

where P_s is the scattered power, P_{inc} the incident power, and n_0 the plasma density. The σ thus calculated is in the order of 10^{-14} cm², i.e., about 10^9 times larger than $\sigma_0 \simeq 6.7 \times 10^{-24}$ cm², the Thomson cross section. As is known, the latter is an upper limit for the cross section of electromagnetic scattering from an equilibrium plasma.

This large value of σ of course results from the presence of a strong driving term (the dc voltage between the electrodes) which continuously replenishes the bump in the ion distribution function, and thus pro-

duces a high level of the excitation in the unstable modes.

In addition, it may be observed that the geometry of the setup favors the detection of strong scattered signals, because the optical ray-path corresponds to the whole length of the plasma.

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Structure and Resistivity of Liquid Metals*

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Ion-ion repulsion in a liquid metal is regarded as the principal factor determining the ionic arrangement. This interaction is idealized in a hard-sphere model; the known solution of the Percus-Yevick equation for this model gives a simple closed form for $a(K)$ (the liquid structure factor) which depends only on the effective packing density of the fluid. This fact enables us to make an estimate for the resistivities of most liquid metals for which model potentials are available. Agreement with experiment is generally good, particularly when the potential is known to be accurate. The sensitivity of the resistivity to the depth of the model potential well is indicated.

I. INTRODUCTION

RECENTLY, considerable interest has focused on liquid metals as a possible source of information on the interactions within their solid counterparts. Crystalline metals have obvious simplicity of structure, with considerable simplification yielded in some problems by the use of group theory. Yet the same structural simplicity often gives rise to severe problems in deducing the ion-electron interactions within a solid. One has only to reflect on the consequences of umklapp contributions to scattering processes to realize that inverting, say, the electrical resistivity to give the electron-photon interaction or the effective electron-ion potential is a formidable problem.

At first sight the irregular arrangement of ions in the liquid would seem to increase these difficulties. This is not so, however, since the liquid structure factor $a(K)$, which is needed in the determination of transport properties, is directly observed in x-ray and neutron-diffraction experiments. If $a(K)$ is known, some properties of the condensed state may be elucidated. For

example, Ziman,¹ and Bradley *et al.*² deduced an average band gap for some metals from a knowledge of the resistivities in the molten state. The Ziman theory of transport properties for liquid metals is remarkably successful when both the interference function and the electron-ion interaction are known in some detail. The success of the theory appears to rest on two facts. First, *all* structural effects are separated into the interference function, which is taken from experiment.³ Second, the Born approximation on which the theory is based is accurate if calculations are carried out consistently with free-electron-like pseudo wave functions. These wave functions are plane waves orthogonalized to the core states, and satisfy a wave equation where the effective ion-electron potential is small enough to be considered a perturbation. Since the matrix element $V(K)$ is further reduced by the factor $[a(K)]^{1/2}$ in the evaluation of the momentum-transfer integral (see below), the scattering

¹ J. M. Ziman, *Phil. Mag.* 6, 1013 (1961).

² C. C. Bradley, T. E. Faber, E. G. Wilson, and J. M. Ziman, *Phil. Mag.* 7, 865 (1962).

³ It has been pointed out by G. Baym [*Phys. Rev.* 135, A1691 (1964)] that a similar approach to transport properties can be used in a solid. At present the structure factors for solid metals are not sufficiently well determined.

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problem is brought into the region of validity of the Born approximation, namely $a(K)v^2(K) \ll E_F^2$.

Model potentials for ion-electron interaction, introduced by Cohen⁴ for the alkali metals, have recently been refined and extended by Heine and Abarenkov.⁵ Application of these potentials^{6,7} to the evaluation of liquid-metal resistivities has indicated that the interference functions are not always known with sufficient accuracy. In computing the transport integral, $a(K)$ is required in the range $0 < K < 2k_F$ and thus includes the forward-scattering region in which experimental difficulties are encountered.

