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MAGNETIC AND ELECTRONIC PROPERTIES OF SIMPLE, TRANSITION, AND RARE EARTH LIQUID METALS

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In the present research paper we have calculated the Magnetic and electronic properties of liquid simple, transition, and rare earth metals at their melting temperature using recently proposed model potential of Baria and Jani. The parameter of the potential is determined through standard zero pressure technique. The effect of exchange and correlation due to Ichimaru and Utsumi has been incorporated, while the structure factor is derived through charge hard sphere approximation. The beauty of this approximation is that it includes potential in describing the structure factor, so this gives better explanation of structure factor than other such approximations. A good agreement between theoretical investigations and experimental findings proves the strength and ability of the potential.

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1. Introduction

Recently Baria and Jani [1,2] have reported large number of lattice mechanical properties of d and f-shell metals in the fcc phase very successively. In the present paper we thought to calculate some magnetic properties such as Knight-Shift and electronic property such as electronic susceptibility of liquid simple, transition, and rare earth metals at their melting temperature to check the applicability of the pseudopotential.

2. Magnetic Property (Knight- Shift)

In the free electron approximation the temperature coefficient of the Knight- Shift at constant volume in the liquid phase is given by [3-7]

$$\frac{\partial \ln K}{\partial T} = \frac{-3Z}{4T_m E_F k_F^2}\int_0^\infty a(q)\,W(q)\left(\frac{q}{2k_F}\right)\ln\left|\frac{q+2k_F}{q-2k_F}\right| d\left(\frac{q}{2k_F}\right) \quad (1)$$

and the knight-shift of liquid metal is given by [4,6]

$$\frac{K_1}{K_0} = \frac{-3Z}{4E_F k_F^2}\int_0^\infty a(q)\,W(q)\left(\frac{q}{2k_F}\right)\ln\left|\frac{q+2k_F}{q-2k_F}\right| d\left(\frac{q}{2k_F}\right) \quad (2)$$

Here a(q) is the structure factor derived through charged hard sphere approximation [8] and depends only on the packing fraction 'η', W(q) is the screened form factor recently proposed by Baria and Jani [1,2], T_m is the melting temperature, E_F is the Fermi energy, k_F is the Fermi wave vector and K_1/K_0 is the knight shift [4,6] of the liquid metals. The values of T_m, packing fraction 'η',Volume (Ω_0) and valance (Z) are given in table 1 while the value of Fermi wave vector k_F can be determined using the relation $K_F = \left(\frac{3\pi^2 Z}{\Omega_0}\right)^{\frac{1}{3}}$ and Fermi energy $E_F = \frac{\hbar^2 k_F^2}{2m}$ from table 1.

Table 1. Input parameters used in the present calculations.

Metals	r_c (a.u.)	Z	η	ζ_0	Ω_0 (a.u.)	T_m (in K)
Li	1.6331	1	0.46	0.1203	154.30	453.0
Na	2.0087	1	0.46	0.0568	277.62	378.0
K	2.4929	1	0.46	0.0242	530.44	343.0
Rb	2.6643	1	0.43	0.0186	651.61	313.0
Cs	2.8837	1	0.43	0.0135	809.43	323.0
Al	1.7361	3	0.45	0.7403	127.56	943.0
Pb	2.4696	4	0.46	0.4861	217.82	613.0
Cu	1.1054	1.5	0.46	0.2266	89.33	1423.0
Ag	1.5583	1.5	0.45	0.1384	130.40	1273.0
Au	1.6570	2.0	0.46	0.1386	128.34	1423.0
Ni	1.0247	1.5	0.45	0.7480	85.21	1773.0
Pd	1.3682	1.5	0.47	0.4978	113.87	1853.0
Pt	1.3973	1.5	0.47	0.9606	120.31	2053.0
Rh	1.2860	1.5	0.45	0.9607	95.6	2236.0
Ir	1.3214	1.5	0.45	0.3401	99.8	2720.0
La	2.6688	2.0	0.43	0.1777	216.63	1243.0
Yb	2.5150	2.0	0.43	0.1089	312.75	1123.0
Ce	2.4022	2.0	0.42	0.1357	265.24	1143.0
Th	2.3782	2.0	0.42	0.1710	222.98	2031.0

