



Comparative study of transport properties using transition metal model potential (TMMP) for 16 liquid metals

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Abstract. We propose a pseudopotential of Kumar form with two parameters, the core radius (r_c) and the model radius (r_m), which in practice is reduced to a single-parameter potential taking r_m as the experimental atomic radius. The validity of the presently used pseudopotential is verified by carrying out a detailed study of transport properties of 16 liquid metals. The results of the liquid metal resistivities using the nearly free electron (NFE) Ziman's approach and the single-site t-matrix approach are presented and compared with the experimental as well as other theoretical findings. Such comparative study confirms that the t-matrix approach is more appropriate and physically sound for a theoretical understanding of liquid metal resistivity, particularly in the case of transition metals. Furthermore, thermoelectric powers are also calculated using the present method and compared with the available experimental and theoretical results.

Keywords. Pseudopotential; liquid metal resistivity; t-matrix approach; simple and non-simple metals.

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1. Introduction

The study of transport properties of liquid metals is helpful to understand the interactions persisting in the corresponding solid metals using the well-known weak scattering approach [1–4]. Due to such importance, many researchers have studied the transport properties (particularly liquid metal resistivity) of simple and non-simple liquid metals and their alloys [5–9]. In their calculations, they have used different forms to describe the electron–ion interaction called pseudopotential. They have also used different approaches such as (i) nearly free electron (NFE) Ziman's approach [1] and (ii) Evan's transition matrix (t-matrix) approach. Evans *et al* [10] developed the t-matrix approach for the first time as an extension of Ziman's approach for the transition metals. The t-matrix approach, to calculate the liquid metal resistivity, was applied by using a muffin-tin (MT) potential [11] and the pseudopotential approach was used for the first time by Ononwu [12] for the calculations. Some researchers

have also studied the self-consistent resistivity and mean free path by considering blurring of Fermi surface [9]. In all these approaches, one of the main ingredients is the structure factor which explains atomic interactions in a liquid state. Different theoretical methods to evaluate the structure factor are discussed with detailed mathematical expressions by Shimoji [13]. In some theoretical calculations, the experimental values of the structure factor data obtained from neutron scattering experiments are used.

The second main ingredient is the pseudopotential form factor (electron–ion interaction). Due to the simplicity in the electronic structure of simple metals, there are large number of pseudopotentials based on a different philosophy which have been found to be successful for describing the transport properties of simple metals with a good degree of success. In the case of transition metals, due to their unusual electronic and structural behaviour, enough care should be taken for the construction of pseudopotential. As suggested by Moriarty [14], the physical properties of the transition

metals can be well described by selecting valency within the narrow range $1.1 < Z < 1.7$. It has been observed that for the liquid state properties of transition metals, valency does play an important role [9,15]. The use of pseudopotential for transition metals is a long-standing problem and it still remains a problem for a comprehensive understanding of physical properties (static, lattice mechanical and transport). During the literature survey, we have found some model potentials for transition metals which are used to study some physical properties [16–19]. For transition metals, a comprehensive study of the physical properties using the pseudopotential is almost nil. The pseudopotential used for the determination of physical properties of transition metals has many adjustable parameters. Such parameters are determined by favouring particular physical properties and such pseudopotentials are unable to describe the remaining physical properties. On the other hand, for the liquid transition metals, Dubinin [20] described the ion–ion interaction by the transition metal pair potential (TMPP) due to Wills–Harrison approach. In his calculation, the potential was represented as the sum of s and d electron contributions and the Bretonett and Silbert local model pseudopotential was used for the interaction of s electron. Using this potential, Dubinin [20] has studied the thermodynamic properties of liquid Fe–Ni alloys employing a variational method of thermodynamic perturbation theory. He also studied binary liquid transition metal Fe–Co alloys using the same philosophy [21]. The transferability of the pseudopotential to predict physical properties at extreme environment (high temperature and high pressure) is also a hindrance for the use of pseudopotential in condensed matter physics.

