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Study of magnetic susceptibilities in liquid metals

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In the present article, a theoretical investigation of the magnetic susceptibilities of liquid non-transition and transition metals of the different groups of the periodic table at their melting point is reported using model potential formalism. Ashcroft's well-known empty core model (EMC) potential is used for the first time with seven local field correction functions proposed by Hartree, Hubbard–Sham, Vashishta–Singwi, Taylor, Ichimaru–Utsumi, Farid *et al.* and Sarkar *et al.* in the present computation and found suitable for such study. In the calculation of these properties the values of the theoretical structure factors have been used due to hard core fluid theory. It is concluded that comparisons of the present results with theoretical or experimental findings, wherever they exist, are highly encouraging. Also, the successful application of the EMC potential to 51 liquid metals is predicted.

Keywords: pseudopotential; magnetic susceptibilities; liquid non-transition metals; liquid transition metals; local field correction functions

1. Introduction

During the last several years, there has been an increasing interest in the properties of non-crystalline conductors such as liquid metals and liquid metallic alloys. Such a liquid exhibits metallic as well as fluid-like behaviour, and hence can help to make a link between the theory of the liquid states and the theory of the electronic states in metals. And hence the study of transport properties such as magnetic susceptibilities of liquid metals and their alloys remain one of the favourite quantities either experimentally or theoretically [1–13].

During the last several decades the concepts of pseudopotential have played an important role in the theory of liquid metals and their alloys [1–13]. Also, to the best of our knowledge, after 1993 the magnetic susceptibilities of large numbers of the liquid metals of the different groups of the periodic table have been reported by researchers very rarely [1–13]. 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] has also reported on the electronic susceptibility of some simple liquid metals using an approach followed by Timbie and White [6]. Also, March [11] and Khajil [12] have reported magnetic

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susceptibility of some liquid metals. March [11] has studied magnetic properties of some liquid metals using free-electron theory. Khajil [12] has reported magnetic properties using first principle Bachelet–Hamann–Schlüter (BHS) model potential [12] and Timbie–White approach [6]. He has noted that the results obtained by using the (BHS) potential are in good agreement with the experiment. Very recently, magnetic susceptibilities of some liquid non-transition and transition metals using a newly proposed model potential was reported by Baria [13] and found suitable for his study. In most of the above studies, various methods are used with some old fascinating local field correction functions. Also, these studies are restricted to some liquid metals only. But, in contrast with the earlier reported studies, the present study spans the large number of liquid metals of periodic table on a common platform of model potential and a common criterion for evaluating the parameters of the model potential.

Keeping all in the mind the cardinal features of these developments, the present article intends to report the magnetic susceptibilities of several monovalent, divalent and polyvalent liquid metals of the different groups of the periodic table based on the well-known empty core model (EMC) potential of Ashcroft [14].

In the present work, the theoretical structure factors are computed from the well-known Percus–Yevic (PY) hard sphere model with proper packing density η [15]. Seven different types of the local field correction functions proposed by Hubbard and Sham (HS) [16,17], Vashishta and Singwi (VS) [18], Taylor (T) [19], Ichimaru and Utsumi (IU) [20], Farid *et al.* (F) [21] and Sarkar *et al.* (S) [22] are employed for the first time to investigate the influence of exchange and correlation effects with reference to the static Hartree (H) [23] screening function in the present computations.

2. Computational methodology

The formulation of the electronic susceptibility is derived by employing the pseudopotential perturbation theory, and by making use of the lattice periodicity and the inverse Laplace transform relationship between the partition function $Z(\beta)$ and the thermodynamic potential Φ per unit volume [6, 7]

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

where,

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

and f_0 is the Fermi function given by

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

Here ξ is the chemical potential and $\beta = k_B T$. Using the standard techniques we write [6,7]

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

Here $\Gamma(r)$ is the gamma function and

$$\begin{aligned} \theta(x) &= 0; & x > 0 \\ &= 1; & x < 0. \end{aligned} \tag{5}$$

The introduction of the potential W shifts the chemical potential ξ away from the Fermi energy. This shift may be calculated to the second order in W using the relation $\partial\Phi/\partial\xi|_{T,\Omega} = n$ where n is the number density of the electrons.

Ignoring the field dependence of ξ , the expression for ξ is given by [6,7]

$$\xi = \xi_0 \left[1 + \frac{W(0)}{\xi_0} - \frac{1}{4\xi_0^{2/3}} \frac{\Omega}{(2\pi)^3} \int d^3q \frac{|S(q)W(q)|^2}{\sqrt{E(q)}} \ln \left| \frac{1 + \sqrt{a_0}}{1 - \sqrt{a_0}} \right| \right], \tag{6}$$

where, $a_0 = 4\xi_0^{2/3}/E(q)$ with $E(q) = \hbar^2 q^2/2m$.

