Annals of Computing (2025), 1(6):36-43
https: doi.org /10.5281/zenodo.15729419
Research Article

Calculation of Electronic Susceptibility of Liquid Akali Metals Using Model Pseudopotential

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Received 13 May 20025; Acceptance 6 June 2025; Published 24 June 2025.

Abstract

In this work, the electronic susceptibility of (Li, Na, K, Rb, and Cs) liquid metals were calculated using the model pseudopotential form factor and the structure factor derived through the charge hard sphere model. From the work, the calculated values for each of these liquid metals were respectively obtained as 3.694, 2.398, 2.062, 2.044 and 2.013 while their experimental values are respectively given as 3.650, 1.880, 2.029, 2.031, and 2.733. A good agreement between theoretical investigation and experimental findings proves the strength and ability of this potential.

Keywords: *Electronic Susceptibility, Form Factor, Structure Factor, Model Pseudopotential.*

Introduction

Liquid metals are regarded as a collection of suitably screened ions, interacting via effective ion-ion pair potentials. The effective ion-ion interactions are mediated by the (almost totally degenerate) assembly of conduction electrons. In these metals the mean free path is about one hundred times the inter-atomic distance [2]. They are electrically conductive due to delocalized electrons which do not belong to a specific atom but are shared by all the ions in the metal, so that current can flow [5]. In a system of positive charges and electrons, polarization of the medium can be induced by applying an external field (E) or introducing impurity charge(s). This will induce dipole moments in the system. Electronic susceptibility is a dimensionless proportionality constant that indicates the degree of polarization of a material in response to applied electric field. [6]. The Pseudopotential method is one of the simplest tools to study various physical and chemical properties of materials [3]. It is an advancement of earlier one electron theory of solid. There are two types of pseudopotentials: the local pseudopotential called the model pseudopotential and non-local pseudopotential. The local pseudopotential is the type of pseudopotential that depends on ion

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positions while the non-local pseudopotential is the type of pseudopotential that depends on energy/momentum [10].

The form factor gives very precious information about the interactions inside the metals / core. It is often referred to simply as the pseudopotential, denoted by W (**q**) and is available from a variety in the ion-cores [11]. The structure factor of a liquid provides information about the detail internal structure of the liquid, that is, internal arrangement of atoms inside the liquid [14]. There are two types of structure factors, static and dynamic. The static structure factors are only wave vector dependent, *S(q)* and are useful when static or bulk properties are to be calculated, such as electrical resistivity etc. Whereas dynamic structure factors are wave vector as well as frequency ω dependent, that is, S (q, ω) and is important when the determination of time dependent properties (vary in time and reciprocal space) will be required [7].

The investigation, based on the pseudopotential theory of the electronic susceptibility of liquid metals is very rare theoretical. Previously, Baria and Jani [4] calculated the electronic properties of liquid simple metals using model pseudopotential, Timbie and White [15] have also calculated the Electronic Susceptibility of Liquid metal to second order in the electron ion potential, Janaka [8] has also reported the Spin-Susceptibilities of some metallic elements by using fully self - consistent non-magnetic ground state energy bands and wave functions but the results obtained by these authors are not too very close to the experimental values. Hence, there is need for an improvement on the previous calculated values of electronic susceptibility of liquid alkali metals. In this work, the electronic susceptibility of alkali metals were differently calculated using model pseudopotential proposed by *Pandya et al.,* [10] and the structure factor derived through the charge hard sphere model.

Research Method

Theoretical Background

The formulation of the electronic susceptibility is derived by employing pseudopotential perturbation theory and making use of lattice periodicity and inverse Laplace transform relationship between partition function Z(β) and thermodynamic potential Φ per unit volume [4], where,

$$\Phi = \int_0^\infty ds\bar{Z}(s)\frac{\partial f_0}{\partial s} \tag{1}$$

$$\bar{Z}(s) = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} dt\, e^{st}\frac{Z(t)}{t^2}\ ,\ c > 0 \tag{2}$$

And $f_0$is the Fermi function given by

$$f_0 = \frac{1}{(e^{\beta(s-\xi)}+1)} \tag{3}$$

Here, ξ is chemical potential and $\beta = k_B T$. Using the standard techniques we write (1) as

$$\Phi = \frac{1}{2\pi i}\int_{c-i\infty}^{c+i\infty} dt\ \frac{e^{xt}}{t^r} = \frac{x^{r-1}}{\Gamma(r)}\theta(x),\ \Gamma > 0 \quad (4)$$

Here Γ(r) is the gamma function and

$$\theta(x) = 0 \qquad x < 0,$$

$$= 1 \qquad x > 0 \quad (5)$$

By knowing the chemical potential, the first derivative of thermodynamic potential Φ, gives the relation for the electronic susceptibility χ as [4].

