Electronic transport properties of some transition liquid metals

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The electronic transport properties of electrical resistivity (ρ), thermoelectric power (Q) and thermal conductivity (σ) of some transition liquid metals (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Pd, Ag, Cd, Pt, Au and Hg) are evaluated using Ziman's formula, along with our newly constructed parameter-free model potential. To describe the structural information, the structure factor $S(q)$ from the Percus–Yevick Hard Sphere (PYHS) reference system is used. The various local-field correction functions, namely Hartree (H), Vashishta–Singwi (VS), Hubbard–Shamm (HS), Sarkar et al. (SS), Ichimaru–Utsumi (IU), Taylor (T) and Farid et al. (F), have been incorporated to see the influence of exchange and correlation effects on electronic transport properties. The proper choice of the model potential, along with the local field correction function and the oxidation state (valency Z), plays a vital role in the study of the electronic transport properties of some transition liquid metals.

Keywords: pseudopotential; electronic transport properties; electrical resistivity; thermo electric power; thermal conductivity; liquid transition metals

1. Introduction

Considerable interest has caused the investigation of the properties of non-crystalline conductors such as liquid metals and their alloys for several years now. Such a liquid shows metallic as well as fluid-like behaviour and hence can facilitate a link between the theory of the liquid states and the theory of the electronic states in metals. Therefore, the study of electronic transport properties of liquid metals and their alloys remains one of the most important areas of research.

The properties of liquid metals make them highly beneficial for numerous applications. Liquid metals are used as defence goods, industrial coating, electronic casings, medical tools, sports equipments, jewellery, for decoration, etc.

The theoretical investigation of electronic transport properties of liquid metals has been of considerable interest [1–17] for several years within pseudopotential formalism. Basically, there are three theoretical methods to study electronic transport properties of liquid metals. The first is based on the nearly free-electron picture [1–15], the second is based on the finite mean free path approach [2–6], and the third is based on the tight-binding approximation [2,3,16,17]. The most popular method for studying the electronic

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transport properties of liquid metals is the electrical conduction theory developed by Ziman [1–15], using the concept of model pseudopotentials. This concept has been extremely useful over the last few decades for simple liquid metals [1,2,4–14]. However, this concept has not been found adequate to explain the electronic transport properties of liquid transition metals.

An important application of pseudopotentials is the calculation of transport properties of disordered materials such as liquids, amorphous materials and their alloys. The problem with model pseudopotentials is that of their transferability, because there is still no accurate method to obtain the form factor by which all the properties of liquid metals may be successfully investigated. It is found that a particular pseudopotential may be suitable for some properties of some metals and unsuitable for other properties of other metals. The usefulness of any model potential depends on how many parameters it involves. Generally, the potential involving fewer parameters is considered to be comparatively better than one involving more parameters, because it avoids more complexities in the calculation. It has been observed that a unique method of determination of the potential parameters has not been elucidated so far. A number of investigators have used a fitting procedure in which the potential parameters are fitted in such a way that a good agreement with experimental findings can be obtained [1–3]. Such a procedure will generally give good results for a certain property, but the same set of parameters will not give good results for other properties. Hence, we thought it was worthwhile to construct a parameter-free model potential which, in employment, can explain the physical as well as chemical properties of condensed matter.

A pseudopotential method employing a simple model of a solid composed of atomic cores and valence electrons can predict the existence and properties of new solids and their properties [18]. By implementing this idea, we construct a new model potential which is split into three regions:

$$
\begin{aligned}
W_B(r) &= 0; & r < r_{\mathrm{i}}, \\
&= -\left(\frac{Ze^2}{r_{\mathrm{a}}}\right)\left\{2 - \exp\left(\frac{r}{r_a} - 1\right)\right\}; & r_{\mathrm{i}} \leq r \leq r_{\mathrm{a}}, \\
&= -\left(\frac{Ze^2}{r}\right); & r > r_{\mathrm{a}}.
\end{aligned}
\tag{1}
$$

Basically, this form of pseudopotential is a modified version of Ashcroft's empty core model [19]. Here we have considered the actual core of an ion as an empty core rather than pseudising it. The whole effective region is split into three parts. The effective weak potential felt by an electron is sandwiched between an empty core and a long-range coulomb potential which is continuous at $r = r_{\mathrm{a}}$ and is considered between the ionic radius (r_{i}) and atomic radius (r_{a}). It may be noted that most of the pseudopotentials [1–17,19–21] are always represented by two-fold splitting in their influence. In the present potential, we have included both the features of the pseudopotential – cancellation as well as a weak remaining interaction around the ion. Another important part of the model potential is that it is parameter free. Looking to the success of the present approach, we believe that it would be interesting to try out all of the local forms of the pseudopotential in line with the present approach.