Non-local pseudopotentials are better than local ones but due to the mathematical and computational complexity, their use for such study is rare. Recently, first-principles calculations using the plane-wave pseudopotential method were used for the study of electronic and optical properties of the metal halide, CsPbI₃ [22]. It may be noted that the study of liquid-state properties of metals is still beyond the scope of *ab-initio* calculations [23]. Given the aforementioned facts, in the present communication, we use the pseudopotential form introduced by Kumar [24] having two parameters r_c (core radius) and r_m (some model radius) for the study of liquid metal resistivity using NFE Ziman’s approach and the t-matrix approach. Kumar has used such pseudopotential successfully for the study of lattice dynamics of f-shell metal thorium and he has concluded that the potential contains s–d–f hybridisation in a phenomenological manner. Thus, one should not require any extra term to account for such hybridisation.

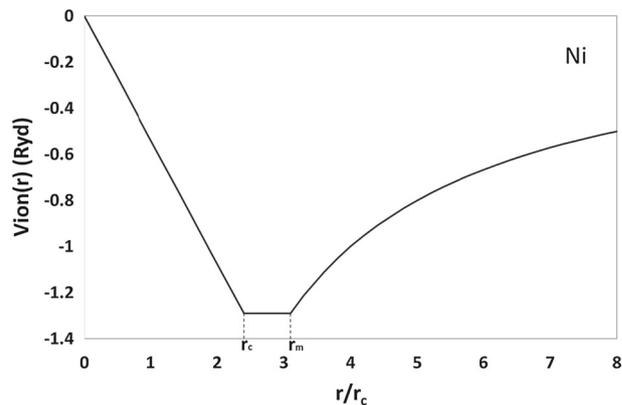


Figure 1. Pseudopotential in real space for Ni.

2. Theory

The pseudopotential in the r -space has the following form:

$$V_{\text{ion}}(r) = \begin{cases} \frac{-Ze^2 r}{r_m r_c} & \text{for } 0 < r < r_c, \\ \frac{-Ze^2}{r_m} & \text{for } r_c < r < r_m, \\ \frac{-Ze^2}{r} & \text{for } r_m < r, \end{cases} \quad (1)$$

where Z is the valency. In the region $r < r_c$, there is no complete cancellation of the potential but it decreases linearly and in the region r_c to r_m it remains constant. It possesses pure Coulombic behaviour for the region outside r_m . The potential between the regions r_c and r_m accounts for hybridisation effects because in the case of d-band metals there is no complete cancellation of potential within this range. Kumar has used empirical relation to determine r_c and r_m was adjusted to tune phonon frequencies at zone boundary in the case of actinide thorium. We have employed a simpler method, in which the two parameters r_c and r_m were reduced to a single one. First, we have approximated r_m by experimental values of atomic radii for all the elements [25]. It has been observed in many studies that the first zero of the screened pseudopotential is found to be near the Fermi surface at metallic densities. Keeping this in mind, we have adjusted r_c to get first zero near the Fermi surface for all the metals at liquid densities. The behaviour of pseudopotential $V_{\text{ion}}(r)$ against r/r_c for Ni as a test case is shown in figure 1. From this study, we wanted to verify whether the present form of the pseudopotential could account for the hybridisation effect properly.

The bare-ion pseudopotential $V_{\text{ion}}(q)$ obtained by taking the Fourier transform of eq. (1) is given in [24]. The bare-ion pseudopotential is screened by the

usual procedure, the screened pseudopotential $V(q) = (V_{\text{ion}}(q))/\epsilon(q)$. Here, $\epsilon(q)$ is the modified Hartree dielectric function with exchange and correlation function due to Hubbard [26] and Sham [27]. We have adopted the method discussed by Wallace [28] for the calculation of $\epsilon(q)$. Using NFE Ziman’s approach, the expression for liquid metal resistivity is given by [11]