$$\chi = \frac{u^2 n}{E_0}\left[1 - \frac{\Omega_o}{8\,E_o^2\,(2\pi)^3}\int d^3q |S(q)W(q)|^2 F(q)\right] \quad (6)$$

$\boldsymbol{\mu}$ is the reduce mass, n is the effective number of free electrons per atom in liquid metals, E_0 is the Fermi energy, $S(q)$ is the structure factor and $W(q)$ is the screened form factor, F(q) is the normalized energy wave number characteristic of the form

$$F(q) = \frac{b_0^{\frac{1}{2}} n}{2}\ln\left|\frac{1+\sqrt{b_0}}{1-\sqrt{b_0}}\right| + \frac{b_0}{b_0-1} - \frac{q_x^2+q_y^2}{q^2}\left[\frac{b_0^2(5-3b_0)}{8(b_0-1)^2} + \frac{3}{16}b_0^{\frac{3}{2}}\ln\left|\frac{1+\sqrt{b_0}}{1-\sqrt{b_0}}\right|\right] \quad (7)$$

Where $b_0 = \frac{4E_0}{E(q)}$, with E (q) = $\frac{\hbar^2 q^2}{2m}$, E (q) is the energy wave number characteristic, E_o is the Fermi energy within the free electron theory. If the above volume integral in equation (20) is solved by integrating from 0 to $2K_f$, then, electronic susceptibility χ becomes

$$\chi = \chi_0\left[1 - \frac{\Omega_0\,|S(q)W(q)|^2\,F(q)8k_f^3}{8E_o^2(2\pi)^3}\right] \quad (8)$$

Where K_f is the Fermi wave vector $\chi_0 = \frac{\mu^2 n}{E_0}$ is Landan-Pauli free electron susceptibility,

The model pseudopotential in this work is given as [10]

$$W_{ion}(r) = \sum_{n=1}^{2} B_n e^{-(r/na)} \quad r < R_c \text{ (Inside the core)} \quad (9)$$

$$W_{ion}(r) = -\frac{Z_s}{r} \quad r > R_c \qquad \text{(Outside the core)} \qquad (10)$$

The Fourier transform of the model potential in (9) in wave number space (q-space) is given by

$$W_{ion}(q) = 4\pi a^3 \rho \left[\frac{B_1 H_1}{\left(1+a^2q^2\right)^2} + \frac{8B_2 H_2}{\left(1+4a^2q^2\right)^2} \right] - \frac{4\pi Z_s \rho}{q^2}.\cos qR_c \qquad (11)$$

Where q, ρ are wave vector and number density. B_1, B_2 are coefficients of the Dirichlet series and H_1, H_2 are represented as the sum of the repulsive and the oscillatory contributions [10]. The expression for B_1, B_2, H_1 and H_2 are respectively given as

$$B_1 = \frac{Z_s}{R_c}\left[1-\frac{2a}{R_c}\right]e^{\frac{R_c}{a}}, \quad B_2 = \frac{2Z_s}{R_c}\left[\frac{a}{R_c}-1\right]e^{\frac{R_c}{2a}} \qquad (12)$$

$$H_1 = 2 - e^{(Y_1)\left[Y_1(1+X_1)-(1-X_1)\right]} \times \frac{\sin qR_c}{aq} + \left[2+Y_1\left(1+X_1\right)\right] \times \cos qR_c \qquad (13)$$

$$H_2 = 2 - e^{(Y_2)\left[Y_2(1+X_2)-(1-X_2)\right]} \times \frac{\sin qR_c}{2aq} + \left[2+Y_2\left(1+X_2\right)\right] \times \cos qR_c \qquad (14)$$

Where X_1, X_2, Y_1 and Y_2 are respectively given as

$$X_1 = a^2q^2, X_2 = 2^2a^2q^2, Y_1 = \frac{R_c}{a}, Y_2 = \frac{R_c}{2a} \qquad (15)$$

In this work, the Thomas Fermi dielectric function was used to screen the form factor. It is given as

$$\varepsilon(q) = 1 + \frac{k_o^2}{q^2}, \; k_o = 0.815k_F\left(\frac{r_s}{a_o}\right)^{\frac{1}{2}} \qquad (16)$$

Where K_F is the Thomas-Fermi wave vector.