In the reciprocal space, the corresponding bare-ion form factor of the present model potential is given by:

$$
W_B(q) = \frac{-4\pi Z e^2}{q^3 r_a \Omega (1+q^2 r_a^2)^2}
\begin{bmatrix}
2(1+2q^2 r_a^2)\sin(qr_a) - qr_a(1+3q^2 r_a^2)\cos(qr_a) + \\
2(1+q^2 r_a^2)^2 \{qr_i\cos(qr_i) - \sin(qr_i)\} - \\
\exp\left(\dfrac{r_i}{r_a}-1\right)\left\{
\begin{array}{l}
(-2q^3 r_a^3 + q^3 r_a^2 r_i + q^5 r_a^4 r_i)\cos(qr_i) - \\
(-q^2 r_a^2 + q^4 r_a^4 + q^4 r_a^3 r_i + q^2 r_a r_i)\sin(qr_i)
\end{array}
\right\}
\end{bmatrix}, \quad (2)
$$

Here Z, e, Ω, q, r_i and r_a are the valency, electronic charge, atomic volume, wave vector, ionic radius and atomic radius, respectively.

The electronic transport property is one of the most sensitive tests of the pseudopotential form factor and structure factor. Hence, the objective of this article is to test the applicability of the newly constructed model potential to investigate the electronic transport properties of some transition liquid metals. As the newly constructed model potential is a modified version of Ashcroft's empty core model potential [19], it is advisable to compare the present results with those obtained by Ashcroft's empty core model potential [19], and if improvements in the present results are found, it would confirm the applicability of the present model potential. Vora [1] has calculated the electronic transport properties of electrical resistivity (ρ), thermoelectric power (Q) and thermal conductivity (σ) of some transition liquid metals using Ziman's formula along with the Ashcroft's empty core model potential [19]. He used a Percus–Yevick hard sphere (PYHS) structure factor. Therefore, the present article deals with the investigation of the electronic transport properties of electrical resistivity (ρ), thermoelectric power (Q) and thermal conductivity (σ) of some transition liquid metals (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Pd, Ag, Cd, Pt, Au and Hg) using Ziman's formula, along with the newly constructed model potential. To describe the structural information, the structure factor $S(q)$, from the PYHS reference system, is used [22]. To see the influence of exchange and correlation effects on electronic transport properties, we have incorporated various local-field correction functions, namely Hartree (H) [23], Vashishta–Singwi (VS) [24], Hubbard–Shamm (HS) [25], Sarkar et al. (SS) [26], Ichimaru–Utsumi (IU) [27], Taylor (T) [28] and Farid et al. (F) [29].

2. Theory

Within pseudopotential formalism, the widely used Ziman formula [1–15] for the electrical resistivity (ρ) of a nearly free-electron liquid metal is:

$$
\rho = \frac{3\pi m^2}{4e^2 \hbar^3 n k_F^6} \int_0^\infty dq\, q^3 S(q) |W(q)|^2 \theta(2k_F - q). \quad (3)
$$

The thermoelectric power (Q) and thermal conductivity (σ) of liquid metals are respectively given by:

$$
Q = -\frac{\pi^2 k_B^2 T}{3e E_F}\left[3 - \frac{2S(2k_F)|W(2k_F)|^2}{\langle S(q)\rangle |W(q)|^2}\right], \quad (4)
$$

and

$$\sigma = \left(\frac{\pi^2 k_B T}{3|e|^2 \rho}\right). \tag{5}$$

In Equations (3)–(5) m, e, n, k_F, $S(q)$, $W(q)$, $\theta(2k_F - q)$, k_B, T and E_F are the electron mass, electronic charge, electron density, Fermi wave number, structure factor, screened electron ion pseudopotential form factor, unit step function, Boltzmann's constant, temperature and Fermi energy, respectively.

3. Results and discussion

The input parameters [30] used in the present computations are tabulated in Table 1. The electrical resistivity (ρ), thermoelectric power (Q) and thermal conductivity (σ) of some transition liquid metals (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Pd, Ag, Cd, Pt, Au and Hg) are presented in Tables 2–4, respectively, along with the available experimental data [30] and other theoretical data [1].