The interference function enters the formal theory of electrical resistance as follows. Consider a metal with N ions in a volume Ω , or number density $n = N/\Omega$. In the liquid state all scattering is supposed to be confined to a spherical Fermi-energy shell. In the relaxation time approximation the solution of the Boltzmann equation for the relaxation time yields⁸

$$1/\tau_F = v_F n 2\pi \int_0^\pi d\theta \sin\theta (1 - \cos\theta) \sigma(k_F, \theta),$$

where $\sigma(k_F, \theta)$ is the differential scattering cross section per scattering center and v_F is the carrier velocity at the Fermi surface, $v_F = \hbar k_F / m^*$. Ziman's theory uses the Born approximation to determine σ . This in turn requires the square of the matrix element, in the plane-wave representation, of the model or pseudopotential scattering the electrons:

$$\begin{aligned} |\langle \mathbf{k} | V | \mathbf{k}' \rangle|_{av}^2 &= |\langle \mathbf{k} | \sum_{\text{ions}} v(\mathbf{r} - \mathbf{r}_{\text{ion}}) | \mathbf{k}' \rangle|_{av}^2 \\ &= N a(K) v^2(K). \end{aligned}$$

Here

$$\mathbf{K} = \mathbf{k}' - \mathbf{k}$$

and

$$a(K) = N^{-1} \left| \sum_{\text{ions}} \exp(i\mathbf{K} \cdot \mathbf{r}_{\text{ion}}) \right|_{av}^2$$

is the liquid structure factor, depending only on the ionic arrangement. Since the scattering occurs on the (spherical) Fermi surface, we have $K = 2k_F \sin(\theta/2)$, and hence

$$\frac{1}{\tau_F} = v_F n \left(\frac{m^*}{2\pi\hbar^2} \right)^2 \frac{\pi}{k_F^4} \int_0^{2k_F} dK K^3 a(K) v^2(K). \quad (1)$$

The resistivity ρ may now be calculated from

$$1/\rho = Z(n e^2 / m^*) \tau_F, \quad (2)$$

where Z is the number of valence electrons per atom.

The purpose of this paper is to point out that for the calculation of resistivities, the known solution of a

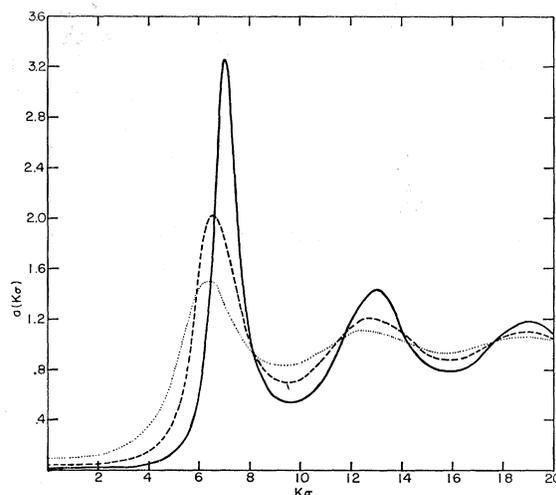


Fig. 1. Structure factor $a(K)$ for a fluid of hard spheres according to the Percus-Yevick equation. The dotted, dashed and full lines are appropriate to packing densities of 30, 40, and 50%.

simple model fluid provides a liquid structure factor of sufficient accuracy (Sec. II). In Sec. III this result is used in calculations with available model potentials. The effects of changes in the liquid structure factor and in the model potential are indicated. For sodium and rubidium, we also compare the temperature dependence of the resistivity predicted by the model potentials.

II. THE LIQUID STRUCTURE FACTOR

Of the existing theories of the liquid state, the theory of Percus and Yevick⁹ has proved to be the most successful, both on the grounds of self-consistency between the pressure and compressibility equation of state for hard spheres,¹⁰ and in the agreement with machine calculations for Lennard-Jones fluids.¹¹ The usefulness of the Percus-Yevick integral equation for the pair distribution function is the greater since a rigorous solution, for the special case of a fluid of hard spheres, has been given independently by Wertheim¹² and by Thiele.¹³ Both the methods of these authors permit the liquid structure factor for this model fluid to be obtained directly. The result (given below) follows immediately from Wertheim's Eqs. (2), (4), and (5) and the definition of the direct correlation function.¹⁴ Alternatively,¹⁵ elementary manipulation of Thiele's Eq. (10) from one-dimensional Laplace transform to

⁹ J. K. Percus and G. J. Yevick, *Phys. Rev.* **110**, 1 (1958).
J. K. Percus, *Phys. Rev. Letters* **8**, 462 (1962).