By knowing the chemical potential ξ , the first derivative of the thermodynamic potential Φ gives the relation for the electronic susceptibility χ as [6,7]

$$\chi = \frac{\mu_n^2}{\xi_0} \left[1 - \frac{1}{8\xi_0^2} \frac{\Omega}{(2\pi)^3} \int d^3q |S(q)W(q)|^2 F(q) \right], \tag{7}$$

where

$$F(q) = \frac{a_0^{1/2}}{2} \ln \left| \frac{1 + \sqrt{a_0}}{1 - \sqrt{a_0}} \right| + \frac{a_0}{a_0 - 1} - \frac{q_x^2 + q_y^2}{q^2} \left[\frac{a_0^2(5 - 3a_0)}{8(a_0 - 1)^2} + \frac{3}{16} a_0^{3/2} \ln \left| \frac{1 + \sqrt{a_0}}{1 - \sqrt{a_0}} \right| \right]. \tag{8}$$

Here $\chi_0 = \mu_n^2/\xi_0$ is the Landau–Pauli free-electron susceptibility.

Assuming that $W(q)$ depends only on the magnitude of q , the above volume integral can be solved using $a(q) = N|S(q)|^2$, and the integration variable is then changed to the dimensionless parameter $k = q/2k_F$. The liquid metal analogue of Glasser’s [7] result for the total electronic susceptibility is thus obtained as

$$\chi = \chi_0(1 + \Delta), \tag{9}$$

here

$$\Delta = \frac{-3Z}{32\xi_0^2} \int_0^\infty dk a(k) W(k)^2 G(k), \tag{10}$$

and

$$G(k) = \frac{2}{k} (k^2 - 1) \ln \left| \frac{k + 2}{k - 2} \right| + \frac{8}{3} \left(\frac{12 + 7k^2 - 3k^4}{(k^2 - 4)^2} \right). \tag{11}$$

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

$$\chi_L = -\frac{1}{2} \chi_0(1 + \Delta_L), \tag{12}$$

with

$$\Delta_L = \frac{-3Z}{32\xi_0^2} \int_0^\infty dk a(k) W(k)^2 G_L(k), \tag{13}$$

and

$$G_L(k) = \frac{2}{k}(k^2 - 1) \ln \left| \frac{k+2}{k-2} \right| + \frac{8}{3} \left(\frac{24 - 22k^2 + 3k^4}{(k^2 - 4)^2} \right) \quad (14)$$

$$\chi_P = -\frac{3}{2} \chi_0 (1 + \Delta_P), \quad (15)$$

with

$$\Delta_P = \frac{-3Z}{32\xi_0^2} \int_0^\infty dk a(k) W(k)^2 G_P(k), \quad (16)$$

and

$$G_P(k) = 2(k^2 - 1) \ln \left| \frac{k+2}{k-2} \right| + \frac{8k^2}{(k^2 - 4)}. \quad (17)$$

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]

$$\chi_{\text{ele}} = -\frac{\chi_0}{1 - \Delta_P + \delta_{\text{ex.}+\text{corr.}}} - \chi_0(1 - \Delta_L), \quad (18)$$

with

$$\delta_{\text{ex.}+\text{corr.}} = [-0.166r_S + 0.204r_S^2(0.225 - 0.0676 \ln r_S)], \quad (19)$$

where the value of r_S can be determined from the relation $r_S = (3\Omega_0/4\pi Z)^{1/3}$.

In the present work, we have used Ashcroft's well-known EMC potential [14] including five different types of the local field correlation functions [16–23]. The form factor explored in the present investigation is of the form [14],

$$W(q) = \frac{-4\pi Z e^2}{\Omega_0 q^2 \varepsilon(q)} \cos(qr_C), \quad (20)$$

where, Z is the valence, Ω_0 the atomic volume, r_C the parameter of the potential and $\varepsilon(q)$ the modified Hartree dielectric function [23] is given by

$$\varepsilon(q) = 1 + (\varepsilon_H(X) - 1)(1 - f(X)); X = \frac{q}{2k_F}. \quad (21)$$

Here, $\varepsilon_H(X)$ is the static Hartree dielectric function and the expression of $\varepsilon_H(X)$ is given by [23]

$$\varepsilon_H(X) = 1 + \frac{me^2}{2\pi k_F \hbar^2 \eta^2} \left(\frac{1 - \eta^2}{2\eta} \ln \left| \frac{1 + \eta}{1 - \eta} \right| + 1 \right); \eta = \frac{q}{2k_F}, \quad (22)$$

while $f(X)$ is the local field correction function. In the present investigation, the local field correction functions due to H [23], HS [16,17], VS [18], T [19], IU [20], F [21] and S [22] are incorporated to see the impact of exchange and correlation effects. The details of all the local field corrections are below.