The elements in the d block of the periodic table are known as transition metals. Many interesting properties of the transition liquid metals as a group are due to the results of their partly filled d subshell. In general, their properties are dependent on the electronic configuration of the electrons in the outer shell and in the penultimate outer shell.

The transition metals have different oxidation states, which make them useful as catalysts. Ions in higher oxidation states tend to make good oxidising agents, whereas elements in low oxidation states become reducing agents. They form coloured compounds, complex ions and also form alloys with themselves and with other elements. The presence of the unpaired and paired electrons in the d sub-orbital makes them paramagnetic and diamagnetic, respectively. To the best of our knowledge, no one has previously reported such a study which investigates electronic transport properties for different oxidation states (valencies Z). For this reason, we have computed for the first time the electronic

Table 1. The input parameters used in the present computations.

Metal	Z	T (K) [30]	Density n (gm cm^{-3}) [30]	η [30]	r_i (Å)	r_a (Å)
Sc	3	1833	2.92	0.43	0.81	1.61
Ti	3, 4	1973	4.15	0.44	0.68	1.45
V	2, 3, 4, 5	2173	5.36	0.44	0.59	1.31
Cr	2, 3, 6	2173	6.27	0.45	0.64	1.25
Mn	2, 3, 6, 7	1533	5.97	0.45	0.80	1.37
Fe	2, 3, 6	1823	7.01	0.44	0.64	1.24
Co	2, 3	1823	7.70	0.45	0.74	1.25
Ni	2, 3	1773	7.72	0.45	0.72	1.25
Cu	1, 2	1423	7.97	0.46	0.72	1.28
Zn	2	723	6.91	0.46	0.74	1.33
Zr	4	2173	5.93	0.44	0.79	1.59
Pd	2, 4	1853	10.5	0.47	0.86	1.38
Ag	1, 2	1273	9.27	0.45	1.26	1.45
Cd	2	623	7.954	0.45	0.97	1.49
Pt	2, 4	2053	18.7	0.47	0.70	1.37
Au	1, 3	1423	17.2	0.46	0.91	1.44
Hg	1, 2	293	13.55	0.45	1.10	1.50

Table 2. Electrical resistivity (μΩcm) of the liquid transition metals.

Metal	Z	Electrical resistivity (μΩcm)								
		H [23]	HS [25]	VS [24]	S [26]	T [28]	IU [27]	F [29]	Other [1]	Expt. [30]
Sc	3	155	179	206	209	246	261	264	–	–
Ti	3	85	98	111	114	131	140	161	53.3, 64.12, 75.55, 87.87, 92.73, 94.90, 70.05	400
	4	107	123	138	141	159	171	212		
V	2	25	28	32	32	38	39	42	47.17, 56.25, 65.44, 75.64, 79.57, 81.37, 60.6	200
	3	48	54	61	62	71	75	85		
	4	64	72	81	82	93	98	118		
	5	78	88	98	100	110	117	148		
Cr	2	48	54	61	62	72	75	78	44.77, 52.99, 61.12, 70.49, 73.87, 75.55, 56.6	80
	3	80	91	102	103	118	125	141		
	6	127	143	158	160	174	185	246		
Mn	2	126	144	164	166	195	205	218	62.85, 74.50, 86.48, 100.4, 105.11, 107.67, 80.13	180
	3	182	207	235	239	272	291	339		
	6	220	249	277	282	306	326	475		
	7	224	253	279	285	306	326	500		
Fe	2	47	54	61	61	74	74	78	57.84, 68.24, 78.52, 90.63, 94.78, 96.69, 72.6	140
	3	81	92	103	105	119	126	142		
	6	129	145	160	162	177	187	249		
Co	2	100	113	128	130	151	158	166	60.08, 70.62, 81.05, 93.63, 97.67, 100.01, 74.9	100
	3	147	168	188	191	218	230	263		
Ni	2	90	115	101	116	135	141	148	65.83, 77.30, 88.68, 102.52, 106.84, 109.43, 81.96	85
	3	134	171	152	174	196	209	283		
Cu	2	4	4.9	5.6	5.7	6.8	6.9	7	79.13, 94.16, 110.33, 129.16, 135.08, 138.62, 102.39	20
	1	90	101	115	116	136	142	149		
Zn	2	90	102	117	119	139	146	154	36.22, 41.82, 47.49, 55.29, 56.77, 58.40, 43.9	37
Zr	2	169	195	220	228	260	280	363	67.86, 82.65, 99.44, 116.93, 123.9,127	400
	4	165	188	215	219	259	272	290		
Pd	4	241	276	310	317	354	381	496	75.46, 89.49, 104.49, 122, 127.58, 130.96, 96.96	83
Ag	1	48	56	66	67	84	88	90	62.72, 76.37, 91.9, 108.15, 114.52, 117.41, 85.16	19
Cd	2	311	359	413	423	501	535	596	30.44, 37.09, 43.35, 49.06, 82.8, 53.56, 40.0	34
Pt	2	214	247	284	292	351	372	404	82.11, 97.58, 114.34, 134.11, 140, 143.76, 106.15	90
	2	65	73	84	85	101	106	111		
	4	122	139	156	160	179	192	240		
Au	1	11	13	15	15.4	19.2	19.7	20	251.61, 306.55, 371.01, 39.93, 469.39, 481.29, 43.22	31
	3	257	296	336	345	395	426	510		
Hg	1	25	29	34	35	45	47	48	83.32, 97.92, 114.43, 135.81, 140.46, 144.81, 106.43	95
	2	309	358	413	427	514	546	600		