¹⁰ G. S. Rushbrooke, *J. Chem. Phys.* **38**, 1262 (1963).

¹¹ A. A. Broyles, S. U. Chung, and H. L. Sahlin, *J. Chem. Phys.* **37**, 2462 (1962).

¹² M. S. Wertheim, *Phys. Rev. Letters* **10**, 321 (1963).

¹³ E. Thiele, *J. Chem. Phys.* **39**, 474 (1963).

¹⁴ L. S. Ornstein and F. Zernike, *Proc. Akad. Sci. (Amsterdam)* **17**, 793 (1914).

¹⁵ This was pointed out to one of the authors by Professor M. H. Cohen.

⁴ M. H. Cohen, *J. Phys. Radium* **23**, 643 (1962).

⁵ V. Heine and I. Abarenkov, *Phil. Mag.* **9**, 451 (1964).

⁶ Lorna J. Sundström, *Phil. Mag.* **11**, 657 (1965).

⁷ A. O. E. Animalu, *Phil. Mag.* **11**, 379 (1965).

⁸ N. F. Mott and H. Jones, *The Theory of the Properties of Metals and Alloys* (Oxford University Press, New York, 1936), p. 262.

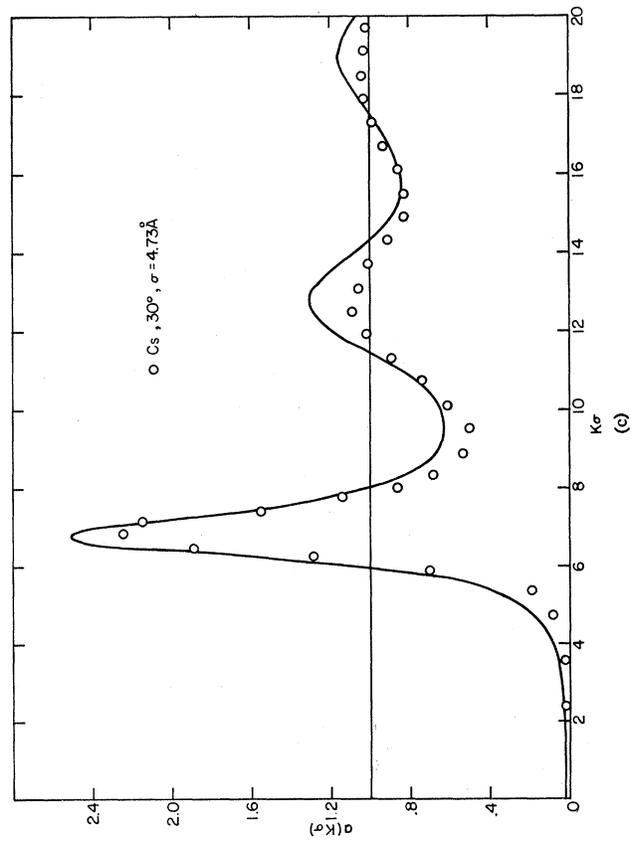
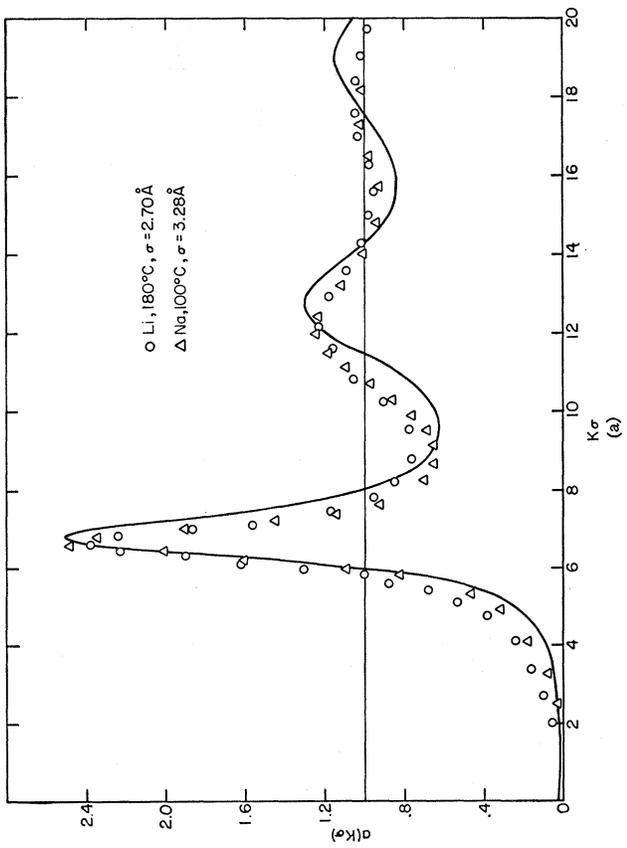
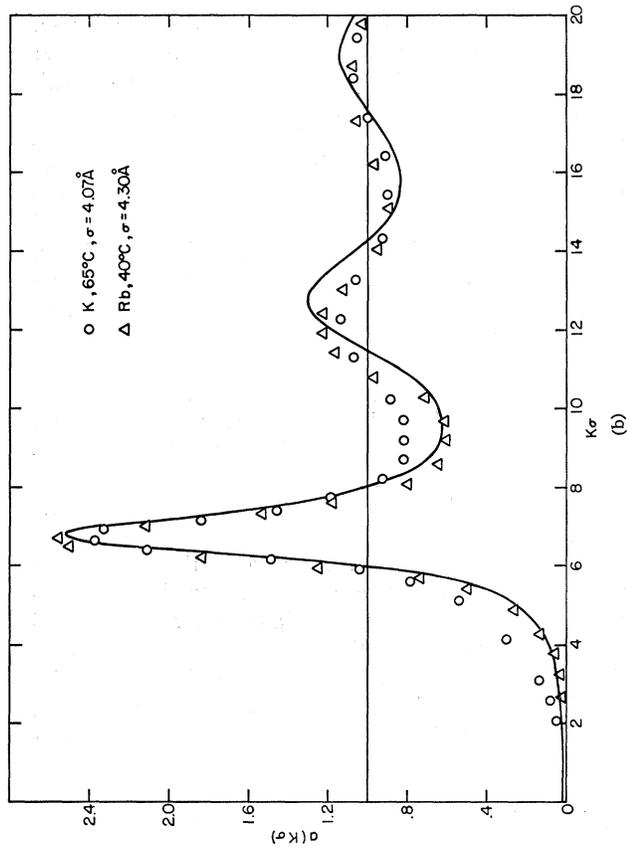