$$\rho_{\text{Ziman}} = \frac{3\pi\Omega}{e^2\hbar^2v_F^2} \int_0^1 4|V(q)|^2 S(q) y^3 dy, \quad (2)$$

where $y = q/2k_F$, Ω is the atomic volume $\hbar = h/2\pi$ (h is the Planck’s constant), k_F is the Fermi wave vector, $V(q)$ is the screened pseudopotential, v_F is the Fermi velocity and $S(q)$ is the structure factor. In the present study, for the calculation, we have used the Percus–Yevick analytical form of structure factor with packing fraction $\eta = 0.45$ [11]. We have adopted atomic unit for the numerical calculations in which $m = 1/2$, $\hbar = 1$ and $e^2 = 2$. The solution of the radial Schrödinger equation gives values of the phase shifts for an l th partial wave in terms of screened electron–ion interactions [29,30]:

$$\begin{aligned} & \langle \vec{k} + \vec{q} | V(q) | \vec{k} \rangle \\ &= -\frac{2\pi\hbar^2}{\Omega} \sum_l (2l + 1) \Delta_l P_l(\cos \theta). \end{aligned} \quad (3)$$

In eq. (3), l is the orbital quantum number and for $l = 0, 1$ and $2 - \Delta_0, \Delta_1$ and Δ_2 are the phase shifts due to s, p and d waves due to pseudopotential. $P_l(\cos \theta)$ is the l th-order Legendre polynomial with θ being the angle between \vec{k} and $\vec{k} + \vec{q}$. Once all Δ_l ’s are calculated in the t-matrix approach, the t-matrix form factor with ‘On

Fermi Surface’ approximation ($|\vec{k}| = |\vec{k}'| = |\vec{k} + \vec{q}| = |k_F|$) takes the following form [11]:

$$\begin{aligned} t(k, k') &= -\frac{2\pi\hbar^3}{m(2mE_F)^{1/2}} \left(\frac{1}{\Omega} \right) \\ &\times \sum_l (2l + 1) \sin \Delta_l(E_F) \\ &\times \exp[i\Delta_l(E_F)] P_l(\cos \theta), \end{aligned} \quad (4)$$

where E_F is the Fermi energy and m is the electron mass. Finally, in the t-matrix approach ρ_t takes the following form [30]:

$$\rho_t = \frac{3\pi\Omega}{e^2\hbar^2v_F^2} \int_0^1 4y^3 S(q) |t(\vec{k}, \vec{k}')|^2 dy. \quad (5)$$

In t-matrix approach, the thermoelectric power at melting temperature T_m can be written as [31]

$$Q = \frac{-\pi^2 k_B^2 T_m}{3eE_F} \left[3 - \frac{2S(2k_F) |t(2k_F)|^2}{4 \int_0^1 S(q) |t(k, k')|^2 y^3 dy} \right], \quad (6)$$

where $k_B\pi$ is the Boltzmann constant.

3. Results and discussion

We have discussed our method in §2 to determine the pseudopotential parameters (r_c and r_m). The values of the parameters, along with the input parameters used in the calculations, are presented in table 1.

The first zero ($q = q_0$) at which $V(q_0) = 0$ is found to be near the Fermi surface within the narrow

Table 1. Values of the input parameters, atomic volume Ω (in atomic unit) at melting temperature (in K, in parentheses), taken from Waseda [11], pseudopotential parameters r_c and r_m [25] (in atomic unit).

Metal	Ω	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

Table 2. The calculated values of phase shifts Δ_l (in rad) and the comparison of liquid metal resistivities ρ_{Ziman} and ρ_t with experimental and other theoretical results. The tabulated values of liquid metal resistivities are in $\mu\Omega$ cm.

