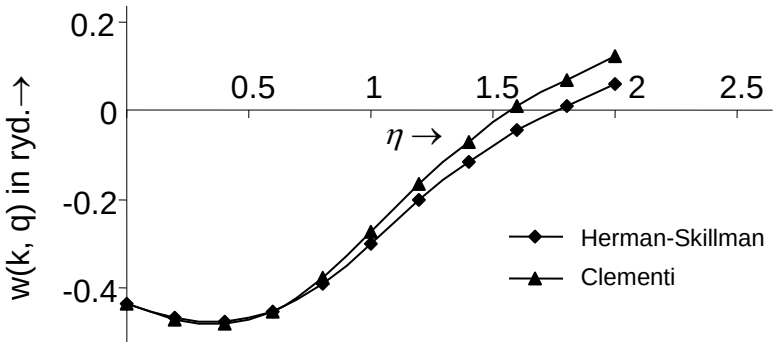

Fig.4 : Form factor of Zn

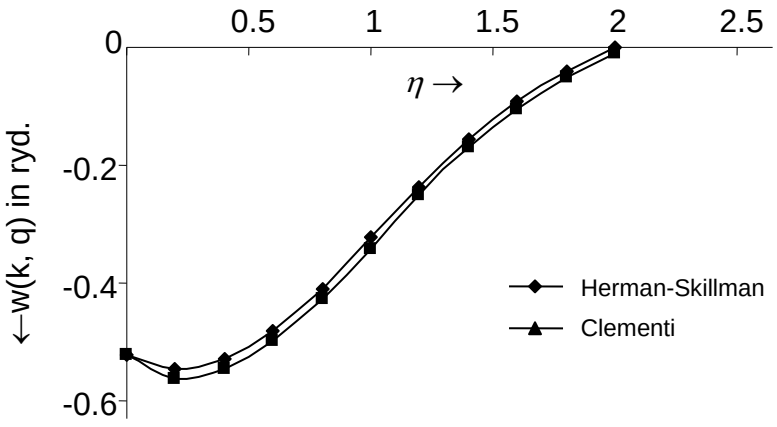

Fig.5 : Form factor of Al

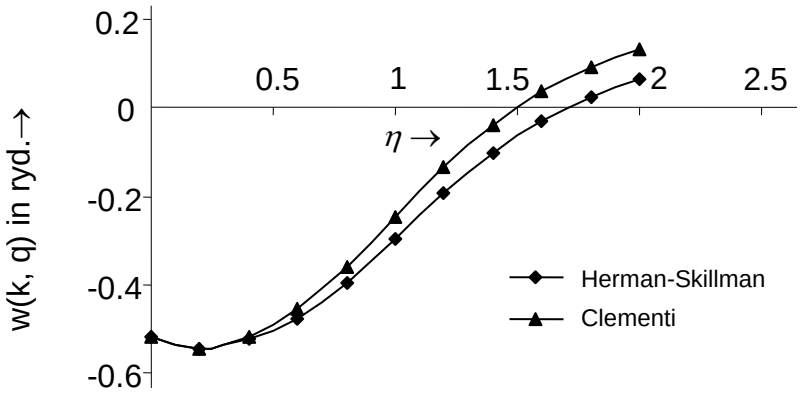

Fig.6 : Form factor of Ga

It is found that in case of Mg 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* [8].

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 [9].

In case of Al the form factor calculated through the eigenvalues of Clementi with $\alpha = \alpha_S = 0.72795$ gives better agreement with the structure factor of Stallard and Davis [10].

In case of Ga the form factor found out on using the eigenvalues of Clementi with α = 2/3 and $\alpha = \alpha_S = 0.70644$ gives better result than the structure factor of Pake [11].

It has been observed that in case of Na, K and Mg only the eigenvalues of Herman-Skillman give reasonable agreement; otherwise in case of Zn, Al and Ga the eigenvalues of Clementi based on Thomas-Fermi technique present better picture.

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

4. Conclusion

During our investigation it has been observed that unlike other properties such as electrical resistivity, thermo-electric power, Fermi energy, density of states etc., which involve the square of the form factor, the integrand of 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 resistivity 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 resistivity having larger magnitude and more sensitiveness to the nature and magnitude of the form factor serves this purpose quite satisfactorily.

References

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