Table 3. Thermoelectric power (μV K) of the liquid transition metals.

Metal	Z	Thermoelectric power (μ V K)								
		H [23]	HS [25]	VS [24]	S [26]	T [28]	IU [27]	F [29]	Other [1]	Expt. [30]
Sc	3	−13.62	−13.55	−13.43	−13.43	−13.11	−13.35	−13.37	−17.83, −18.09, −18.22, −18.14, −18.11, −18.52, −18.44	—
Ti	3	−11.96	−11.90	−11.79	−11.80	−11.51	−11.71	−11.73	–	—
V	4	−10.10	−10.07	−10.00	−10.01	−9.83	−9.96	−10.01	−17.16, −17.40, −17.52, −17.45, −17.43, −17.81, −17.73	—
	2	−12.56	−12.32	−11.94	−11.92	−11.03	−11.54	−11.50		
	3	−11.31	−11.24	−11.12	−11.12	−10.83	−11.04	−11.04		
	4	−9.56	−9.53	−9.45	−9.46	−9.27	−9.41	−9.44		
	5	−8.25	−8.23	−8.17	−8.17	−8.02	−8.13	−8.18		
Cr	2	−11.90	−11.72	−11.45	−11.44	−10.82	−11.21	−11.16	−15.27, −15.50, −15.62, −15.55, −15.54, −15.89, −15.82	—
	3	−10.53	−10.49	−10.41	−10.41	−10.21	−10.37	−10.39		
Mn	6	−6.77	−6.74	−6.73	−6.74	−6.65	−6.71	−6.78	−11.22, −11.42, −11.52, −11.46, −11.46, −11.77, −11.71	—
	2	−9.67	−9.56	−9.40	−9.39	−8.99	−9.26	−9.25		
	3	−8.38	−8.36	−8.31	−8.32	−8.20	−8.29	−8.32		
	6	−5.48	−5.48	−5.47	−5.47	−5.44	−5.46	−5.50		
	7	−4.99	−4.99	−4.98	−4.98	−4.95	−4.97	−5.01		
Fe	2	−9.78	−9.63	−9.41	−9.40	−8.88	−9.20	−9.14	−12.29, −12.49, −12.60, −12.53, −12.53, −12.84, −12.78	—
	3	−8.69	−8.65	−8.59	−8.59	−8.42	−8.55	−8.57		
	6	−5.63	−5.62	−5.59	−5.60	−5.53	−5.58	−5.63		
Co	2	−10.08	−9.97	−9.80	−9.80	−9.39	−9.66	−9.65	−11.54, −11.75, −11.85, −11.79, −11.80, −12.11, −12.05	0.6
	3	−8.77	−8.75	−8.70	−8.71	−8.59	−8.68	−8.71		
Ni	2	−9.69	−9.58	−9.41	−9.41	−9.01	−9.27	−9.26	−10.44, −10.63, −10.73, −10.66, −10.68, −10.97, −10.92	7.8
	3	−8.45	−8.43	−8.39	−8.39	−8.27	−8.36	−8.39		
Cu	1	−8.29	−7.82	−6.99	−6.98	−4.86	−5.87	−5.53	−10.32, −10.52, −10.64, −10.57, −10.58, −10.92, − 10.85	−3.5
	2	−8.08	−7.98	−7.84	−7.84	−7.51	−7.73	−7.71		
Zn	2	−4.56	−4.50	−4.42	−4.41	−4.21	−4.34	−4.33	−4.11, −4.18, −4.23, −4.20, −4.22, −4.35, −4.33	0.10
Zr	4	−13.60	−13.56	−13.47	−13.48	−13.23	−13.41	−13.49	−23.44, −23.81, −23.99, −23.88, −23.83, −24.44, −24.32	–
Pd	2	−12.75	−12.62	−12.43	−12.42	−11.94	−12.26	−12.25	−12.71, −12.98, −13.12, −13.04, −13.06, −13.49, −13.41	5.5
	4	−9.20	−9.19	−9.17	−9.17	−9.09	−9.15	−9.20		
Ag	1	−11.80	−11.40	−10.76	−10.72	−8.97	−10.07	−9.73	−13.11, −13.32, −13.43, −13.36, −13.33, −13.61, −13.36	−1.9
	2	−10.42	−10.37	−10.29	−10.29	−10.06	−10.22	−10.27		
Cd	2	−5.29	−5.23	−5.13	−5.13	−4.88	−5.05	−5.03	−7.01, −7.02, −7.03, −7.02, −7.01, −7.02, −7.02	0.5
Pt	2	−13.62	−13.43	−13.14	−13.12	−12.43	−12.87	−10.31	−14.49, −14.79, −14.97, −14.87, −14.89, −15.41, −15.31	–
	4	−9.97	−9.95	−9.90	−9.90	−9.75	−9.87	−8.80		
Au	1	−10.36	−9.68	−8.60	−8.52	−5.74	−7.73	−6.71	−16.42, −16.55, −16.64, −16.59, −16.60, −16.83, −16.79	−0.6
	3	−9.10	−9.08	−9.04	−9.04	−8.92	−9.02	−9.05		
Hg	1	−2.76	−2.60	−2.37	−2.34	−1.68	−2.06	−1.93	−2.69, −2.74, −2.77, −2.77, −2.75, −2.86, −2.85	2.7
	2	−2.64	−2.61	−2.57	−2.57	−2.47	−2.54	−2.54		