Equations (1) and (2) were used to estimate the temperature coefficient of Knight shift of liquid metals at constant volume and Knight shift of liquid non-transition and transition metals at melting point temperature. We have performed the integration from 0 to $2k_F$. Very few experimental and theoretical data of Knight shift are available. Our present investigation of temperature coefficient of Knight-shift at constant volume of liquid metal, Knight-shift and Knight-shift in percentage are shown in table 2. It is the evident that the present investigations of Knight-shift in percentage for Li, Na, K, Rb, Cs, Al, Cu, Ag, Au, Rh and Ir are very close to the experimental findings while for rest of the metals the results are predictive in nature. The experimental or theoretical result of the temperature coefficient of the Knight-shit at constant volume and Knight-shift are not available so present investigations have the predictive mean.

3. Electronic Property (electronic susceptibility)

The theoretical investigation, based on the pseudopotential theory of the magnetic susceptibility of liquid metals is very rare. Baltensperger [11] calculated the correction due to the electron-ion potential to the Landau diamagnetism in liquid metals by the theory of the free electron susceptibility of solid phase to the liquid phase by employing the pseudopotential perturbation technique. Takahashi and Shimizu [12] have investigated the magnetic susceptibility of liquid metals by taking account of the higher order terms due to the electron-ion potential in

Green's function method. Srivastava [13] has also reported electronic susceptibility of some simple liquid metals using an approach followed by Timbie and White [14].

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 [14, 15].

$$\Phi = \int_0^\infty ds\, \bar{Z}(s) \frac{\partial f_0}{\partial s} \tag{3}$$

where

$$\bar{Z}(s) = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dt\, e^{st} \frac{Z(t)}{t^2}, \qquad c>0 \tag{4}$$

and f_0 is the Fermi function

$$f_0 = \frac{1}{(e^{\beta(s-\xi)}+1)} \tag{5}$$

Here ξ is chemical potential and $\beta = k_B T$. Using the standard techniques we write [14,15]

$$\Phi = \frac{1}{2\pi i} \int_{c-i\infty}^{c+i\infty} dt \frac{e^{xt}}{t^r} = \frac{x^{r-1}}{\Gamma(r)}\theta(x), \qquad \Gamma > 0 \tag{6}$$

Here Γ(r) is the gamma function and

$$\begin{aligned} \theta(x) &= 0 \quad x < 0 \\ &= 1 \quad x > 0 \end{aligned} \tag{7}$$

The introduction of the potential W(q) shifts the chemical potential ξ away from the Fermi energy. This shift may be calculated to second order in W using the relation

$\left.\frac{\partial\Phi}{\partial\xi}\right|_{T,\Omega}$ = -n, where n being number density of electrons

Ignoring the field dependence of ξ, the expression for ξ is given by [14, 15]

$$\xi = \xi_0 \left(1 + \frac{W(0)}{\xi_0} - \frac{1}{4\,\xi_0^{2/3}} \frac{\Omega}{(2\pi)^3} \int d^3q \frac{|S(q)\,W(q)|^2}{\sqrt{E}} \ln \left| \frac{1+\sqrt{a_0}}{1-\sqrt{a_0}} \right| \right) \tag{8}$$

were $a_0 = \frac{4\xi_0^{2/3}}{E(q)}$ with $E(q) = \frac{\hbar^2 q^2}{2m}$

By knowing the chemical potential ξ, the first derivative of thermodynamic potential Φ gives the relation for the electronic susceptibility χ as [14, 15]

$$\chi = \frac{\mu^2 n}{\xi_0}\left[1 - \frac{1}{8\,\xi_0^2}\frac{\Omega}{(2\,\pi)^3}\int d^3q \,\big|\, S(q)\, W(q) \,\big|^2 F(q)\right] \tag{9}$$

where

$$F(q) = \frac{a_0^{1/2}}{2}\ln\left|\frac{1+\sqrt{a_0}}{1-\sqrt{a_0}}\right| + \frac{a_0}{a_0 - 1} - \frac{q_x^2 + q_y^2}{q^2}\left[\frac{a_0^2\,(5 - 3a_0)}{8(a_0 - 1)^2} + \frac{3}{16}a_0^{3/2}\ln\left|\frac{1+\sqrt{a_0}}{1-\sqrt{a_0}}\right|\right] \tag{10}$$