Metal	Δ_l			ρ_{Ziman}	ρ_t	Expt results	Other results
	Δ_0	Δ_1	Δ_2				
Cr	-0.20963	0.31619	0.37089	36.0	83.5	150 [32]	120 [11], 80 [33]a, 91 [33]b, 102 [33]c, 103 [33]d, 118 [33]e, 125 [33]f, 141 [33] g
Fe	-0.46026	0.25004	0.42440	66.0	121.0	138 [34–36]	182 [11], 92 [12], 81 [33]a, 92 [33]b, 103 [33]c, 105 [33]d, 119 [33]e, 126 [33]f, 142 [33] g
Co	-0.29422	0.32690	0.28750	68.9	93.4	115 [35,36]	83.3 [11], 90 [12], 100 [33]a, 113 [33]b, 128 [33]c, 130 [33]d, 151 [33]e, 158 [33]f, 166 [33] g
Ni	-0.20582	0.37542	0.27002	72.0	88.2	87 [35,36]	54.9 [11], 87 [12], 90 [33]a, 115 [33]b, 101 [33]c, 116 [33]d, 135 [33]e, 141 [33]f, 148 [33] g
Pd	-0.11976	0.40470	0.25884	73.3	85.2	83 [37]	58.1 [11], 79 [12], 165 [33]a, 188 [33]b, 215 [33]c, 219 [33]d, 259 [33]e, 272 [33]f, 290 [33] g
Pt	-0.12308	0.39838	0.26021	24.1	85.0	–	94.6 [11], 22 [12], 65 [33]a, 73 [33]b, 84 [33]c, 85 [33]d, 101 [26]e, 106 [33]f, 111 [33] g
Si	-0.07607	0.74068	0.48589	72.4	75.3	75 [38]	67.3 [11], 66.6 [38]
Ge	0.10444	0.77876	0.46768	57.9	55.6	67 [38]	66.7 [11], 41.2 [38]
Sn	0.25375	0.76119	0.46421	43.7	45.9	48 [39]	63.3 [11]
Pb	-0.07506	0.79696	0.49877	100.7	95.1	95 [39]	121 [11]
Sb	-0.22603	1.04700	0.62473	121.7	76.5	115 [40]	112 [11]
La	-0.30003	0.28456	0.39440	58.3	137.9	140 [41]	354 [7]a, 498 [7]b, 599 [7]c, 644 [7]d, 652 [7]e, 165 [31]
Ce	-0.28855	0.25584	0.38205	47.5	122.5	125 [41]	332 [7]a, 461 [7]b, 552 [7]c, 592 [7]d, 599 [7]e, 134 [31]
Gd	-0.41240	0.36346	0.42804	105.4	185.2	244 [41]	227 [7]a, 317 [7]b, 382 [7]c, 409 [7]d, 414 [7]e, 146 [31]
Eu	-0.29960	0.47649	0.28346	242.5	241.2	195 [41]	184 [7]a, 264 [7]b, 326 [7]c, 350 [7]d, 355 [7]e, 193 [31]
Yb	-0.01755	0.48165	0.24771	116.1	112.9	110 [41]	134 [7]a, 189 [7]b, 230 [7]c, 246 [7]d, 250 [7]e, 137 [31]

References: Thakor *et al* [7] (a) Hartree (H), (b) Sarkar *et al* (S), (c) Taylor (T), (d) Ichimaru–Utsumi (IU) and (e) Farid *et al* (F) local field correction function. Thakor *et al* [33] (a) Hartree (H), (b) Hubbard–Sham (HS), (c) Vashishta–Singwi (VS), (d) Sarkar *et al* (S), (e) Taylor (T), (f) Ichimaru–Utsumi (IU) and (g) Farid *et al* (F) local field correction function.

range $(0.9–1.1)k_F$ for all the metals. Using such screened pseudopotential, we have calculated the liquid metal resistivity ρ_{Ziman} and compared it with experimental results, as shown in table 2.

