

## The Theoretical Study of Electron Dispersion of Some Liquid Metals Using Transition Metal Model Potential (TMMP)

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In the present communication, we have proposed a simple method using which two parameters of Kumar's pseudopotential can be reduced to effectively single parameter. Further the reliability of our proposed method is examined by carrying out electron dispersion curves ( $E(k) \rightarrow k$ ), Fermi energy ( $E_F$ ) and density of states at Fermi energy ( $N(E_F)$ ) for sixteen liquid metals. In absence of any experimental or theoretical results of aforesaid properties, our results will throw some light in the determination of interactions persisting in the liquid state of transition metals.

**Keywords:** Pseudopotential, Liquid metals, Electron dispersion, Density of states.

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### 1. INTRODUCTION

The pseudopotential formalism in its different form (local and non-local) has been used successfully for theoretical understanding of almost all the physical properties (static, dynamic and transport) for solid and liquid metals, metallic alloys and metallic glasses with good degree of success [1-4]. The reason behind such applicability of pseudopotential is due to its physical transparency and computational simplicity. Recently, it has been observed that local form of the pseudopotential can be used successfully for the theoretical study of thermodynamic properties of metals at extreme environment (high temperatures and high pressures). In case of metals and their alloys, first principles methods are more powerful but at the same time less transparent, computationally lengthy and time consuming. The first principles or ab initio methods has a limitation for the study of physical properties of liquid state (for more details See Ref. [5]). The study of physical properties at liquid density has a great importance in many areas of science like fusion and fission reactors, geophysics, astrophysics etc. Transport properties of liquid metals provide better understanding about nature of the interactions persisting among atoms at melting temperature. For such study one requires two main ingredients, first electron ion interaction called pseudopotential and structure factor which gives information about atomic distributions. The later can be measured with the help of X-ray scattering experiments or with the help of theoretical approaches. Looking to the importance of study of liquid state

properties, we in the present study calculate total energy as a function of propagation vector  $k$  known as electron dispersion for some liquid transition and rare earth metals. In order to understand electron ion interaction we use Kumar's [6] pseudopotential with two parameters. During literature survey we find that the theoretical study of electron dispersion is very rare and limited for simple liquid metals. The form of Kumar's pseudopotential in real space is as following [6],

$$\begin{aligned} V_{ion}(r) &= \frac{-Ze^2 r}{r_m r_c} \text{ for } 0 < r < r_c, \\ V_{ion}(r) &= \frac{-Ze^2}{r_m} \text{ for } r_c < r < r_m, \\ V_{ion}(r) &= \frac{-Ze^2}{r} \text{ for } r_m < r. \end{aligned} \quad (1.1)$$

where  $Z$  is the valency. In the region  $r < r_c$ , there is no complete cancellation of potential but it decreases linearly and in the region  $r_c$  to  $r_m$  it remains constant. It possesses pure coulombic behavior for the region outside  $r_m$ . The potential between region  $r_c$  to  $r_m$  accounts hybridization effects because in case of  $d$ -band metals there is no complete cancellation of potential within this range.

### 2. THEORY

The Fourier transform of Eq. (1.1) gives bare-ion pseudopotential in momentum space which has the following form [6],

$$\begin{aligned} V_{ion}(q) &= -\frac{4\pi Ze^2}{\Omega q^2} \cos qr_m - \frac{4\pi Ze^2}{\Omega q^4 r_m r_c} \left[ -q^2 r_c^2 \cos qr_c + 2qr_c \sin qr_c + 2 \cos qr_c - Z \right] - \\ &-\frac{4\pi Ze^2}{\Omega q^3 r_m} \left[ (qr_c \cos qr_c - qr_m \cos qr_m) + (\sin qr_m - \sin qr_c) \right]. \end{aligned} \quad (2.1)$$