Here $\chi_0 = \dfrac{\mu^2 n}{\xi_0}$ is Landau-Pauli free electron susceptibility

Assuming that W(q) depends only on the magnitude of q, the above volume integral can be solved using $a(q)=N\left|S(q)\right|^2$ and the integration variable is changed to the dimensionless parameter $k=q/2k_F$. the liquid metal analog of Glasser's [15] result for the total electronic susceptibility is thus obtained as

$$\chi = \chi_0(1 + \Delta) \tag{11}$$

where

$$\Delta = -\frac{3}{32}\frac{Z}{\xi_0^2}\int_0^\infty dk\; a(k)\; W^2(k)\; G(k) \tag{12}$$

and

$$G(k) = \frac{2}{k}(k^2 - 1)\ln\left|\frac{k+2}{k-2}\right| + \frac{8}{3}\frac{12 + 7k^2 - 3k^2}{(k^2 - 4)^2} \tag{13}$$

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

$$\chi_L = -\frac{1}{2}\chi_0(1 + \Delta_L) \tag{14}$$

$$\Delta_L = -\frac{3}{32}\frac{Z}{\xi_0^2}\int_0^\infty dk\; a(k)\; W^2(k)\; G_L(k) \tag{15}$$

and

$$G_L(k) = \frac{2}{k}(k^2 - 1)\ln\left|\frac{k+2}{k-2}\right| + \frac{8}{3}\frac{24 - 22k^2 + 3k^4}{(k^2 - 4)^2} \tag{16}$$

$$\chi_P = -\frac{3}{2}\chi_0(1 + \Delta_P) \tag{17}$$

$$\Delta_P = -\frac{3}{32}\frac{Z}{\xi_0^2}\int_0^\infty dk\, a(k)\, W^2(k)\, G_P(k) \tag{18}$$

and

$$G_P(k) = 2(k^2-1)\ln\left|\frac{k+2}{k-2}\right| + \frac{8k^2}{(k^2-4)} \tag{19}$$

Now, including exchange and correlation due to Brueckner and Sawada [16], we get the relation for total electronic susceptibility for liquid metals [17],

$$\chi_{ele} = -\chi_o(1-\Delta_P+\delta_{ex.+corr.})^{-1} - \chi_o(1-\Delta_L) \tag{20}$$

with

$$\delta_{ex.+corr.} = [-0.166\, r_s + 0.204\, r_s^2\ (0.225 - 0.0676 \ln r_s)] \tag{21}$$

The value of ζ_0 is given in table 1 while the value of r_s can be determined using the relation $r_s = \left(\frac{3\,\Omega_0}{4\,\pi\,Z}\right)^{\frac{1}{3}}$ from table 1.The obtained values of electronic susceptibilities are displayed in table 2 with available other such experimental as well as theoretical findings. It is seen that present findings for Li, Na, K, Rb, Cs and al agrees very well with the experimental results as well as theoretical results of Janak [18] while for Cu, Ag, Pd and Rb are very similar to the results of Janak [18]. For rest of metals no theoretical as well as experimental data are available for the quantitative comparisons, so they are predictive in nature. The effect of exchange and correlation due to Ichimaru and Utsumi [19] is incorporated while calculating structure factor a(q).

Table 2. The temperature coefficient of Knight-shift at constant volume, Knight shift and Knight-shift in % of some liquid simple, transition, and rare earth metals at melting temperature.

Metal	$\frac{\partial \ln K}{\partial T}$ in $10^{-4}\,{}^0K^{-1}$	$\frac{K_1}{K_0}$	K%	K% Expt. [9,10]	Others [3-7,9]
Li	3.9	0.126	0.0274	0.026	0.028, 0.030
Na	3.5	0.206	0.1146	0.116	0.125, 0.100, 0.116
K	2.5	0.303	0.2399	0.265	0.357, 0.296
Rb	3.8	0.378	0.5743	0.662	0.588, 0.534
Cs	1.9	0.425	1.3416	1.44	1.13, 1.254
Al	7.7	0.220	0.2051	0.164	0.111, 0.173
Pb	4.4	0.148	1.1973	1.49	1.32
Cu	0.85	0.1371	0.2629	0.232	0.260
Ag	0.48	0.5992	0.5554	0.522	-
Au	0.40	0.7856	4.2344	4.00	4.361
Ni	0.01	0.5441	1.1879	-	-
Pd	0.35	1.3064	0.7757	-	-
Pt	0.24	1.2300	0.4805	-	-
Rh	0.50	0.8978	0.4109	0.35	0.385

