Plasma and liquid-metal resistivity calculations using the Ziman theory

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Liquid-metal and dense plasma resistivities are calculated for some transition metals and for Al using the Ziman theory together with the self-consistent average atom INFERNO code. The hypernetted-chain equation is used for calculating the structure factors when no experimental data are available. Attempts are made to improve upon previous calculations by including more accurate electron densities of states as well as the second and third order terms in the multiple scattering expansion of the T matrix. Calculated resistivities with the exception of low density Cu plasma are up to a factor of 4 higher than the experiment for transition metals and between three to four times smaller for Al liquid metal and plasma. The results of the model used in this paper do not seem to agree with the recent experimental data for Cu at a density of the order of a gram and temperatures of several eV as recently obtained by DeSilva and Kunze [Phys. Rev. E **49**, 4448 (1994)]. [S1063-651X(96)00207-3]

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I. INTRODUCTION

Extensive and systematic calculations of plasma and liquid-metal resistivities were recently carried out by Rinker [1] using the extended Ziman formula. This author, who also analyzed the derivation of the formula, pointed out that several approximations made in these calculations could be improved upon. Among these we cite the use of more accurate electron densities of states and multiple scattering effects. Lee and More [2] also calculated plasma resistivities, covering a wide range of density and temperature. Another recent development is the experimental work of DeSilva and Kunze who measured the conductivities of dense Cu plasmas [3].

In this paper three major topics are addressed. (a) In Sec. II, liquid-metal resistivities of some transition metals are calculated from the Ziman theory using the self-consistent average atom INFERNO code [4] model, the extended Ziman theory was derived by Evans, Greenwood, and Lloyd [5]. An attempt to improve the calculation is made by using more realistic electron densities of states thereby improving the accuracy of the chemical potential and thus also of the number of conducting electrons. In addition comparisons were also made to recent high temperature liquid metal resistivity data for Cu and Ni [6,7]; here use is made of the hypernetted-chain (HNC) equation [8] for calculating the ion structure factor. (b) The effect of the second and third order terms of the T matrix expansion of the multiple scattering series on the resistivity of liquid-metal Cu is evaluated and described in Sec. III. (c) The resistivity of Cu plasma as a function of temperature was studied by means of the Ziman theory. It was found that for the experimental conditions in Ref. [3] the mean free path (mfp) obtained on the basis of the Ziman theory is smaller than the interparticle distance. Aluminum plasma were also studied and the results of calculations using the Ziman theory were compared to recent experimental data [9].

The basic motivation for the present research is to attempt to ascertain the accuracy of dense plasma resistivity calculations using the Ziman theory. There is presently a considerable demand for dense plasma resistivities particularly in connection with recent femtosecond pulsed laser experiments [9] as well as other laser plasma experiments [10]. Thus to test the Ziman theory the detailed comparisons of experiment to theory, which included effects not accounted for previously were carried out for liquid metals, as well as the comparisons with very recently obtained plasma resistivities in Cu and Al. The conclusions drawn from these comparisons are presented in Sec. V.

II. LIQUID-METAL RESISTIVITIES

The extended Ziman formula as derived by Evans, Greenwood, and Lloyd [5] was used here in calculating the resistivity of the liquid transition metals. This formula in its simple form is given by

$$R=\hbar/(3\pi\overline{z^2}e^2\overline{\rho})\int_0^\infty dE\ f'(E)\int_0^{2k}dq\ q^3S(q)\sigma(q). \quad (1)$$

It employs the single site t matrix approximation for the scattering,

$$\sigma(q)=\langle k|t|k'\rangle^2 = \left|\frac{1}{2ik}\sum_l\ (2l+1)(e^{2i\delta(k)}-1)P_l\ \cos\ \theta_{kk'}\right|^2. \quad (2)$$

Here q is the momentum transferred from the incident electron with energy E, $f(E)$ is the electron fermi distribution, ρ is the ion density, and θ is the scattering angle.