The Hartree screening function [23] is purely static, and it does not include the exchange and correlation effects. The expression of it is

$$f(X) = 0. \tag{23}$$

Hubbard and Sham [16,17] have introduced an analytical expression for the local field correction function, which satisfies the compressibility sum rule exactly. The mathematical expression of the HS local field correction functions is given by

$$f(X) = \frac{q^2}{2(q^2 + \xi k_F^2)}, \tag{24}$$

with

$$\xi = \frac{0.916}{(0.458 + 0.012r_S)}. \tag{25}$$

Vashishta and Singwi [18] have introduced an analytical expression for the local field correction function, which is written as

$$f(X) = A_{VS} \left\{ 1 - \exp\left(\frac{-B_{VS}q^2}{k_F^2}\right) \right\}. \tag{26}$$

Taylor [19] has introduced an analytical expression for the local field correction function which satisfies the compressibility sum rule exactly. This is the most commonly used local field correction function and covers the overall features of the various local field correction functions proposed before 1972. According to T [19],

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

The IU local field correction function [20] is a fitting formula for the dielectric screening function of the degenerate electron liquids at metallic and lower densities, which accurately reproduces the Monte-Carlo results as well, as it also satisfies the self-consistency condition in the compressibility sum-rule and short range correlations. The fitting formula is

$$f(X) = A_{IU}Q^4 + B_{IU}Q^2 + C_{IU} + \left[A_{IU}Q^4 + \left(B_{IU} + \frac{8A_{IU}}{3} \right)Q^2 - C_{IU} \right] \left\{ \frac{4 - Q^2}{4Q} \ln \left| \frac{2 + Q}{2 - Q} \right| \right\}. \tag{28}$$

On the basis of the IU [20] local field correction function, F [21] have given a local field correction function of the form

$$f(X) = A_FQ^4 + B_FQ^2 + C_F + [A_FQ^4 + D_FQ^2 - C_F] \left\{ \frac{4 - Q^2}{4Q} \ln \left| \frac{2 + Q}{2 - Q} \right| \right\}. \tag{29}$$

Based on Equations (28)–(29), S [22] have proposed a simple form of local field correction function, which is of the form

$$f(X) = A_S \{ 1 - (1 + B_SQ^4) \exp(-C_SQ^2) \}, \tag{30}$$

where $Q = 2X$ with $X = q/2k_F$. The parameters A_{VS} , B_{VS} , A_{IU} , B_{IU} , C_{IU} , A_F , B_F , C_F , D_F , A_S , B_S and C_S are the atomic volume-dependent parameters of VS, IU, F and S local field correction functions. The mathematical expressions of these parameters are narrated in the respective papers of the local field correction functions [18, 20–22].

3. Results and discussion

The input parameters and constants used in the present calculations are given in Table 1. The parameter of the model potential r_C is determined using the first zero of the form factor. We have performed the integrations from 0 to $2k_F$ at the melting points of the liquid metals. Very few experimental [1,6] and theoretical [6,10,13] data of the electronic susceptibility (χ_{ele}/χ_O) and total electronic susceptibility (χ) are available in the literature.

Our present investigation of the electronic susceptibility (χ_{ele}/χ_O) and total electronic susceptibility (χ) of 51 metallic elements of the different groups of the periodic table computed from Equations (1) to (30) are narrated in Tables 2 and 3 with experimental [1,6] and theoretical [6,10,13] yielding wherever it exists in the literature.

From the study of Table 2, it can be noted that among the seven employed local field correction functions, the local field correction function due to H (without exchange and correlation) gives the minimum value of electronic susceptibility (χ_{ele}/χ_O) of liquid metals at melting point, while the local field correction function due to T gives the maximum value. The presently computed results of electronic susceptibility (χ_{ele}/χ_O) are found in qualitative agreement with the available experimental [6] and theoretical [6,10,13] data.

The computed results of the electronic susceptibility (χ_{ele}/χ_O) for Li, Na, K, Rb and Cs metallic elements are found to be in qualitative agreement with the other available experimental [6] and theoretical [6,10,13] data. Also, the present data of the electronic susceptibility (χ_{ele}/χ_O) for Li and Cs metals are found to be lower while those for Rh, Ir, Cu, Ag, Ni, Pd, Pt, Au, La, Yb, Ce, Th, Al and Pb metals are found to be higher than the other experimental [6] and theoretical [6,10,13] yielding.

The calculated results of the electronic susceptibility (χ_{ele}/χ_O) for Li, Na, K, Rb, Cs, Al and Pb liquid metals deviate in the range of 36.59–36.79%, 23.18–23.37%, 14.24–14.43%, 14.33–14.70%, 14.62–15.02%, 50.94–51.67% and 254.81–291.01% from the experimental data [6], respectively.