Table 4. Thermal conductivity (watt K^{-1} cm^{-1}) of the liquid transition metals.

Metal	Z	Thermal conductivity (watt K^{-1} cm^{-1})							
		H [23]	HS [25]	VS [24]	S [26]	T [28]	IU [27]	F [29]	Other [1]
Sc	3	0.289	0.250	0.220	0.212	0.182	0.169	0.142	—
Ti	3	0.562	0.492	0.434	0.424	0.368	0.345	0.300	0.95, 0.79, 0.67, 0.72, 0.58, 0.55, 0.53
V	4	0.447	0.393	0.349	0.341	0.302	0.282	0.227	
	2	2.138	1.884	1.664	1.637	1.403	1.350	1.271	1.18, 0.99, 0.85, 0.92, 0.73, 0.70, 0.68
	3	1.102	0.974	0.864	0.850	0.744	0.703	0.622	
	4	0.829	0.734	0.656	0.645	0.575	0.541	0.449	
Cr	5	0.678	0.603	0.542	0.533	0.481	0.453	0.539	
	2	1.114	0.986	0.871	0.860	0.738	0.708	0.676	1.24, 1.05, 0.91, 0.98, 0.79, 0.75, 0.73
	3	0.661	0.585	0.52	0.513	0.451	0.425	0.377	
Mn	6	0.417	0.372	0.337	0.332	0.305	0.288	0.215	
	2	0.296	0.260	0.229	0.225	0.191	0.182	0.172	0.63, 0.54, 0.46, 0.50, 0.40, 0.38, 0.37
	3	0.206	0.180	0.159	0.157	0.138	0.129	0.110	
	6	0.170	0.150	0.135	0.133	0.122	0.115	0.079	
	7	0.167	0.148	0.134	0.132	0.122	0.115	0.075	
Fe	2	0.938	0.831	0.734	0.725	0.623	0.598	0.571	0.82, 0.69, 0.60, 0.65, 0.52, 0.50, 0.49
	3	0.546	0.484	0.43	0.424	0.374	0.353	0.313	
	6	0.344	0.307	0.278	0.274	0.252	0.238	0.179	
Co	2	0.444	0.393	0.343	0.343	0.295	0.281	0.267	0.78, 0.66, 0.58, 0.63, 0.50, 0.48, 0.47
	3	0.302	0.267	0.237	0.234	0.206	0.194	0.169	
Ni	2	0.483	0.428	0.378	0.373	0.321	0.307	0.292	0.66, 0.56, 0.49, 0.53,0.42, 0.41, 0.40
	3	0.322	0.285	0.253	0.249	0.221	0.207	0.181	
Cu	1	8.064	7.001	6.130	6.034	5.112	4.987	4.913	0.44, 0.37, 0.31, 0.34, 0.27, 0.26, 0.25
	2	0.387	0.342	0.302	0.298	0.256	0.245	0.233	
Zn	2	0.196	0.172	0.151	0.149	0.127	0.121	0.114	0.55, 0.48, 0.42, 0.46, 0.36, 0.35, 0.34
Zr	4	0.313	0.272	0.241	0.233	0.204	0.189	0.146	0.82, 0.67, 0.56, 0.60, 0.47, 0.45, 0.44
Pd	2	0.274	0.240	0.210	0.206	0.175	0.166	0.156	0.60, 0.51, 0.43, 0.47, 0.37, 0.35, 0.35
	4	0.188	0.164	0.146	0.143	0.128	0.119	0.091	