One interesting observation emerging from these results is that the calculated values of ρ_{Ziman} are in good agreement with experimental results particularly for non-transition metals Si, Ge, Sn, Pb and Sb (except for Eu and Yb), while in the case of transition metals, Cr, Fe, Co, Ni, Pd, Pt, La, Ce and Gd, the percentage deviations of the calculated results from the experimental

ones are more than 50%. This is because the formulation to compute liquid metal resistivity ρ_{Ziman} is based on the NFE approach or weak scattering approach.

For the completeness of the present calculation, we have displayed variations of Δ_0 , Δ_1 and Δ_2 up to the Fermi surface for Eu in figure 2. Here, for all the metals, values of the phase shifts are less than π which means that the use of perturbation theory or Born approximation is justified. The variations of the t-matrix form factors as a function of q/k_F are plotted for La, Ce and Gd as a test case in figure 3. The variations of the

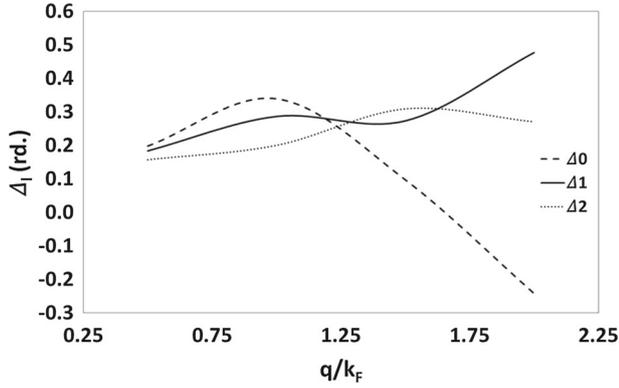


Figure 2. Variations of phase shifts against q/k_F for Eu.

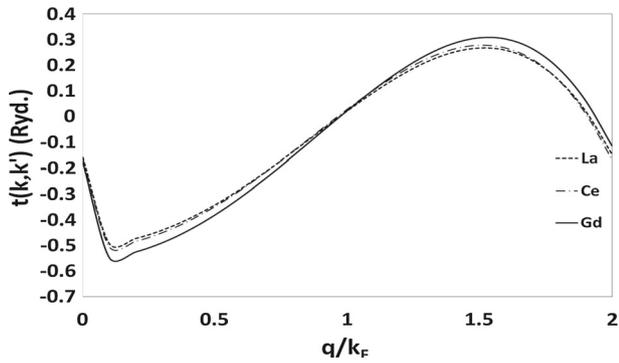


Figure 3. Variations of t-matrix form factors for La, Ce and Gd.

t-matrix form factors for the remaining metals are not presented here but the behaviours of the t-matrix form factors for all the metals studied are wiggles free and no spurious oscillations are observed up to $2k_F$. The first zeros of the t-matrix form factors for all the metals are also found to be near the Fermi surface (within the range $(0.9-1.1)k_F$). The values of the t-matrix form factors at $q = 0$ can be found by taking the limit of eq. (4) as $q \rightarrow 0$. This limiting value takes the following form in the atomic unit:

$$t(k, k') = -\frac{4\pi}{\Omega k_F} [\sin \Delta_0 \cos \Delta_0 + 3 \sin \Delta_1 \cos \Delta_1 + 5 \sin \Delta_2 \cos \Delta_2]. \quad (7)$$

For all the transition metals, the computed results of ρ_t are in excellent agreement with experimental findings except for Cr, Co and Fe and are far better than the results computed using the same pseudopotential with NFE Ziman's approach (see table 2). For non-transition metals, the results obtained using both the approaches are not changing appreciably except for antimony. A bigger discrepancy is observed in the results of liquid metal resistivity (ρ_{Ziman} and ρ_t) in the case of Cr

which may be due to exchange and correlation function used in the present study. The pseudopotential parameter r_c , determined from first zero of the pseudopotential form factor, is highly sensitive to the use of exchange and correlation function. It has been observed that the values of liquid metal resistivity have a strong dependency on exchange and correlation function [33]. We have also verified that results can be improved by using Ichimaru and Utsumi [44] and Farid *et al* [45] exchange and correlation function but our aim is to use the present conjunction scheme of Kumar's pseudopotential with exchange and correlation function due to Hubbard [26] and Sham [27] to carry out the study of comprehensive physical properties of transition metals with the same set of parameters.