The three basic elements in the calculation are the number of conducting electrons per ion $\overline{z}$, the scattering phase shifts δ, and the ion structure factor $S(q)$. The INFERNO calculation gives the number of bound electrons N_b. Let $n(E)$ denote the sum of the free electrons up to energy E, $N_0(E)$, plus the resonance electrons up to this energy. $n(E)$ is given where E is positive by

$$n(E)=N_0(E)+\frac{2}{\pi}\sum_l\ (2l+1)\,\delta_l(E)+N_{\rm MS}(E), \quad (3)$$

where δ_l is the phase shift of the l partial wave. $N_{\rm MS}$ is the multiple scattering contribution to the density of states (DOS) in the formalism of the Lloyd theory which together

TABLE I. Table of liquid-metal resistivities, resistivities in $\mu\Omega$ cm. MS denotes the inclusion of the ''multiple scattering'' term in the DOS. (a) Near melting. (b) Comparisons with higher temperature cases; see text for source of experimental data.

(a)

	ρ (cgs)	T (eV)	expt. [1]	Rinker [1]	espos [9]	noMS	MS	Z(noMS)	Z(MS)
Mn	6.43	0.131	174	640		732		1.38	
Fe	7.05	0.156	139	423	1130	571	491	1.24	1.34
Ni	7.85	0.149	85	440	74	76		1.07	
Cu	7.96	0.117	21	45	41	19.8	18	1.34	1.42
Al	2.70	0.060	25			10.9		3.0	

(b)

	ρ (cgs)	T (eV)	expt.	noMS	Z(noMS)	$S(q)$	τ(sec)
Cu	7.96	0.117	21	19.8	1.34	exp	1.7×10^{-15}
	8.00	0.117	19.1	24.5	1.34	HNC	1.8×10^{-15}
	6.42	0.302	32.3	8.8	1.20	HNC	1.5×10^{-15}
Ni	7.85	0.149	85	76	1.07	exp	4.8×10^{-16}
	7.71	0.164	97.3	103	1.04	HNC	4.4×10^{-16}
	6.57	0.319	117	70.6	0.891	HNC	5.0×10^{-16}

with the second term, the Friedel term, should give the correct DOS [11,12]. In the case of Cu the sum of these terms was taken from the experiment [13], while in the case of Fe they were based on calculations [14]. The sum of both the terms was assumed equal to the number of particles under the resonance as calculated by the INFERNO code. Thus the N_{MS} term only alters the shape of the DOS curve here, compared to the calculation without the N_{MS} term.

The chemical potential is obtained from where Z_0 is the nuclear charge from

$$Z_0 - N_b = \int n(E) f(E) dE. \tag{4}$$

The improvement in the present calculations over previous ones lies in the inclusion of the N_{MS} term in Eq. (1). This influences the chemical potential and thus the ratio of free to resonance electrons, see Table I. A point worth mentioning, which was not accounted for here, is the exact location of the lowest energy of the free electrons relative to the jellium continuum. This topic has been discussed by Ziman [15] in connection with liquid metals, where it is pointed out that this energy is influenced by the surrounding ions.

The scattering phase shifts are obtained from the INFERNO calculation. The basic assumption of the Ziman model is the muffin tin picture where the electrons are scattered by the core potentials. Thus the use of the INFERNO model for calculating the phase shifts is open to some question since what is needed is the scattering at the core boundary by the core potential and not at the Wigner-Seitz (WS) radius as in INFERNO. The ion structure factors are taken from the experiment [16], for the liquid metals near melting, while for the higher temperature calculations the ion structure factor was obtained from the HNC model [8].

In Table I(a) are presented results of our calculations for liquid metals near melting together with experimental data as well as results of other calculations. MS denotes our results with the more accurate DOS, i.e., with the N_{MS} term in Eq. (3), while noMS is our calculation using Eq. (1) just with the Friedel term. Z(MS) and Z(noMS) denote the number of conducting electrons in both these cases.

The resistivities obtained for Cu and Ni are in very good agreement with the experiment, while for Al the experimental resistivity is of the order of twice the one calculated here. The calculated results for Fe and Mn are about four times larger than the experimental result, the results of Rinker are in fair agreement with ours for the latter two elements, while Esposito, Ehrenreich, and Gelatt [11] obtain an even higher calculated result for Fe. Our results and those of Rinker [1] should be similar but not exactly the same, since although both calculations are essentially the same they differ in details such as the values of the potentials which are evaluated somewhat differently. The reason for the large difference in the calculated resistivity of Ni is not clear.

