

# Study of Magnetic Susceptibilities in Liquid Alkali Metals

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**Abstract**— The theoretical study of the magnetic susceptibilities of liquid alkali metals at their melting temperature is reported using a universal model potential proposed by Fiolhais *et al.* Five different local field correction functions known by Hartree (H), Taylor (T), Ichimaru-Utsumi (IU), Farid *et al.* (F) and Sarkar *et al.* (S) in the present computation for the first time with such model potential and found suitable. It is concluded that, the comparisons of present results with theoretical or experimental findings wherever exists are highly encouraging and found qualitative in nature.

**Keywords**— Pseudopotential; Magnetic susceptibilities; Liquid alkali metals; Local field correction functions

## I. INTRODUCTION

During the last several decades the concepts of pseudopotential have played an important role in the theory of liquid metals and their alloys [1]-[12]. Baltensperger [3] has calculated the correction due to the electron-ion potential to the Landau diamagnetism in liquid metals, using the theory of the free electron susceptibility from the solid phase to the liquid phase, by employing the pseudopotential perturbation technique. Takahashi and Shimizu [4] have investigated the magnetic susceptibility of liquid metals by taking into account the higher order terms due to the electron-ion potential in the Green's function method. Srivastava [5] and Jani *et al.* [10] have reported on the electronic susceptibility of some simple liquid metals using an approach followed by Timbie and White [6]. The magnetic susceptibilities of some liquid non-transition and transition metals using newly proposed model potential was reported by Baria [11] and found suitable for his study. Also, we have [9] reported magnetic susceptibilities of large number of liquid metals using Ashcroft's empty core [13] single parametric pseudopotential. In the present article, we report the magnetic susceptibilities of liquid alkali metals based on the well-known universal model potential of Fiolhais *et al.* [14]. The theoretical structure factors are computed from the well-known Percus-Yevic (PY) hard sphere model with proper packing density  $\eta$  [15]. Five different types of the local field correction functions proposed by Taylor (T) [16], Ichimaru-Utsumi (IU) [17], Farid *et al.* (F) [18] and Sarkar *et al.* (S) [19] are employed for the first time to investigate the influence of exchange and correlation effects with reference to the static Hartree (H) [20] screening function in the present computations.

## II. THEORY

The liquid metal analogy of Glasser's [7] result for the total electronic susceptibility is thus obtained as

$$\chi = \chi_O(1 + \Delta), \quad (1)$$

here

$$\Delta = \frac{-3Z}{32\xi_0^2} \int_0^\infty dk a(k)W(k)^2 G(k), \quad (2)$$

and

$$G(k) = \frac{2}{k}(k^2 - 1) \ln \left| \frac{k+2}{k-2} \right| + \frac{8}{3} \left( \frac{12 + 7k^2 - 3k^4}{(k^2 - 4)^2} \right). \quad (3)$$

The orbital susceptibility in the liquid phase may be calculated separately in much the same way by omitting the spin term from the Hamiltonian. The relation is given by

$$\chi_L = -\frac{1}{2} \chi_O(1 + \Delta_L), \quad (4)$$

with

$$\Delta_L = \frac{-3Z}{32\xi_0^2} \int_0^\infty dk a(k)W(k)^2 G_L(k). \quad (5)$$

and

$$G_L(k) = \frac{2}{k}(k^2 - 1) \ln \left| \frac{k+2}{k-2} \right| + \frac{8}{3} \left( \frac{24 - 22k^2 + 3k^4}{(k^2 - 4)^2} \right). \quad (6)$$

$$\chi_P = -\frac{3}{2} \chi_O(1 + \Delta_P), \quad (7)$$

with

$$\Delta_P = \frac{-3Z}{32\xi_0^2} \int_0^\infty dk a(k)W(k)^2 G_P(k). \quad (8)$$

and

$$G_P(k) = 2(k^2 - 1) \ln \left| \frac{k+2}{k-2} \right| + \frac{8k^2}{(k^2 - 4)}. \quad (9)$$

Now, by including the exchange and the correlation due to Brueckner and Sawada[8], we get the relation for the total electronic susceptibility of liquid metals [9]

$$\chi_{ele} = -\frac{\chi_O}{1 - \Delta_P + \delta_{ex+corr}} - \chi_O(1 - \Delta_L). \quad (10)$$

with

$$\delta_{ex+corr} = \left[ -0.166r_S + 0.204r_S^2(0.225 - 0.0676 \ln r_S) \right]. \quad (11)$$

Where, the value of  $r_s$  can be determined from the relation  $r_s = (3\Omega_0/4\pi Z)^{1/3}$ . Also,  $\chi_0$  the Landau-Pauli free electron susceptibility is computed directly from the given relation. The universal model potential of Fiolhais *et al.* [14] is used in the present computation including five different types of the local field correlation functions [16]-[20]. The form factor used in the present investigation is of the form [14],

$$W(q) = \frac{4\pi Ze^2 R^2}{\Omega_0 \varepsilon(q)} \left[ \frac{-1}{(qR)^2} + \frac{1}{[(qR)^2 + \alpha^2]} + \frac{2\alpha\beta}{[(qR)^2 + \alpha^2]^2} + \frac{2A}{[(qR)^2 + 1]^2} \right],$$