From the study of Table 3, it is noticed that among all the local field correction functions employed, the local field correction function due to T gives the minimum value of the total electronic susceptibility (χ) of liquid metals at melting point while the local field correction function due to H (without exchange and correlation) gives the maximum value. The presently computed results of the total electronic susceptibility (χ) are found to be in qualitative agreement with the available experimental [1] findings wherever they exist in the literature.

The calculated results of the total electronic susceptibility (χ) for Li, Na, K, Rb, Cs, Cu, Ag, Ni, Cr, Mn, Fe, Co, Zn, Cd, Hg, Al, Ga, In, Tl, Sn, Pb, Sb and Bi liquid metals deviate in the range of 56.31–56.52%, 2.70–2.83%, 36.31–36.44%, 61.97–62.27%, 22.19–22.51%, 170.45–174.43%, 131.89–132.88%, 84.52–85.49%, 83.52–84.14%, 92.28–92.66%, 96.13–96.33%, 98.12–98.22%, 255.08–263.85%, 170.31–172.75%, 133.31–136.42%, 1.37–8.50%, 533.93–582.33%, 297.00–309.30%, 144.75–152.30%, 362.30–440.52%, 145.97–180.03%, 38.38–489.38% and 17.24–128.17% from the experimental data [1], respectively.

Table 1. The input parameters and constants.

Metals	Z	Ω_{O} (au)	η	r_C (au)
Li	1.0	146.46	0.46	0.9700
Na	1.0	266.08	0.46	1.6000
K	1.0	480.84	0.46	2.0000
Rb	1.0	627.15	0.43	2.0500
Cs	1.0	775.73	0.43	2.0700
Rh	1.5	95.60	0.45	0.7100
Ir	1.5	99.80	0.45	0.7200
Cu	1.5	119.60	0.46	0.6900
Ag	1.5	173.06	0.45	0.9400
Ni	1.5	85.21	0.45	0.5900
Pd	1.5	113.87	0.47	0.6800
Pt	1.5	120.31	0.47	0.6800
Ti	1.5	129.30	0.44	0.8400
V	1.5	106.47	0.44	0.7800
Cr	1.5	92.90	0.45	0.7300
Mn	1.5	103.09	0.45	0.6900
Fe	1.5	89.25	0.44	0.6500
Co	1.5	85.74	0.45	0.6200
Zr	1.5	172.32	0.44	0.9200
Sc	1.5	172.48	0.43	0.9100
Nb	1.5	121.31	0.45	0.8700
Mo	1.5	105.16	0.45	0.8300
Ta	1.5	121.67	0.45	0.9000
W	1.5	107.05	0.45	0.8500
Os	1.5	94.36	0.45	0.7600
Be	2.0	54.78	0.45	0.7500
Mg	2.0	157.68	0.46	1.3600
Ca	2.0	292.93	0.46	1.6100
Sr	2.0	381.17	0.46	1.8700
Ba	2.0	427.80	0.46	2.3800
Zn	2.0	103.27	0.46	1.2800
Cd	2.0	145.55	0.45	1.0100
Hg	2.0	157.68	0.45	1.5700
Au	2.0	228.46	0.46	0.7400
La	2.0	216.63	0.43	0.8400
Yb	2.0	312.75	0.43	0.8000
Ce	2.0	265.24	0.42	0.8100
Th	2.0	222.98	0.42	0.8800
Eu	2.0	369.26	0.42	0.9500
Al	3.0	111.46	0.45	1.1200
Ga	3.0	131.99	0.43	1.1700
In	3.0	175.90	0.45	1.2800
Tl	3.0	194.00	0.45	1.4500
Gd	3.0	254.93	0.43	0.7900
Tb	3.0	245.91	0.43	1.4551
Si	4.0	121.48	0.38	0.9700
Ge	4.0	146.25	0.38	1.0070
Sn	4.0	180.85	0.43	1.0400
Pb	4.0	203.86	0.46	1.4100
Sb	5.0	205.26	0.4	1.3300
Bi	5.0	238.56	0.4	1.4000

Table 2. Electronic susceptibility (χ_{ele}/χ_0) for some liquid metals at melting point.