The effect of using the more accurate DOS is seen to significantly decrease the resistivity of Fe by bringing about an increase in the number of conduction electrons. For Cu this effect does not alter the result significantly.

Another point also connected to multiple scattering which could bring the calculated results, especially for Fe and Mn, in closer agreement with the experiment, relates to the problem of scattering from a cluster as opposed to scattering from a single scatterer as assumed in the calculations presented here. Scattering from a cluster could be represented by generalized phase shifts, which decrease and broadens the scattering integral $\int_0^{2k} dq\, q^3 S(q)\sigma(q)$ as a function of energy [17,18]. The scattering cross section of Fe is maximum at the resonance energy, at which $f'(E)$ also attains its maximum, see Fig. 1(a). Smearing the resonance will lower the scattering cross section and hence the resistivity. Such an explanation has been put forward by Fresard and Germond [17] in connection with the resistivities of transition liquid metals. This effect should be more pronounced in Fe than in Cu; in the latter the resonance energy is considerably lower than the maximum in $f'(E)$, see Fig. 1(b).

In Table I(b) we compare our calculated results to the experimental data of Gathers for Cu [6] and to those of Hix-

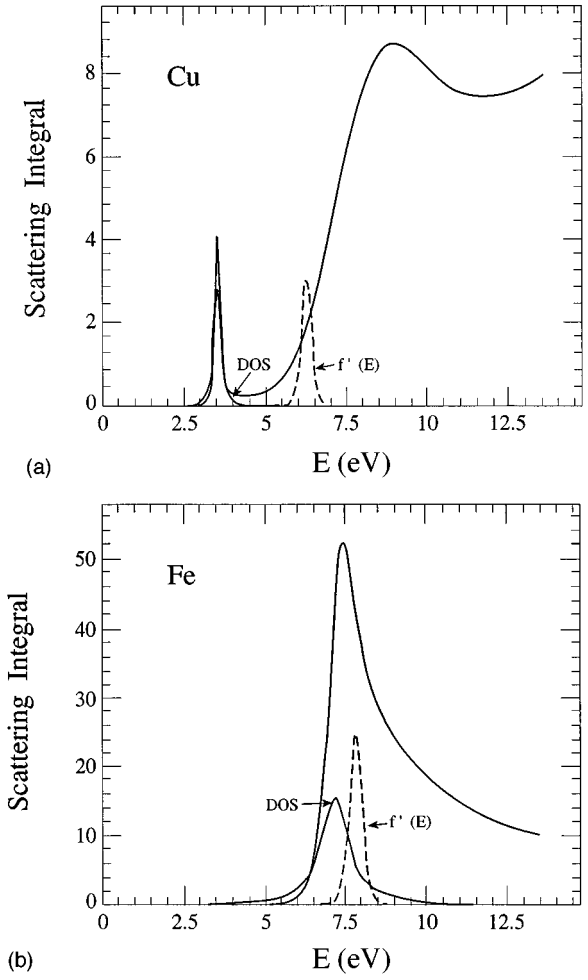

FIG. 1. Scattering integral as a function of energy; also plotted are $f'(E)$ and the density of states of the resonance. (a) For Fe, (b) for Cu.