We have also compared the presently computed results of t-matrix resistivity with other theoretical results due to Waseda [11], Ononiwu [12] and Thakor *et al* [7,33].

From a detailed comparison, we find that, for all the metals, our computed results are better than the results obtained by Waseda, except for chromium (Cr), germanium (Ge) and antimony (Sb). Here, we would like to comment in brief about the method used by Waseda to compute the t-matrix resistivity. He has used linear MT potential to calculate s, p and d waves phase shifts at Fermi energy and using such phase shifts, the t-matrix form factors have been computed as a function of q/k_F . According to him, $|T^2|$ represents the total t-matrix form factor which, in single-site approximation, can be expressed as the product of the structure factor $S(q)$ and the t-matrix form factor $|t(k, k')|^2$ describing the electron-ion interactions. Finally, using eq. (5), he has calculated the t-matrix resistivity. He has constructed the MT potential using experimental structural data and used Mattheiss' prescription [46], commonly used for solids, in which the total charge density at any point in the liquid is obtained by superposing the atomic charge densities.

Ononiwu [12] has calculated the transport properties of transition metals using Ziman's theory which was modified by Evans *et al* [10]. He has simulated the effect of d-band resonance in transition metals in NFE approximation and V-matrix pseudopotential form factor has been replaced by the t-matrix form factor in the equation of t-matrix resistivity. In order to account for the deviation of electron density of states at Fermi level from its free electron value, he has introduced a factor g , such that $g = (N(E_F)/N_0(E_F))$, where $N(E_F)$ is the density of states at the Fermi level and $N_0(E_F)$ is the bare density of states. He has estimated the mean value of g ($g \approx 2$) using experimental heat capacity and electron renormalisation constant using McMillan's theory for transition metals.

Table 3. The calculated values of thermoelectric power and the comparison of thermoelectric powers with experimental and other theoretical results. The tabulated values of thermoelectric powers are in $\mu\text{V}/\text{K}$.

Metal	Q	Expt results	Other results
Cr	12.07	—	–10.53 [33]a, –10.49 [33]b, –10.41 [33]c, –10.41 [33]d, –10.21 [33]e, –10.37 [33]f, –10.39 [33]g
Fe	–9.92	–4.697 [42]	–8.69 [33]a, –8.65 [33]b, –8.59 [33]c, –8.59 [33]d, –8.42 [33]e, –8.55 [33]f, –8.57 [33]g
Co	–12.45	–3.000 [42]	–10.08 [33]a, –9.97 [33]b, –9.80 [33]c, –9.80 [33]d, –9.39 [33]e, –9.66 [33]f, –9.65 [33]g
Ni	–11.98	–39.000 [42]	–9.69 [33]a, –9.58 [33]b, –9.41 [33]c, –9.41 [33]d, –9.01 [33]e, –9.27 [33]f, –9.26 [33]g
Pd	–14.66	–48.221 [37]	–12.75 [33]a, –12.62 [33]b, –12.43 [33]c, –12.42 [33]d, –11.94 [33]e, –12.26 [33]f, –12.25 [33]g
Pt	–17.28	—	–13.62 [33]a, –13.43 [33]b, –13.14 [33]c, –13.12 [33]d, –12.43 [33]e, –12.87 [33]f, –10.31 [33]g
Si	–9.46	–2.506 [38]	—
Ge	–7.75	–0.387 [38]	—
Sn	–7.44	—	—
Pb	–8.55	—	—
Sb	–6.35	0.500 [40]	—
La	–13.72	–7.500 [43]	–11.98 [7]a, –12.13 [7]b, –12.12 [7]c, –12.29 [7]d, –12.27 [7]e, –2.42 [24]
Ce	–11.73	–4.500 [43]	–10.25 [7]a, –10.38 [7]b, –10.37 [7]c, –10.51 [7]d, –10.50 [7]e, –6.34 [24]
Gd	–17.43	—	–14.68 [7]a, –14.91 [7]b, –14.89 [7]c, –15.14 [7]d, –15.11 [7]e, 3.35 [24]
Eu	–20.09	—	–12.31 [7]a, –12.55 [7]b, –12.54 [7]c, –12.83 [7]d, –12.80 [7]e, –2.64 [24]
Yb	–18.22	—	–11.27 [7]a, –11.48 [7]b, –11.47 [7]c, –11.72 [7]d, –11.69 [7]e, –0.87 [24]