Metals	Present results											Expt. [6]	Others [6,10,13]	Percentile influence (%)
	H	HS	VS	T	IU	F	S							
Li	2.3070	2.3100	2.3127	2.3146	2.3085	2.3092	2.3086	3.65	1.89, 2.11, 2.25	0.07-0.33				
Na	2.3157	2.3174	2.3188	2.3193	2.3164	2.3164	2.3163	1.88	1.51, 1.71, 1.84	0.03-0.16				
K	2.3191	2.3208	2.3224	2.3230	2.3198	2.3195	2.3195	2.03	1.5, 1.77, 1.95	0.02-0.17				
Rb	2.3210	2.3238	2.3270	2.3284	2.3223	2.3216	2.3215	2.03	1.46, 2.12, 2.34	0.02-0.32				
Cs	2.3200	2.3237	2.3283	2.3309	2.3218	2.3207	2.3206	2.73	1.46, 1.79	0.03-0.47				
Rh	2.3119	2.3218	2.3300	2.3371	2.3171	2.3271	2.3206	—	1.79, 1.88	0.38-1.09				
Ir	2.3157	2.3261	2.3347	2.3424	2.3212	2.3312	2.3247	—	0.97	0.39-1.15				
Cu	2.3390	2.3530	2.3661	2.3787	2.3471	2.3586	2.3506	—	1.11, 1.12	0.50-1.70				
Ag	2.3439	2.3566	2.3688	2.3792	2.3509	2.3564	2.3523	—	1.00, 1.12	0.36-1.51				
Ni	2.3108	2.3220	2.3311	2.3395	2.3167	2.3300	2.3212	—	-0.98, 1.17	0.45-1.24				
Pd	2.3317	2.3446	2.3564	2.3681	2.3391	2.3505	2.3427	—	4.46, 4.98	0.47-1.56				
Pt	2.3386	2.3524	2.3656	2.3787	2.3467	2.3583	2.3502	—	0.98	0.50-1.71				
Ti	2.3308	2.3424	2.3525	2.3611	2.3370	2.3447	2.3396	—	—	0.38-1.30				
V	2.3180	2.3283	2.3368	2.3439	2.3234	2.3322	2.3265	—	—	0.37-1.12				
Cr	2.3061	2.3152	2.3223	2.3283	2.3107	2.3199	2.3140	—	—	0.34-0.96				
Mn	2.3236	2.3354	2.3456	2.3550	2.3300	2.3413	2.3338	—	—	0.44-1.35				
Fe	2.3135	2.3245	2.3333	2.3412	2.3192	2.3312	2.3234	—	—	0.43-1.20				
Co	2.3084	2.3189	2.3273	2.3350	2.3138	2.3260	2.3180	—	—	0.42-1.15				
Zr	2.3494	2.3633	2.3767	2.3881	2.3570	2.3630	2.3586	—	—	0.39-1.65				
Sc	2.3540	2.3690	2.3833	2.3953	2.3622	2.3686	2.3638	—	—	0.42-1.75				
Nb	2.3173	2.3265	2.3342	2.3404	2.3221	2.3286	2.3244	—	—	0.31-1.00				
Mo	2.3079	2.3161	2.3227	2.3279	2.3120	2.3190	2.3146	—	—	0.29-0.87				
Ta	2.3139	2.3223	2.3292	2.3346	2.3182	2.3240	2.3203	—	—	0.28-0.89				
W	2.3073	2.3153	2.3216	2.3266	2.3113	2.3178	2.3138	—	—	0.28-0.84				
Os	2.3045	2.3130	2.3196	2.3252	2.3088	2.3171	2.3119	—	—	0.32-0.90				

Be	1.9468	2.4080	2.8442	3.5954	2.3288	3.7596	2.3863	—	—	22.58-84.68
Mg	2.3143	2.3215	2.3267	2.3310	2.3179	2.3227	2.3197	—	—	0.23-0.72
Ca	2.3408	2.3496	2.3569	2.3621	2.3451	2.3470	2.3453	—	—	0.19-0.91
Sr	2.3659	2.3790	2.3933	2.4073	2.3738	2.3753	2.3726	—	—	0.28-1.75
Ba	2.5408	2.6019	2.6921	2.7989	2.5850	2.5886	2.5744	—	—	1.32-10.16
Zn	2.2854	2.2910	2.2947	2.2983	2.2881	2.2947	2.2904	—	—	0.22-0.56
Cd	2.3422	2.3573	2.3687	2.3765	2.3493	2.3604	2.3539	—	—	0.50-1.46
Hg	2.3590	2.3750	2.3911	2.4106	2.3694	2.3849	2.3733	—	—	0.61-2.19
Au	2.5937	2.6754	2.7711	2.8720	2.6436	2.6852	2.6521	—	0.97	2.25-10.73
La	2.5219	2.5813	2.6444	2.7036	2.5558	2.5865	2.5637	—	5.01	1.66-7.20
Yb	2.6664	2.7730	2.9074	3.0428	2.7306	2.7566	2.7286	—	4.29	2.33-14.12
Ce	2.6092	2.6954	2.7954	2.8922	2.6596	2.6903	2.6638	—	3.77	2.09-10.85
Th	2.5113	2.5674	2.6258	2.6783	2.5427	2.5694	2.5496	—	3.64	1.53-6.65
Eu	2.6197	2.7114	2.8267	2.9338	2.6737	2.6856	2.6669	—	—	1.80-11.99
Al	2.2641	2.2736	2.2751	2.2699	2.2644	2.2688	2.2721	1.5	—	0.21-0.35
Ga	2.3543	2.3733	2.3824	2.3861	2.3608	2.3799	2.3709	—	—	0.71-1.35
In	2.3805	2.4015	2.4144	2.4229	2.3894	2.4077	2.3976	—	—	0.72-1.78
Tl	2.4316	2.4637	2.4913	2.5207	2.4492	2.4839	2.4601	—	—	1.17-3.66
Gd	3.4445	3.9765	4.7259	5.6946	3.7102	4.1483	3.8464	—	—	11.67-65.32
Tb	2.4359	2.4652	2.4866	2.5031	2.4497	2.4681	2.4568	—	—	0.86-2.76
Si	1.4158	1.5290	1.5977	1.6449	1.4059	1.7643	1.5388	—	—	8.69-24.62
Ge	2.7952	2.9290	3.0061	3.0481	2.8440	3.0396	2.9271	—	—	4.72-9.05
Sn	2.7818	2.9143	3.0031	3.0550	2.8349	2.9975	2.9045	—	—	4.41-9.82
Pb	2.5901	2.6762	2.7556	2.8544	2.6366	2.7767	2.6745	—	—	3.26-10.20
Sb	4.2092	5.8067	8.8876	31.1418	5.0375	19.2589	5.9447	0.73	1.20, 1.37	41.23-639.85
Bi	3.6724	4.3912	5.3485	7.4704	4.0470	6.0245	4.4018	—	—	19.86-103.42