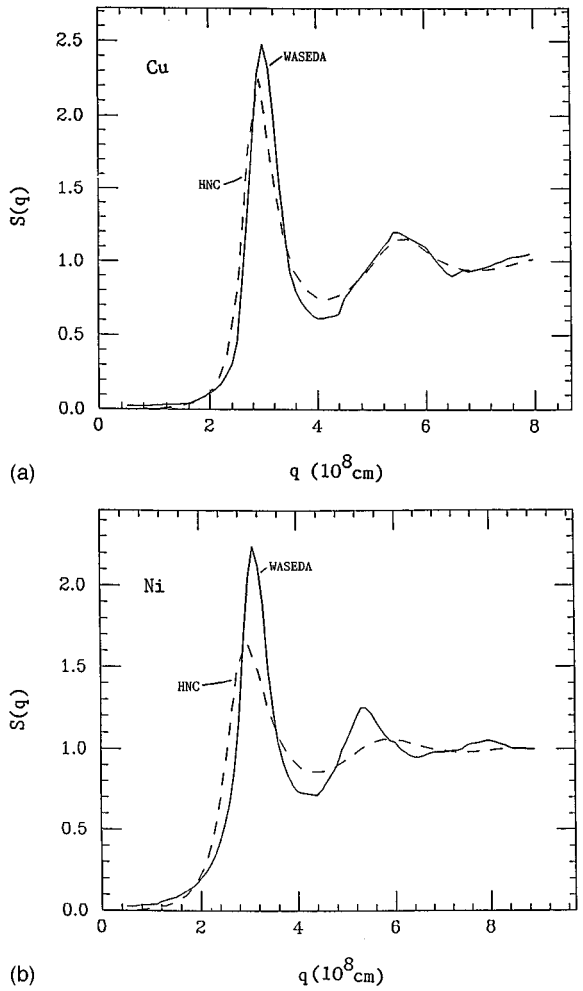

FIG. 2. Comparison of the structure factor $S(q)$, between experimental data as given by Waseda [14] and results of the HNC calculations, for liquid Cu in (a) and liquid Ni in (b).

son, Winkler, and Hodgdon for Ni [7]. Structure factors were obtained from the HNC model since experimental data are not available at these higher temperatures. It is of interest to compare resistivity results using experimental structure factors to those calculated by means of the HNC model at the lower temperatures. In the latter case the liquid metal is assumed to be composed of a plasma of ions and electrons with the number of free electrons calculated as described above and given in the fifth column of Table I(b). For Cu a comparison is made for densities of 7.96 g/cm^3 and 8.0 g/cm^3 both at the temperature of 0.117 eV. The latter case is adopted from the experimental data of Gathers [6] and is essentially the same as the former case which is given in Table I(a). In Fig. 2(a) we compare the experimental $S(q)$ at a density of 7.96 g/cm^3 to the calculated $S(q)$ at 8.0 g/cm^3 and the agreement is satisfactory (it could be significantly improved if the ''bridge function'' was accounted for [19]). The calculated resistivities, using the same phase shifts, differ, however, by about 25%, indicating the sensitivity of the resistivity on the structure factor. A similar comparison was carried out for Ni and in Fig. 2(b) we compare the structure factors which are seen to differ substantially as does the calculated resistivity. Table I(b) affords a comparison of calculated resistivities of Cu and Ni as a function of temperature. The results are presented without multiple scattering effects in the DOS since neither the experimental nor theoretical densities of states are available for the cases studied in Table I(b). Table I(b) also includes in the last column the collision times τ for each of the cases treated. The experimental resistivity of Cu at the higher temperature is seen to increase by 69% compared to the lower temperature value while the calculation based on the HNC structure factors is observed to decrease drastically. For Ni the experimental value increases by 20% while the calculated result decreases again this time by about 30%.

Although we do not reproduce the trend of the experimental data for Ni the results still agree within less than a factor of 2. In Cu the experimental resistivity is almost four times higher than that calculated here, and again the trend of the experimental data as a function of temperature is opposite to the calculated result. Although the number of calculated conducting electrons decreases with expansion and heating, a factor which should cause an increase in the calculated resistivity, our calculation yields a decrease in the resistivity, especially very significant in the case of Cu. This discrepancy should be investigated in more detail in the future.

III. MULTIPLE SCATTERING EXPANSION OF THE *T* MATRIX EFFECT ON RESISTIVITY

In this section we investigate the effect of the second and third order terms of the multiple scattering expansion on the resistivity result of liquid Cu obtained above where only the first order term as given by Eq. (1) was used.