Ag	1	0.653	0.557	0.474	0.461	0.369	0.353	0.346	0.50, 0.41, 0.34, 0.36, 0.29, 0.27, 0.26
	2	0.100	0.087	0.075	0.073	0.062	0.058	0.052	
Cd	2	0.071	0.062	0.054	0.052	0.043	0.041	0.038	0.58, 0.48, 0.41, 0.44, 0.36, 0.33, 0.33
Pt	2	0.777	0.682	0.598	0.587	0.497	0.474	0.450	0.61, 0.51, 0.44, 0.47, 0.37, 0.36, 0.35
	4	0.41	0.36	0.32	0.314	0.28	0.261	0.209	
Au	1	3.111	2.672	2.296	2.242	1.810	1.761	1.724	0.14, 0.11, 0.09, 0.10, 0.08, 0.07, 0.07
	3	0.135	0.117	0.103	0.101	0.088	0.082	0.068	
Hg	1	0.290	0.246	0.209	0.202	0.159	0.153	0.150	0.12, 0.10, 0.08, 0.09, 0.07, 0.07, 0.07
	2	0.023	0.02	0.017	0.017	0.014	0.013	0.012	

transport properties for different oxidation states, i.e. for different valencies (Z) of transition metals.

From Table 2, it is seen that the electrical resistivity (ρ) has minimum numerical values due to the Hartree (H) [23] local field correction function, while maximum due to the Farid *et al.* (F) [29] for all the liquid transition metals. Another important point is that the different forms of the exchange and correlation functions have a sensible effect on the numerical values of the electrical resistivity (ρ). As the oxidation states (valencies Z) increase, the value of electrical resistivity (ρ) increases. The present results are far better than the other available theoretical data [1]. The present results are in good agreement with the available experimental data [30]. A good agreement between the present results and experimental data [30] has been achieved due to the Farid *et al.* [29] local field correction function with oxidation states (valencies Z) equal to 4, 5, 3, 1, 4, 1 and 1 for Ti, V, Fe, Cu, Zr, Au and Hg, respectively. For Cr, Mn, Co, Ni, Zn, Pd and Ag, it is due to the Hartree [23] local field correction function with oxidation states (valencies Z) equal to 3, 3, 2, 2, 2, 2 and 1, respectively, whereas for Pt, it is due to Sarkar *et al.* [26] with oxidation states (valencies Z) equal to 2.