References: Thakor *et al* [7] (a) Hartree (H), (b) Sarkar *et al* (S), (c) Taylor (T), (d) Ichimaru–Utsumi (IU) and (e) Farid *et al* (F) local field correction function. Thakor *et al* [33] (a) Hartree (H), (b) Hubbard–Sham (HS), (c) Vashishta–Singwi (VS), (d) Sarkar *et al* (S), (e) Taylor (T), (f) Ichimaru–Utsumi (IU) and (g) Farid *et al* (F) local field correction function.

Thakor *et al* [33] have studied the transport properties of liquid transition metals (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Pd, Ag, Cd, Pt, Au and Hg). Using their proposed pseudopotential, which is parameter free, they have studied liquid metal resistivity using Ziman's approach with different forms of exchange and correlation function and proper choice of valency. We have quoted only results obtained using original valency (for more details, see tables 2 and 3). Here, we would like to point out that such a study cannot explain the merits and demerits of the pseudopotential. Moreover, the use of Ziman's weak scattering approach for a group of transition metals is really questionable. Using the same philosophy, Thakor *et al* [7] have computed the transport properties of liquid lanthanides with valency $Z = 3$ for all metals while Eu and Yb are divalent. Our results for La, Ce and Eu are better than theirs.

The presently computed results for thermoelectric power Q are negative except for chromium and the values are not in good agreement with the experimental results in general. We have also found that the theoretical results obtained by Thakor *et al* [7,33] are highly deviating from the experimental values. Such disagreement and change in the sign of Q can be further explained in the following way: during the course of numerical calculation, we found that the computed values of the structure factor at $2k_F$ change appreciably with experimental values for all the metals [11]. From the equation (see eq. (6)), it can be seen that the values of Q depend upon the values of the structure factor at $q = 2k_F$ (i.e. on the Fermi sphere). For a free electron, the value around three has been calculated where plasma potential is dominant. When q is less than $2k_F$, most of the contribution is due to the structure factor $S(q)$ which is the reason for the positive value of Q (e.g. Cr). The resistance depends upon scattering vectors at $q = 2k_F$ at which the pseudopotential is large. At the region near $q = 2k_F$, the structure factor $S(q)$ increases rapidly. In such a condition, the values of Q are found to be negative [7]. In a liquid, the structure factor $S(q)$ increases more sharply near $q = 2k_F$ [11].

4. Conclusions

From the present study, we have found that transport properties of the liquid transition metals can be well understood with the local form of transition metal model potential with the single adjustable parameter core radius r_c . The maximum interactions of electrons are found to be near the Fermi surface. Keeping this fact in mind, we have determined the core radius r_c from the first zero of the pseudopotential near the Fermi surface. Such a method used to determine the pseudopotential is found to be successful for the study

of transport properties. The present form of the local pseudopotential accounts for s, p and d hybridisation properly and adjustment of valency is not required for the better understanding of physical properties as suggested by Moriarty. Looking at the computed results of transport properties, particularly liquid metal resistivity, we may conclude that, for transition metals, the t-matrix approach is more realistic and physically sound than Ziman's NFE weak scattering approach.

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