(12) with  $x = r/R$ ,  $R$  being a core decay length, and with  $\alpha > 0$ . An analyticity condition at  $r = 0$  determines the parameters  $A$  and  $\beta$  in terms of  $\alpha$  as follows,

$$\beta = \frac{\alpha^3 - 2\alpha}{4(\alpha^2 - 1)} \text{ and } A = \frac{1}{2}\alpha^2 - \alpha\beta. \quad (13)$$

Also,  $Z$  is the valence,  $\Omega_0$  the atomic volume and  $\varepsilon(q)$  the modified Hartree dielectric function [20].

### III. RESULTS AND DISCUSSION

The input parameters and constants used in the present calculations are tabulated in Table I. Our present investigation of the electronic susceptibility ( $\chi_{ele}/\chi_0$ ) and total electronic susceptibility ( $\chi$ ) of alkali metallic elements are narrated in Tables II-III with experimental [1],[6] and theoretical [6],[11],[12] data wherever exists in the literature.

TABLE I  
Input parameters and other constants

Metals	Z	$\Omega_0$ (au)	T (K)	$\eta$	$\alpha$	R
Li	1	142.47	453	0.46	3.546	0.361
Na	1	254.25	378	0.46	3.074	0.528
K	1	480.84	343	0.46	2.806	0.745
Rb	1	588.98	313	0.43	2.749	0.823
Cs	1	743.53	323	0.43	2.692	0.919

TABLE II  
Electronic susceptibility ( $\chi_{ele}/\chi_0$ ) for liquid alkali metals

Metals	Present results					Expt. [6]	Others [6, 11, 12]
	H	T	IU	F	S		
Li	2.37	2.40	2.38	2.38	2.38	3.65	1.89, 2.11, 2.25
Na	2.38	2.42	2.39	2.39	2.39	1.88	1.51, 1.71, 1.84
K	2.38	2.42	2.39	2.39	2.39	2.03	1.5, 1.77, 1.95
Rb	2.40	2.45	2.41	2.40	2.40	2.03	1.46, 2.12, 2.34
Cs	2.39	2.45	2.40	2.40	2.40	2.73	1.46, 1.79

TABLE III  
Total electronic susceptibility ( $\chi$ ) for liquid alkali metals

Metals	Present results					Expt. [1]
	H	T	IU	F	S	
Li	0.7810	0.7697	0.7788	0.7777	0.7786	1.80
Na	0.6484	0.6407	0.6470	0.6471	0.6474	0.63
K	0.5271	0.5219	0.5262	0.5266	0.5267	0.39
Rb	0.4921	0.4865	0.4912	0.4916	0.4917	0.30
Cs	0.4560	0.4512	0.4553	0.4557	0.4558	0.37

From the present study, it is observed that for electronic susceptibility ( $\chi_{ele}/\chi_0$ ) for liquid alkali metals among all the employed five local field correction function the H (without exchange and correlation) shows the lowest value while T-function shows highest values. Also for the values of the total electronic susceptibility ( $\chi$ ) for liquid alkali metals, H-function shows higher values than the others. The presently computed data are found in good and qualitative agreement with the available experimental [1], [6] and theoretical [6], [11], [12] yielding. The presently reported magnetic susceptibility of liquid alkali elements have predicted positive values of susceptibility in comparison with negative experimental susceptibilities. Also, certain difference between the theoretically computed values and experimental data are attributed to the exchange enhancement of the conduction-electron spin life time. Also, the ionic potential factors  $\Delta_L$  and  $\Delta_P$  are much less important than the electron-electron enhancement factor  $\delta_{ex+corr}$  used in the present computation [1]. The magnetic susceptibility calculations are not particularly sensitive to the exact values of the structure factor of the metallic elements and uncertainties in the results cannot account for the differences between theory and experiment. Also, the numerical values of the magnetic susceptibilities are found to be quite sensitive to the selection of the local field correction functions and showing a minor variation with the change in the functions. Also, the discrepancies of the present results of the magnetic susceptibilities are found because of the principal contributions such as  $\Delta_L$  and  $\Delta_P$  which are structural dependent corrections. Also, the diamagnetic term is little affected by local field correction functions, but in real metal it may well be influenced by the distortion of the conduction electron wave function inside the cores which may causes approximately same results of the magnetic susceptibility of metallic elements computed from the various local field correction functions [1],[2].

### IV. CONCLUSIONS

It is concluded that, the magnetic susceptibilities of some liquid alkali metals reported for the first time based on a Fiolhais *et al.*'s universal model potential with PY structure factor and H, T, IU, F and S-local field correction functions. Hence, such potential can predict the trend of the potential over the alkali elements.

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