From Table 3, it is found that the effect of the local field correction function on the numerical values of thermoelectric power (Q) is not very sensible when compared to the electrical resistivity. The minimum numerical values have been obtained due to the Hartree [23] local field correction function, while maximum is due to the Taylor [28] local field correction function. An improvement in the present results is observed over the theoretical data [1] if it compares more closely to the available experimental data [30]. As the oxidation state (valencies Z) increases, the numerical value of thermoelectric power (Q) also increases. As we have seen from Equation (4), the thermoelectric power (Q) is very sensitive to the size of the Fermi surface and hence depends on the behaviour of the scattering as k_F increases. It also depends on the magnitude of the pseudopotential $W(q)$ and the structure factor $S(q)$. The value of around 3 has been calculated for a free electron, i.e. where the plasma potential is dominant, so that most of the weightage comes from the values of the structure factor $S(q)$, where q is not too close to $2k_F$. This gives a positive sign to the thermoelectric power (Q). But when the pseudopotential is large, the resistance is determined by scattering vectors near $2k_F$ and the structure factor $S(q)$ rises quickly in this region. At this time the negative values of the thermoelectric power (Q) are shown easily, simply by the great increase of scattering that occurs when q is increased slightly. In liquid, the structure factor $S(q)$ increases more sharply near $q = 2k_F$. This makes no difference where only small values of q are effective, but clearly makes the thermoelectric power (Q) more negative when the effect of the ion core is large. In transition liquid metals, the effect of the d shell above the Fermi level appears to give rise to a considerable increase in the scattering amplitude, as k_F is high. Due to this, all values of the thermoelectric power (Q) become negative.

From Table 4, it has been noticed that the influence of the local field correction function is very effective on the numerical values of thermal conductivity (σ). Hartree [23] produces maximum numerical values of thermal conductivity (σ), while Farid *et al.* [29] produces the minimum. As the oxidation states (valencies Z) increase, the value of thermal conductivity (σ) decreases.

Vora [1] has also conducted a similar study for transition liquid metals using the Ashcroft empty core model potential [19]. He has taken $Z = 1.5$ for Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zr, Pd, Ag and Pt liquid metals and $Z = 2$ for Zn Cd, Au and Hg liquid metals. He has also fitted the parameter of the potential r_c in such a way that the results are found in

good agreement with experimental data [30]. But the present study is free from any such type of fitting procedure. We have taken actual possible oxidation states (valencies Z) rather than taking $Z = 1$, 1.5 or 2. Our potential is also a parameter-free model potential. Even though we have not taken any fitting procedures, our results are in quite good agreement with available experimental data [30] and also better fit the experimental data than the other data generated by Vora [1]. In the case of electrical resistivity (ρ), the excellent agreement between the present results and the experimental data [30] has been achieved due to the Farid *et al.* [29] local field correction function with oxidation states (valencies Z) equal to 3 for Fe. For Cr, Mn, Co and Ni, it is due to Hartree [23] local field correction functions with oxidation states (valencies Z) equal to 3, 3, 2 and 2, respectively, whereas for Pt, it is due to Sarkar *et al.* [26] with oxidation states (valencies Z) equal to 2. Significant improvements in the present results have been found in the case of electrical resistivity (ρ) (except Zn, Pd, Cd and Hg) and thermoelectric power (Q) (except Zn) than in the other results obtained by Vora [1] using Ashcroft's empty core model potential [19]. This confirms the validity of our model potential to explain electronic transport properties of some transition liquid metals.

4. Conclusion

The electronic transport properties of some transition liquid metals (Sc, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Zr, Pd, Ag, Cd, Pt, Au and Hg) have been successfully investigated by Ziman's [1–15] formula, along with our newly constructed parameter-free model potential. Electronic transport properties are very sensitive to the choice of different forms of local field correction functions and different oxidation states (valencies Z). Good qualitative and quantitative data of the electronic transport properties of some transition liquid metals have been obtained, and these could be beneficial to other theoreticians as well as experimentalists working in the same field. The presently obtained results using our newly constructed parameter-free model potential seems to lead to better results than those results obtained by Vora [1] using the Ashcroft empty core model potential [19]. The structure factor $S(q)$, from the PYHS reference system [22], is also capable of explaining electronic transport properties of some transition liquid metals. Our significantly improved results could be obtained by the use of other local field correction functions and structure factor $S(q)$. So, the application of our newly proposed model potential in the present study definitely adds a new contribution to the understanding of electronic transport properties of some transition metals in the liquid state. Thus, the proper choice of the model potential along with the local field correction function and oxidation state (valency Z) plays a vital role in the study of the electronic transport properties of some transition liquid metals.

Looking to the success of the newly modelled potential in the present study, the use of the presently constructed parameter-free model potential in the investigation of electronic transport properties using two further methods (i.e. a mean free path and a tight binding), and also using other structure factors, is in progress. It will be communicated within due course.

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