Table 3. Total electronic susceptibility (χ) for some liquid metals at melting point.

Metals	Present results										Expt. [1]	Percentile influence (%)
	H	HS	VS	T	IU	F	S	S	S	S		
Li	0.7865	0.7852	0.7838	0.7826	0.7857	0.7854	0.7857	0.7857	0.7857	0.7857	1.80	0.10-0.50
Na	0.6478	0.6475	0.6472	0.6470	0.6477	0.6477	0.6477	0.6477	0.6477	0.6477	0.63	0.02-0.12
K	0.5321	0.5320	0.5317	0.5316	0.5320	0.5321	0.5321	0.5321	0.5321	0.5321	0.39	0.00-0.09
Rb	0.4868	0.4865	0.4861	0.4859	0.4866	0.4867	0.4867	0.4867	0.4867	0.4867	0.30	0.02-0.18
Cs	0.4533	0.4529	0.4524	0.4521	0.4531	0.4532	0.4532	0.4532	0.4532	0.4532	0.37	0.02-0.26
Rh	0.9729	0.9597	0.9467	0.9318	0.9643	0.9475	0.9475	0.9475	0.9475	0.9475	-	0.88-4.22
Ir	0.9605	0.9475	0.9347	0.9201	0.9520	0.9364	0.9364	0.9364	0.9364	0.9364	-	0.88-4.21
Cu	0.8932	0.8785	0.8631	0.8454	0.8833	0.8690	0.8690	0.8690	0.8690	0.8690	-1.2	1.11-5.35
Ag	0.8221	0.8143	0.8058	0.7972	0.8171	0.8132	0.8132	0.8132	0.8132	0.8132	-2.5	0.61-3.03
Ni	0.9751	0.9558	0.9369	0.9143	0.9621	0.9331	0.9331	0.9331	0.9331	0.9331	6.3	1.33-6.24
Pd	0.9070	0.8923	0.8768	0.8588	0.8970	0.8815	0.8815	0.8815	0.8815	0.8815	-	1.10-5.31
Pt	0.8895	0.8746	0.8588	0.8405	0.8793	0.8648	0.8648	0.8648	0.8648	0.8648	-	1.15-5.51
Ti	0.8979	0.8884	0.8785	0.8682	0.8918	0.8841	0.8841	0.8841	0.8841	0.8841	-	0.68-3.31
V	0.9518	0.9409	0.9302	0.9186	0.9449	0.9332	0.9332	0.9332	0.9332	0.9332	-	0.72-3.49
Cr	0.9888	0.9767	0.9649	0.9516	0.9809	0.9651	0.9651	0.9651	0.9651	0.9651	~ 6.0	0.80-3.76
Mn	0.9413	0.9268	0.9122	0.8956	0.9317	0.9148	0.9148	0.9148	0.9148	0.9148	12.2	1.02-4.85
Fe	0.9785	0.9621	0.9463	0.9279	0.9677	0.9451	0.9451	0.9451	0.9451	0.9451	25.3	1.10-5.17
Co	0.9834	0.9658	0.9486	0.9282	0.9716	0.9455	0.9455	0.9455	0.9455	0.9455	52.2	1.20-5.61
Zr	0.8201	0.8117	0.8024	0.7930	0.8147	0.8104	0.8104	0.8104	0.8104	0.8104	-	0.66-3.30
Sc	0.8179	0.8090	0.7992	0.7894	0.8122	0.8077	0.8077	0.8077	0.8077	0.8077	-	0.70-3.48
Nb	0.9256	0.9177	0.9096	0.9013	0.9206	0.9136	0.9136	0.9136	0.9136	0.9136	-	0.54-2.63
Mo	0.9681	0.9595	0.9512	0.9423	0.9627	0.9535	0.9535	0.9535	0.9535	0.9535	-	0.56-2.67
Ta	0.9298	0.9228	0.9158	0.9088	0.9255	0.9194	0.9194	0.9194	0.9194	0.9194	-	0.46-2.26
W	0.9658	0.9578	0.9501	0.9421	0.9608	0.9526	0.9526	0.9526	0.9526	0.9526	-	0.52-2.45