Following a suggestion by Ziman [20] and elaborated on by Dreirach *et al.* [21], what is needed in Eq. (1) is the total T matrix of the system. Calculations using the T matrix were carried out by Dunleavy and Jones [22] for liquid transition metals and by Perrot and Dharma-wardana [23] for hydrogen plasma as well as Fe at 5 keV. We therefore write

$$R=\hbar/3\pi\overline{z^2}e^2\overline{\rho}\int_0^\infty d\epsilon f'(\epsilon)\int_0^{2k} dq\ q^3T^2. \tag{5}$$

The T matrix can be written [24–26] in the form of the multiple scattering expansion, when the initial scattering commences at ion i,

$$T=\sum_i t_i+\sum_{ij} t_iG_0t_j,+\sum_{ijk} t_iG_0t_jG_0t_k, \tag{6}$$

where the first term represents simple scattering by particle i. The second term represents double scattering, first by particle i then propagation of the scattered particle to j where it is scattered by the latter. The nth term represents n successive scatterings, in all cases the incident momentum is k_0, while the outgoing momentum is k.

It can be shown that by invoking the approximation that the surroundings of the scatterers are identical (the quasicrystalline approximation QCA) the resistivity is now

$$R=\hbar/3\pi\overline{z^2}e^2\overline{p}\int_0^\infty d\epsilon\ f'(\epsilon)\int_0^{2k} dq \times q^3S(q)\left|t_1+\sum_j t_1G_0t_j+\sum_{jk} t_1G_0t_jG_0t_k+\cdots\right|^2. \tag{7}$$

As noted above the widely used extended Ziman formula employs only the first term of this series. It is our purpose to examine the influence of the second and third terms on the calculated resistivity of liquid metals, near melting, which bear strong d resonances. Our example here is Cu at $T=0.117$ keV and $\rho=7.96$ g/cm^3. As mentioned above three of the basic ingredients needed for the resistivity calculation were obtained from the self-consistent average atom model (INFERNO) [4]. These are the phase shifts of the electron ion scattering, the number of conducting electrons, and the free electron energy distribution. The ion structure factor were obtained from the experimental data [16].

As a first step in ascertaining the influence of the second term of Eq. (2) on the scattering, the positions of the neighboring scatterers are determined. In the present calculations the influence of the nearest neighbors only, defined as all the ions comprising the first peak of the radial distribution function $g(r)$ or first coordination shell, were considered. $g(r)$ was taken from Waseda [16] and the number of scatterers thus obtained is ten. The distribution of the scatterers about the central ions was obtained by means of the Monte Carlo technique by sampling, $g(r)r^2dr$ for the radial coordinate, while the $\cos(\theta)$ and ϕ were sampled with equal probability. In the equal probability scatterer configurations thus generated, no correlations were assumed between the ions of the configuration.

TABLE II. Effects of second order term in the multiple scattering series on the resistivity of liquid Cu. The resistivities are in units of $\mu\Omega$ cm, and the result for the single site approximation here is 19.8.

Configuration	with 2nd order term
1	21.4
3	20.8
5	21.2
7	21.4
9	20.8

The second term of the series given in Eq. (2) is evaluated as in Messiah [25]. The propagator G_0 between r_1 and r_2 is given by [24]

$$G_0=\exp(ik_p|r_1-r_2|)/(4\pi|r_1-r_2|),$$

where $k_p=|k_0|\vec{R}/R$, $\vec{R}$ is the vector connecting the central ion to the given scatterer.

The term to be determined for each of the ten neighboring ions each denoted by the index j is obtained by assuming the core radius to be small relative to R. The result is

$$\langle k|t_iG_0t_j|k_0\rangle=-1/(4\pi R)\langle k|t_i|k_p\rangle\langle k_p|t_j|k_0\rangle. \tag{8}$$

Summing these terms over all ten scatterers in a given nearest neighbor configuration and inserting the result into Eq. (7), gives the resistivity which includes the second term of the multiple scattering series of Eq. (6).

The results of resistivities which include the second term of the series, obtained from five different configurations of the ten scatterers, are presented in Table II. The resistivity with no multiple scattering corrections obtained here is 19.8 $\mu\Omega$ cm (the experimental result is 21 $\mu\Omega$ cm), while the resistivity averaged over the five configuration in Table II is 21.1 $\mu\Omega$ cm. Thus inserting the second term of the multiple scattering series therefore causes an average increase of only 7% in the calculated resistivity.