The bare-ion pseudopotential is screened by usual procedure, the screened pseudopotential  $V(q) = (V_{ion}(q))/\epsilon(q)$ . Here  $\epsilon(q)$  is the modified Hartree dielectric function. Due to the weakness of the pseudo-

potential, one can use conventional perturbation theory to calculate total energy as a sum of ground state, first and second order corrections to the energy. In case of liquid state, the analogy of the total energy can be un-

derstood in terms of screened pseudopotential  $V(q)$  and structure factor  $S(q)$  as [7],

$$E(k) = \frac{\hbar^2 k^2}{2m} + \frac{2m}{\hbar^2} \left[ \sum_q \frac{S(q)|V(q)|^2}{k^2 - |k+q|^2} - \frac{S(q)|V(q)|^2}{q^2} \right], \quad (2.2)$$

$$= \frac{\hbar^2 k^2}{2m} + \Delta(k) - \Delta(0), \quad (2.3)$$

where,

$$\Delta(k) \equiv \frac{3Z}{8k_F E_F \bar{k}} \int_0^\infty S(q) |V(q)|^2 |q| \ln \left| \frac{2\bar{k} + q}{2\bar{k} - q} \right| dq, \quad (2.4)$$

$S(q)$  is the structure factor. In the present study, we have used the hard sphere solution of the Percus-Yevick equation with packing fraction  $\eta = 0.45$  [5].

$$\Delta(0) = \frac{3Z}{2k_F E_F \bar{k}} \int_0^\infty S(q) |V(q)|^2 dq. \quad (2.5)$$

### 3. RESULTS AND DISCUSSION

We have proposed simple scheme in which we have approximated  $r_m$  by experimental values of atomic radii for all the elements [9]. It has been observed in many studies that the first zero of the screened pseudopotential is found near the Fermi surface at metallic densities. Keeping this in our mind we have adjusted  $r_c$  to get first zero near Fermi surface for all the metals at liquid densities. The values of parameters along with the atomic volume at melting temperature are tabulated in Table 1.

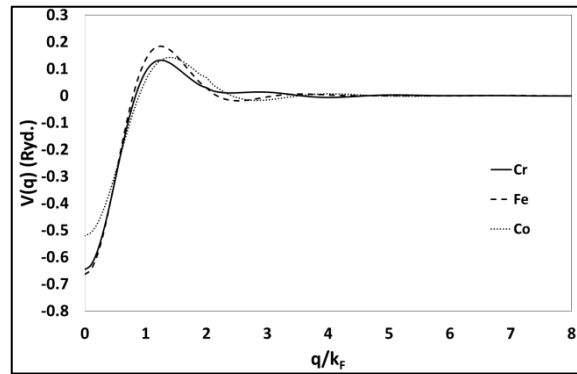
As we have discussed earlier, the main ingredient for the calculation of electron dispersion curves i.e. plot of  $\Delta(k) - \Delta(0)$  against  $k$  is screened pseudopotential  $V(q)$ . For the completeness of the present calculations we have presented variations of  $V(q)$ s for some transition metals (Cr, Fe and Co) in Fig. 1. From such plots, the first zeroes are observed near the Fermi surface, also behaviour of  $V(q)$ s are wiggles free upto  $8k_F$ . In the present calculation the behaviour of pseudopotential at higher values of  $q$  are most important and without using any extra damping factor near or about  $8k_F$  pseudopotential becomes zero. It has also been found during literature survey that the use of artificial damping factor with screened pseudopotential has no physical significance.

The plots of  $\Delta E(k) = \Delta(k) - \Delta(0)$  against  $k$ , calculated using set of equations (2.2-2.5) are plotted in Fig.(2-7) for all sixteen metals. For the study of electron dispersion  $\Delta(k)$  should be calculated precisely. In the expression of  $\Delta(k)$  (See Eq. 2.4), logarithmic term which depends upon  $q$  as well  $k$  has highly oscillatory behaviour even at large values of  $q$  and  $k$ . As a result, in order to achieve proper convergence we have evaluated such integration with upper limit upto  $80k_F$  in step of  $0.1k_F$ . The order of  $\Delta E(k)$  is same as those obtained by Vora [7]. In absence of experimental as well as other theoretical results, the variations of  $\Delta E(k)$  are acceptable.