Ir	0.35	0.7847	2.7464	2.00	2.255
La	-0.062	-3.9592	-0.6635	1.0	-
Yb	-0.062	-4.2120	-0.9945	-	-
Ce	-0.074	-5.0065	-1.1472	-	-
Th	-0.029	-2.2931	-0.7116	-	-

Table 3. Electronic susceptibility (χ_{ele}/χ_0) of some liquid simple, transition, and rare earth metals at melting temperature.

Metal	Present work	Expt. [14]	Others [14]	Others [18]
Li	1.892	3.65	2.11	2.25
Na	1.836	1.88	1.51	1.71
K	1.765	2.029	1.5	1.95
Rb	2.339	2.031	1.46	2.12
Cs	1.792	2.733	1.46	-
Al	1.549	1.5	1.375	1.34
Pb	1.201	0.73	1.369	-
Cu	1.112	-	-	1.12
Ag	1.000	-	-	1.12
Au	0.975	-	-	-
Ni	1.165	-	-	-0.98
Pd	4.975	-	-	4.46
Pt	0.983	-	-	-
Rh	1.878	-	-	1.79
Ir	0.973	-	-	-
La	5.013	-	-	-
Yb	4.289	-	-	-
Ce	3.774	-	-	-
Th	3.641	-	-	-

It is an evident from Table 1 and 2 that the presently proposed pseudopotential have reproduced promising results of the Knight-Shift and susceptibility of liquid simple, transition, and rare earth metals and hence the potential can be exploited further to study the other metallic properties.

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References

[1] J. K. Baria and A. R. Jani, Physica B **328,** 317 (2003).
[2] J. K. Baria and A. R. Jani, Pramana J. of Phys. **60,** 1 (2003).
[3] J. Behari, Phil. Mag. **26,** 737 (1972).

[4] A. L. Ritter and J. A. Gardner, Phys. Rev. B **3,** 46 (1970).
[5] M. Watabe, M. Tahaka, H. Endo and B. K. Jones, Phil. Mag. **12,** 347 (1965).
[6] N. C. Halder, J. Chemical Phys. **52,** 5450 (1970).
[7] B. Mishra, L. K. Das, T. Sahu, G. S. Tripathi, P. K. Mishra, J. Phys.: Condensed Matter **2,** 9891 (1990).
[8] R. V. Gopala Rao and U Bandyopadhyay, Ind. J. Phys. **65A,** 286 (1991).
[9] G. A. Styles and G. Tranfield, J. Phys. F: Metal Phys. **8,** 2035 (1978).
[10] F. Seitz and D. Turnbull, Solid State Physics, Vol. 2, Academic Press, New York, (1956).
[11] W. Baltensperger, J. Phys.: Condensed Matt. **5,** 115 (1966).
[12] Y. Takahashi and M. Shimizu, J. Phys. Soc. Japan **34,** 942 (1973). J. Phys. Soc. Japan **35,** 1046 (1973).
[13] S. K. Srivastava, J. Phys. Chem. Solids **36,** 993 (1975).
[14] J. P. Timbie and R. M. White, Phys. Rev. B **1,** 2409 (1970).
[15] M. L. Glasser, Phys. Rev. **134,** A1296 (1964).
[16] R. K. Bruckner and K. Sawada, Phys. Rev. **112**, 328 (1958).
[17] A. R. Jani, P. N. Gajjar and H. K. Patel, Phys. Stat. Sol. (b) **169,** K105 (1992).
[18] J. F. Janak, Phys. Rev. **16,** 255 (1977).
[43] S. Ichimaru and K. Utsumi, Phys. Rev. B **22,** 1522 (1980)., Phys. Rev. B **22,** 5203 (1980), Phys. Rev. B **23,** 3291 (1981)., Phys. Rev. B **24,** 3220 (1981)., Phys. Rev. B **24,** 7385 (1981).