Os	0.9912	0.9803	0.9699	0.9582	0.9842	0.9706	0.9805	—	0.71–3.33
Be	4.1713	4.4744	4.7631	5.2672	4.4256	5.3674	4.4591	—	6.10–28.67
Mg	0.9377	0.9313	0.9249	0.9173	0.9334	0.9272	0.9319	—	0.46–2.18
Ca	0.7758	0.7723	0.7685	0.7648	0.7736	0.7726	0.7736	—	0.28–1.42
Sr	0.7017	0.6965	0.6897	0.6821	0.6980	0.6973	0.6986	—	0.44–2.79
Ba	0.5984	0.5750	0.5414	0.5036	0.5808	0.5794	0.5850	—	2.24–15.84
Zn	1.0159	0.9997	0.9835	0.9615	1.0041	0.9747	0.9982	–0.62	1.16–5.35
Cd	0.9458	0.9340	0.9234	0.9140	0.9392	0.9287	0.9357	–1.30	0.70–3.36
Hg	0.8559	0.8353	0.8123	0.7827	0.8406	0.8182	0.8358	–2.35	1.79–8.55
Au	0.6560	0.6110	0.5591	0.5046	0.6259	0.6017	0.6216	—	4.59–23.08
La	0.7217	0.6875	0.6496	0.6116	0.6997	0.6803	0.6955	—	3.05–15.26
Yb	0.6074	0.5671	0.5175	0.4687	0.5808	0.5703	0.5820	—	4.18–22.84
Ce	0.6525	0.6138	0.5687	0.5241	0.6274	0.6125	0.6260	—	3.85–19.68
Th	0.7307	0.6999	0.6659	0.6327	0.7112	0.6949	0.7078	—	2.67–13.41
Eu	0.6137	0.5834	0.5452	0.5093	0.5941	0.5898	0.5968	—	2.75–17.01
Al	1.0751	1.0473	1.0246	0.9973	1.0579	0.9977	1.0453	1.09	1.60–7.24
Ga	1.0235	0.9972	0.9757	0.9509	1.0076	0.9611	0.9961	0.15	1.55–7.09
In	0.9628	0.9428	0.9253	0.9062	0.9507	0.9251	0.9434	–0.46	1.26–5.88
Tl	0.8315	0.7944	0.7568	0.7115	0.8062	0.7578	0.7943	–1.59	3.04–14.43
Gd	0.3409	0.2010	0.0614	–0.0616	0.2596	0.1535	0.2261	—	23.85–118.07
Tb	0.8591	0.8396	0.8207	0.8004	0.8469	0.8302	0.8423	—	1.42–6.83
Si	1.7995	1.8116	1.8540	1.9793	1.8438	1.9712	1.8090	—	0.53–9.99
Ge	0.8285	0.7440	0.6910	0.6552	0.7909	0.6573	0.7420	—	4.54–20.92
Sn	0.7832	0.7000	0.6417	0.6033	0.7450	0.6359	0.7024	–0.23	4.88–22.97
Pb	0.6242	0.5386	0.4572	0.3586	0.5672	0.4220	0.5332	–0.78	9.13–42.55
Sb	0.0690	–0.1136	–0.2734	–0.4715	–0.0493	–0.4278	–0.1286	–0.08	171.45–783.33
Bi	0.1296	–0.0401	–0.1940	–0.3807	0.0191	–0.2819	–0.0508	–0.46	85.26–393.75