Further, in order to verify predictivity of the present pseudopotential we have calculated Fermi energy

**Table 1** – The values of Input Parameters: atomic volume  $\Omega$  (in atomic unit) at melting temperature (in K shown in parenthesis) taken from Waseda [8]). The Pseudopotential parameters  $r_c$  and  $r_m$  (in atomic unit)

Metal	$\Omega$	Valency $Z$	Pseudopotential parameter	
			$r_c$	$r_m$
Cr	93.04 (2173)	3	1.90	3.4965
Fe	89.35 (1833)	3	2.60	3.2508
Co	85.94 (1823)	2	2.75	3.1563
Ni	85.29 (1773)	2	2.40	3.0618
Pd	113.72 (1863)	2	2.20	3.3831
Pt	117.07 (2053)	2	1.19	3.4587
Si	121.71 (1733)	4	1.70	2.7594
Ge	146.52 (1253)	4	1.50	2.8728
Sn	200.44 (973)	4	1.20	3.2508
Pb	228.98 (1023)	4	1.90	3.4209
Sb	211.09 (933)	5	2.10	2.8917
La	259.81 (1243)	3	2.60	5.1786
Ce	232.83 (1143)	3	2.55	5.1030
Gd	254.12 (1603)	3	2.85	4.8006
Eu	367.93 (1103)	2	3.50	4.8384
Yb	309.96 (1123)	2	2.35	4.5360



**Fig. 1** – Variations of pseudopotential formfactors against  $q/k_F$  for Cr, Fe and Co

$E_F$  and Density of States at Fermi energy  $N(E_F)$ . The Fermi energy can be evaluated with  $k = k_F$  in Eq. (2.3),