The third term in the multiple scattering series of Eq. (3) is derived in the same manner as the second term. As above the incident momentum is k_0 while the final momentum is k. The two intermediate momenta are k_p and k_{p1} and are given by the positions of the second and third scatterers. Thus the third term of the series is

$$\langle k|t_iG_0t_jG_0t_k|k_0\rangle=\frac{\langle k|t_i|k_{p1}\rangle\langle k_{p1}|t_j|k_p\rangle\langle k_p|t_k|k_0\rangle}{(4\pi)^2R_1R_2}. \tag{9}$$

The summation over k_p is over the nearest ten scatterers to the central ion. For each of these scatterers the third scattering event is assumed to take place at the positions of the ten nearest atoms to that given scatterer. The positions of the latter are obtained by means of a molecular dynamics simulation which gives the correct $g(r)$ curve for liquid Cu. We

TABLE III. Resistivity of Cu at 1.5 g/cm^3. Resistivity Ω cm designates the resistivity assuming the number of conduction electrons is Z. Z is the number of conductors according to the calculations of this paper, ZSAHA is the ionization state obtained from the Saha equation. Resistivities are not corrected in this table for the mfp, see text.

Temp	Z	Resistivity (Ω cm)	ZSAHA
15 000	0.09	10.2×10^{-3}	0.07
17 000	0.13	6.4×10^{-3}	0.08
22 000	0.26	1.9×10^{-3}	0.15
25 000	0.35	1.4×10^{-3}	0.20
30 000	0.44	1.1×10^{-3}	0.29

note that the position of the first scatterers are those used above which were sampled from the $g(r)$ curve. The distance between the central ion and first scatterer is R_1 while that between the second and third scatterer is R_2. The effect of the third term on the resistivity in the case studied here was found to be less than 1%.

The small increase of 7% in the calculated resistivity is not nearly enough to account for the large difference between the calculation and the experiment in the cases of Fe and Mn. It is logical to assume that corrections of similar magnitude would be obtained for Fe, Ni, and Mn. As noted above Dunleavy and Jones [22] performed multiple scattering calculations of the resistivities of liquid transition metals. These authors calculate the complete T matrix also within the QCA, generalizing the solution given by Schwartz and Ehrenreich [26]. They observe a decrease in the resistivity of liquid Cu by the introduction of multiple scattering whereas we here observe an increase in this value. The reason for this difference could be that our calculation does not include all the aspects of the T matrix. Although possibly less accurate, the calculations performed here clearly bring out the relative contribution of the terms in the multiple scattering series.

IV. RESISTIVITY OF Cu AND Al PLASMA

In this section we compare the results of our calculations to the recently obtained experimental conductivities of DeSilva and Kunze [3] for dense Cu plasma. As in Sec. II which dealt with liquid metals we again calculate the resistivity of the Cu plasma using Eq. (1). Resistivities are calculated here at a density of 1 g/cm^3 from 21 000 K to 30 000 K and at 1.5 g/cm^3 from 15 000 K to 30 000 K. The smaller temperature range at the lower density is because the INFERNO calculation fails to converge at temperatures less than 21 000 K due to the relatively low density involved, while at 1.5 g/cm^3 the calculation ceases to converge below 15 000 K. The number of conducting electrons is derived as above using Eq. (3) [without the $N_{MS}(E)$ term] while the phase shifts are also derived from the INFERNO model. The structure factor was obtained by means of the HNC model [8], in the case of the Cu plasma studied here the inclusion of screening in the HNC calculation is of no significance.

In Table III are presented the results of resistivity calculations for Cu at a density of 1.5 g/cm^3 and in the temperature range from 15 000 K up to 30 000 K. Z is the number of free electrons as obtained from the INFERNO calculations,