The structure factor that was used in this work was derived through the charged hard sphere (CHS) model and it is given by [9].

$$S(q)=\frac{S_0(q)}{\left[1+\rho\beta V(q)S_0(q)\right]} \tag{17}$$

$$S_0(q)=\frac{1}{1-\rho C_0(q)} \tag{18}$$

$$V(q)=\left[\frac{W^2(q)}{\phi(q)}\right]\left[\frac{1}{\varepsilon(q)}-1\right],\quad \phi(q)=\frac{4\pi e^2}{q^2} \tag{19}$$

ε(q) is the dielectric function.

$$\begin{aligned}\rho C_0(q)=\left(\frac{24\eta}{q^6}\right)[\,&Aq^3(\sin q-q\cos q)+Bq^2\left\{2q\sin q-\left(q^2-2\right)\cos q-2\right\}\\&+Cq\left\{\left(3q^2-6\right)\sin q-\left(q^2-6\right)\right\}+D\left\{\left(4q^2-24\right)q\sin q-\left(q^4-12q^2+24\right)\cos q+24\right\}\\&+\frac{E}{q^2-\gamma q^4\cos q}\begin{Bmatrix}6\left(q^4-20q^2+120\right)q\sin q\\-\left(q^6-30q^4+360q^2-720\right)\cos q-720\end{Bmatrix}\,]\end{aligned} \tag{20}$$

The coefficients *A, B, C, D* and *E* appearing in equation (20) are respectively expressed in terms of the packing fraction η as

$$A=\frac{(1+2\eta)^2}{(1-\eta)^4}+\frac{Q^2}{4(1-\eta)^2}-\frac{(1+\eta)QK}{12\eta}-\frac{(5+\eta^2)^2}{60\eta} \tag{21}$$

$$B=6\eta M^2,\ C=\frac{K^2}{6},\ D=\left(\frac{\eta}{2}\right)(A-K^2U) \tag{22}$$

$$E=\frac{\eta K^2}{60},\ Q=\frac{(1+2\eta)}{(1-\eta)}\left[1-\left\{\frac{1+2(1-\eta)^3}{(1+2\eta)^2}\right\}^{\frac{1}{2}}\right] \tag{23}$$

$$M=\frac{Q^2}{24\eta}-\frac{(1+0.5\eta)}{(1-\eta)^2},\ U=\frac{1+\eta+\eta^2/5)}{12\eta}-\frac{(1-\eta)Q}{12\eta K} \tag{24}$$

K is the inverse screening length due to Debye-Huckel and is given by K = $\left(24\eta\gamma\right)^{1/2}$ the packing fraction $\eta=\frac{\pi}{6}\rho\sigma^3$.Here ρ is the number density of electrons which is given by the expression $\rho=\frac{1}{\Omega}$ and σ is the charge hard sphere diameter [13]

In this present work, the modified Hartree dielectric function was used. It is given as

$$\varepsilon(q) = 1 + \left[1 - f(q)\right]\left[\varepsilon_H(q) - 1\right] \tag{25}$$

With the static Hartree dielectric function $\varepsilon_H(q)$ given as

$$\varepsilon_H(q) = 1 + \frac{me^2}{2\pi h^2 k_F Y^2}\left[1 + \frac{\left(1-Y^2\right)}{2Y}\ln\left|\frac{1+Y}{1-Y}\right|\right] \tag{26}$$

Where m is the ionic mass, h is planck's constant, K_F is the Fermi wave vector, e is the electronic charge and Y= or q, f(q) is the local field correction function suggested by Talor [12] to incoperate the exchange and correlation among the conduction electrons in the dielectric screening and it is given as

$$f(q) = \frac{q^2}{4K_F^2}\left[1 + \frac{0.1534}{4K_F^2}\right] \tag{27}$$

Results and Discussion

The input parameters used in the calculation are given in Table 1 and the comparison between the calculated values of electronic susceptibility of liquid alkali metals in this work and others previously calculated with the experimental values are given in in Table 2. From Table 1, the Electronic Susceptibility values of this work are in closer agreement with the experimental values when compared with the values obtained by [4, 8,15].

Table 1. Input parameters used in the calculation of Electronic Susceptibility of Different Metals.

Metal	Ω_0 (a.u)^3	E_o(a.u) $^{-1}$	K_f(a.u) ^{1}	F(q)(a.u)	S(q)(a.u)	W(q)(a.u)
Li	154.30	0.1682	0.580	-154.526	0.0016	-29.59
Na	277.62	0.1152	0.480	-6.522	0.001	-41.59
K	530.44	0.0760	0.380	-3751.3	0.0014	-59.47
Rb	651.61	0.0648	0.360	-1507.9	0.0014	-70.60
Cs	809.44	0.0545	0.330	-1321.0	0.0014	-57.50

Table 2. Comparison of Electronic Susceptibility of Different Metals by Different Authors.

Metals	Present work	Others [4]	Others [8]	Others [15]	Exp values [8]
Li	3.694	1.892	2.25	2.11	3.650
Na	2.398	1.836	1.71	1.51	1.880
K	2.062	1.765	1.95	1.50	2.029
Rb	2.044	2.339	2.12	1.46	2.031
Cs	2.013	1.792	--	1.46	2.733

Conclusion

The calculation of electronic susceptibility of liquid metals was done differently by using the Model pseudopotential. The results obtained are in a good agreement with experimental values. This Model pseudopotential has improved previous results obtained and as a result can be used to predict theoretically experimental values of electronic susceptibility of liquid metals.

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