The computed results of the total electronic susceptibility (χ) for Na, Al, Sb and Bi metallic elements are found in qualitative agreement with the available experimental data [1]. Also, The present data of the total electronic susceptibility (χ) for Li, Ni, Cr, Mn, Fe and Co metals are found lower while those for Na, K, Rb, Cs, Cu, Ag, Zn, Cd, Hg, Ga, In, Tl, Sn and Pb metals are found higher than the other experimental yielding [1]. The presently reported magnetic susceptibility of Cu, Ag, Cr, Zn, Cd, Hg, In, Tl, Sn and Pb liquid metals have predicted positive values of susceptibility in comparison with negative experimental susceptibilities. These materials are diamagnetic materials. But, in the present case these materials follow reverse trends in the present study. Also, Fe and Co liquid metals have very large experimental values of susceptibilities in comparison with calculated ones. These types of materials are ferromagnetic materials. But, in the present case both materials are found to have higher values, and this may be due to the free-electronic behaviour. These types of differences between experimental and theoretical values are attributed to the exchange enhancement of the conduction-electron spin life time. Also, the ionic potential factors Δ_L and Δ_P are much less important than the electron–electron enhancement factor $\delta_{\text{ex.}+\text{corr.}}$ used in the present computation [1]. The results may be summarised by saying that electron–ion corrections cause only considerable deviations from electron gas values when calculated by such a nearly free-electron approach.

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 values of the conduction electron spin susceptibility used in the present computation of the magnetic susceptibilities are responsible for significant variations.

The numerical values of the magnetic susceptibilities are found to be quite sensitive to the selection of the local field correction functions and show a minor variation with the change in the functions. Out of 51 metallic elements, we do not have either theoretical or experimental comparisons of the electronic susceptibility (χ_{ele}/χ_0) for 33 elements or of the total electronic susceptibility (χ) for 28 elements. Neither the experimental nor theoretical results of the magnetic susceptibilities for most of the metallic elements at a constant volume are available in the literature, so the present investigations are predictive.

In contrast with the reported studies, the present study spans the metallic elements of the different groups of the periodic table on a common platform of model potential and common criteria for evaluating the parameters of the model potential. This is essential for obtaining concrete conclusions. Our investigation also predicts that the study of the magnetic susceptibilities of metallic elements is sensitive to the selection of the proper local field correction function.

4. Conclusion

It is concluded that to the best of our knowledge we are reporting for the first time a large number of results of the magnetic susceptibilities for a large number of metallic elements of different groups in the periodic table based on local pseudopotential application to non-transition as well as transition metals. Hence, the present formalism of the EMC potential can predict the trend of the potential over the various elements in the periodic table correctly.

References

- [1] M. Shimoji, *Liquid Metals* (Academic Press, London, 1977).
- [2] T.E. Faber, *An Introduction to the Theory of Liquid Metals* (Cambridge University Press, London, 1972).
- [3] W. Baltensperger, *J. Phys.: Cond. Matt.* **5**, 115 (1966).
- [4] Y. Takahashi and M. Shimizu, *J. Phys. Soc. Japan* **34**, 942 (1973), *J. Phys. Soc. Japan* **35**, 1046 (1973).
- [5] S.K. Srivastava, *J. Phys. Chem. Solids* **36**, 993 (1975).
- [6] J.P. Timbie and R.M. White, *Phys. Rev.* **B1**, 2409 (1970).
- [7] M.L. Glasser, *Phys. Rev.* **134**, A1269 (1964).
- [8] R.K. Bruckner and K. Sawada, *Phys. Rev.* **112**, 328 (1958).
- [9] A.R. Jani, P.N. Gajjar, and H.K. Patel, *Phys. Stat. Sol. (b)* **169**, K105 (1992).
- [10] J.F. Janak, *Phys. Rev.* **16**, 255 (1977).
- [11] N. March, *Can. J. Chem.* **55**, 2165 (1977).
- [12] T. Khajil, *Int. J. Modern Physics* **16**, 2221 (2002).
- [13] J.K. Baria, *Chinese J. Phys.* **41**, 528 (2003).
- [14] N.W. Ashcroft, *Phys. Lett.* **23**, 48 (1966).
- [15] J.K. Percus and G.J. Yevick, *Phys. Rev.* **110**, 1 (1958).
- [16] J. Hubbard, *Proc. Roy. Soc. London* **A243**, 336 (1958).
- [17] L.J. Sham, *Proc. Roy. Soc. London* **A283**, 33 (1965).
- [18] P. Vashista and K.S. Singwi, *Phys. Rev.* **B6**, 875 (1972).
- [19] R. Taylor, *J. Phys. F: Metal Phys.* **8**, 1699 (1978).
- [20] S. Ichimaru and K. Utsumi, *Phys. Rev.* **B24**, 7385 (1981).
- [21] B. Farid, V. Heine, G.E. Engel, and I.J. Robertson, *Phys. Rev.* **B48**, 11602 (1993).
- [22] A. Sarkar, D.S. Sen, S. Haldar, and D. Roy, *Mod. Phys. Lett.* **B12**, 639 (1998).
- [23] W.A. Harrison, *Elementary Electronic Structure* (World Scientific, Singapore, 1999).