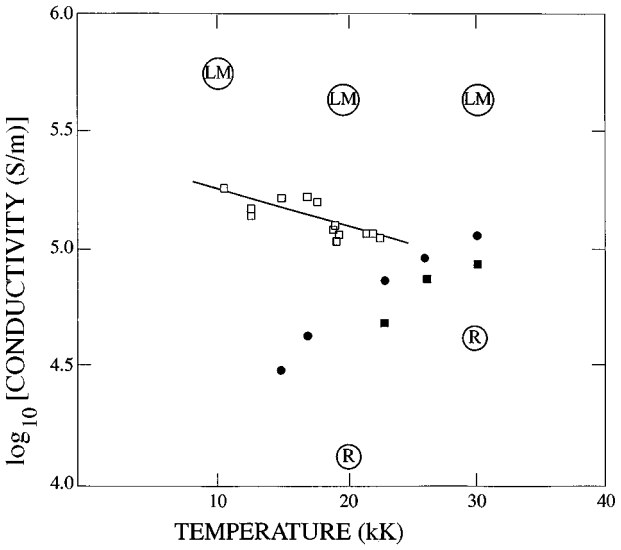

FIG. 3. Conductivity of a Cu plasma at density 1 g/cm^3 as a function of temperature. The squares and full line are the experimental data of DeSilva and Kunze, while R and LM denote the results of Rinker and Lee and More, respectively. Our calculated results are given by the full points and squares and are for 1.5 g/cm^3 and 1.0 g/cm^3, respectively.

which brings into account the p resonance for the cases studied in Table III. In Table III we note the increase in the number of conducting electrons with temperature, similar to the results obtained from the Saha model presented in the fourth column of the table.

By using the resistivities calculated as described above, the mean free path (mfp) of the conduction electrons based on the simple Drude formula [27] were obtained. These values are considerably lower than the distance between the scatterers. The calculated resistivities in Table III therefore were recalculated assuming that the electron mfp is equal to the distance between the scatterers. A similar procedure was carried out by Dharma-wardana and Perrot [28] for aluminum plasma. Conductivities thus obtained are plotted in Fig. 3 in units of Siemens/meter as a function of temperature, for densities of 1 and 1.5 g/m^s together with the recent experimental results of DeSilva and Kunze [3] and with the calculations of Rinker [1] and of Lee and More [2] at 1 gm/cm^3; both these calculations make no *ad hoc* assumption on a number of conducting electrons. At temperatures greater than 15 000 K the trend of our results is similar to Rinker but considerably higher. This trend of rising conductivity as a function of temperature is due to the increase of conducting electrons with temperature above 15 000 K. The experimental data of DeSilva and Kunze [3], however, are of the opposite trend with the conductivity decreasing as a function of temperature as well as being about an order of magnitude higher than our calculated results near 15 K. The very low number of conduction electrons could cast doubt on the applicability of the Ziman theory for the Cu plasma studied here. We should at this point make note of the recent results of Benage *et al.* [29] who measured the resistivity of polyurethane at 1.265 g/cm^3 between the temperatures of 25–30 eV. In these measurements the resistivity was seen to decrease with temperature.

A similar calculation was carried out for the resistivity of

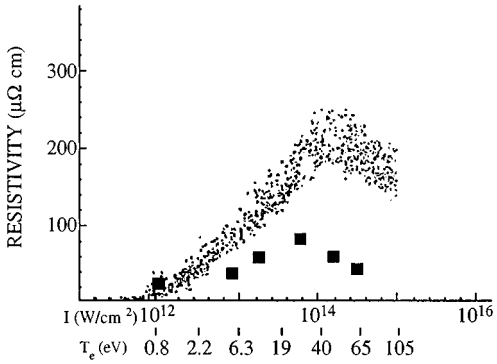

FIG. 4. Resistivity of aluminum plasma as a function of electron temperature; points are experimental data from the femtosecond laser experiments [9]. The squares denote the results of our calculations.

aluminum as a function of temperature at the natural density. The results of the calculations were compared to resistivities obtained from self-reflectivity experiments of an intense femto-second laser pulse [9], see Fig. 4. It is to be noted that the high temperature aluminum plasma exhibits a *d* resonance. As in the case of the transition liquid metals discussed in Sec. II these electrons are assumed not to conduct. Our calculations indicate that ''resistivity saturation'' discussed above for Cu plasma, is not reached here for the aluminum plasma in contradiction to Ref. [28].

Although our results follow the trend of the experimental data as a function of temperature they are between a factor of 3 to 4 less than experiment. The temperatures in Fig. 4 are quoted from Ref. [9] and could be somewhat in error. An analysis of the experiment of Ref. [9] was carried out by Ng *et al.* [10] who showed that the region of laser target interaction extends over a range of plasma temperatures and densities. This renders as somewhat inaccurate the direct correspondence between laser intensity and temperature as quoted in Fig. 4.