$$E_F = \frac{\hbar^2 k_F^2}{2m} + \Delta(k_F) - \Delta(0). \quad (3.1)$$

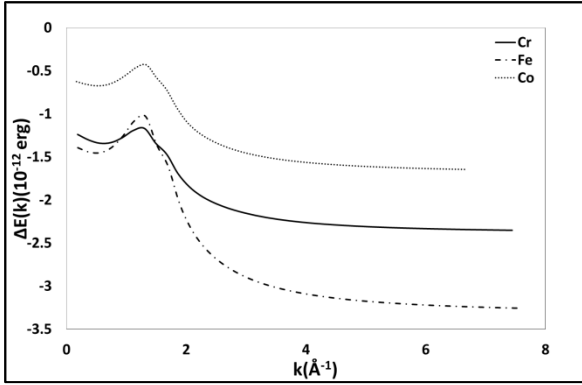


Fig. 2 – Electron Dispersion for Cr, Fe and Co

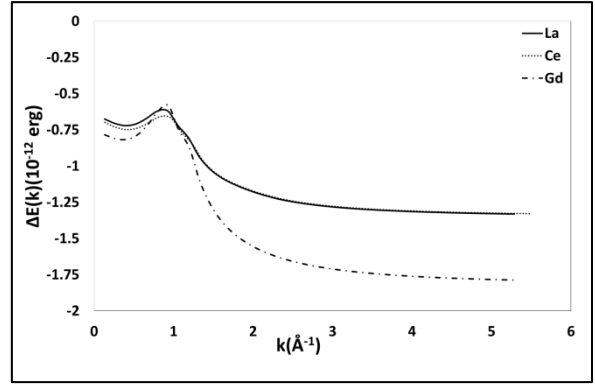


Fig. 6 – Electron Dispersion for La, Ce and Gd

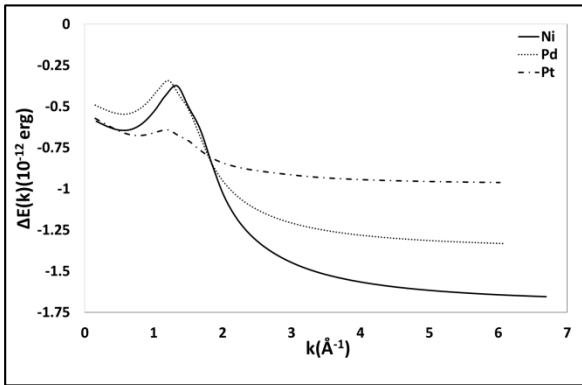


Fig. 3 – Electron Dispersion for Ni, Pd and Pt

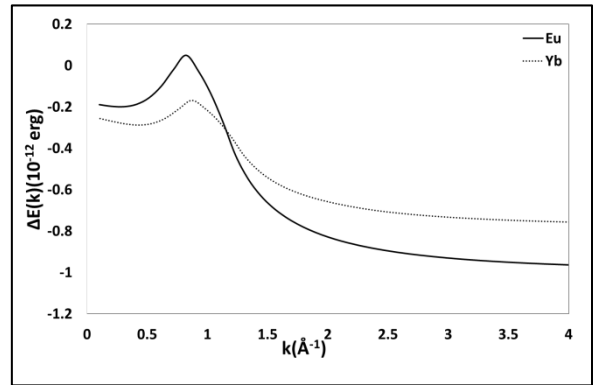


Fig. 7 – Electron Dispersion for Eu and Yb

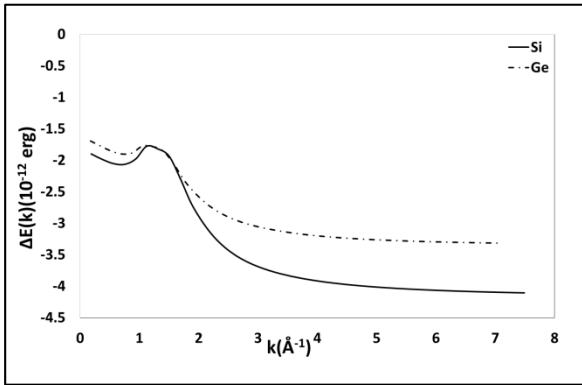


Fig. 4 – Electron Dispersion for Si and Ge

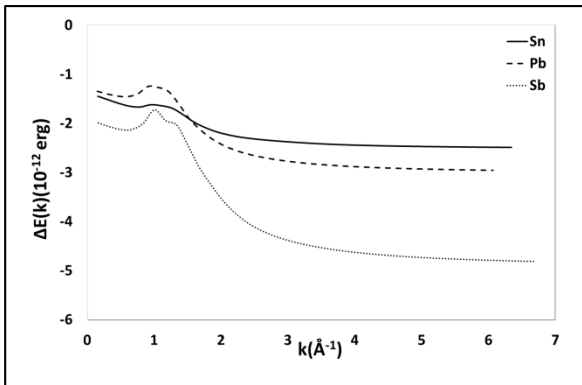


Fig. 5 – Electron Dispersion for Sn, Pb and Sb

Such values of  $E_F$  are displayed in Table 2. The Density of States at Fermi energy  $N(E_F)$  can be calculated as,

$$N(E_F) = \frac{k_F^2}{n\pi^2} \left[ \frac{\partial E}{\partial k} \Big|_{(k=k_F)} \right]^{-1}. \quad (3.2)$$

Table 2 – The calculated values of Fermi energy  $E_F$  ( $\times 10^{-12}$  erg) and density of states at Fermi level  $N(E_F)$  ( $\times 10^{12}$  (energy-atom) $^{-1}$ )

Metal	$E_F$	$N(E_F)$
Cr	19.391	1.4221
Fe	19.624	1.4278
Co	16.247	1.2074
Ni	16.413	1.2017
Pd	13.545	1.4460
Pt	13.097	1.4234
Si	18.671	1.9348
Ge	16.543	2.1509
Sn	13.347	2.6100
Pb	12.123	2.9712
Sb	14.260	3.1046
La	9.697	2.8298
Ce	10.475	2.6137
Gd	9.684	2.8882
Eu	6.299	3.3473
Yb	6.947	2.8218

We could not find experimental as well as theoretical results for  $N(E_F)$  during literature survey. The numerical

results of  $N(E_F)$  are important for the understanding of many liquid state properties like free energy due to electron gas, entropy, thermal conductivity etc.

#### 4. CONCLUSION

The present form of the local pseudopotential with proper form of exchange and correlation function is used for less studied physical properties like electron dispersion, Fermi energy and Density of States at Fermi energy for many transition and rare earth liquid metals for the first time. In absence of experimental and theoretical results, presently obtained results favours the qualities like validity, transferability and capability of the local form of pseudopotential along with the procedure proposed by us to determine pseudopotential parameters for the study of liquid state properties (near melting point). Encouraged by such

study we would like to extend present form of pseudopotential with the same set of parameters for the study of liquid state properties like phonon dispersion, density of states, elastic constants and many thermodynamic functions.

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