V. DISCUSSION

In this paper we have applied the extended Ziman formula to calculating resistivities of transition metals and Al in the liquid state as well as for a dense Cu and Al plasma, using the INFERNO model for calculating phase shifts and the number of conducting electrons and by using the experimental structure factors near melting. Very good agreement between our calculations and experimental results were obtained for Cu and Ni near melting, while for Fe and Mn our resistivities were about four times higher than experiment. On the whole it could be stated that our results are in somewhat better agreement with experiment than those of Rinker [1] and Esposito, Ehrenreich, and Gelatt [11].

A major point in the present paper is the inclusion of higher order terms in the simple extended Ziman formula. Improved DOS were inserted into the calculation for Cu and Fe, which in the latter case brought about a lowering in the number of conducting electrons, thereby causing a decrease of 16% in the calculated Fe resistivity. In Sec. III the effect of the second and third order terms of the multiple scattering expansion of the T matrix on the calculated value of the resistivity was investigated. It was found that for liquid Cu the second order term caused an increase in the resistivity of 7%, while the influence of the third order term was found to be less than 1%. This serves as an indication that at liquid-metal conditions the second and third order terms are essentially insignificant. These terms perhaps could be influential at extremely high densities.

The calculations dealing with the heated and expanded Ni and Cu liquid metals give resistivities which decrease upon heating and expansion, while the experiments indicate the opposite trend. In the case of Cu the calculated result is four times lower than experiment while for Ni the calculation yields a resistivity 1.6 times higher than experiment. These calculations on these and other liquid metals should be pursued in the future.

In the dense Cu plasma case the basic trend of our resistivities as a function of plasma temperature at given temperature is opposite to that of the experimental data and in general the agreement between our calculated results and the experimental data of DeSilva and Kunze [3] is poor. Our results agree within a factor of 3 to those of Rinker with the same basic trend as to be expected. In the case of the aluminum plasma the difference between our calculated results and those of the experiment is between a factor of 3 to 4, but the basic trend in the resistivity as function of temperature is reproduced.

Very recently Yuan, Sun, and Zheng [30] carried out extensive plasma and liquid-metal resistivity calculations very like ours also by using the extended Ziman theory. In a manner similar to the INFERNO calculation carried out by us, these authors also employed a detailed average atom calculation and also made use of the HNC model for the ion-ion correlations. We should, however, point out that our results and those of Yuan, Sun, and Zheng differ with regard to the Fe and Cu liquid metal resistivities. The ratio of the Fe to Cu resistivity is at least an order of magnitude in our calculations as well as those of Rinker [1] and of Esposito, Ehrenreich, and Gelatt [11], with the experimental ratio 6.6. Yuan, Sun, and Zheng on the other hand obtain that both these resistivities are essentially the same. The reason for the higher Fe resistivity is discussed by us in Sec. II and elaborated in Fig. 1. As pointed out below it is our intention to pursue this topic further. The results of Yuan, Sun, and Zheng [30] for the Al plasma are, however, in better agreement with experiment than ours as given in Fig. 4.

The basic question addressed in this paper, as mentioned in Sec. I, deals with the accuracy, especially for plasmas, of the resistivity calculations of the Ziman theory, using the INFERNO atom in the cell model as well as the HNC model for the structure factors. One important reason for this lies in the recent demand for accurate dense plasma resistivity calculations.

Thus with the exception of the Cu plasma the calculational procedure outlined in the present paper agrees with experimental data up to within about a factor of 4. The calculated liquid transition metal resistivities are up to a factor of 4 higher than the experiment, while for Al the calculated resistivities are lower by between three to four times the experimental results for both the plasma and liquid metal cases.

Future work should include the effect of the generalized

scattering phase shifts [17,18] which in the cases of Fe and Mn could bring about a significant reduction in the calculated resistivities. Also as mentioned above additional calculations should be made on expanded and heated liquid metals. Finally, more experimental dense plasma resistivity data would be very beneficial for testing plasma resistivity calculations such as those outlined in this paper.

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