Fig. 2. Neutron-diffraction data of Gingrich and Heaton (Ref. 16) compared with the Percus-Yevick hard-sphere theory (full curve) for a fluid of packing density 45%.

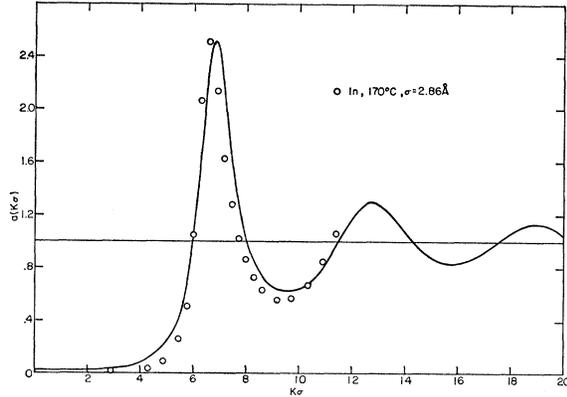


FIG. 3. X-ray-diffraction data for indium (Ref. 17) compared with Percus-Yevick theory $\eta=0.45$.

three-dimensional Fourier transform, with the use of his Eq. (2), yields the same result, namely

$$a(K\sigma) = \{1 - nc(K\sigma)\}^{-1}, \quad (3)$$

where σ is the hard-sphere diameter and the direct correlation function in momentum space is given by

$$c(K\sigma) = -4\pi\sigma^3 \int_0^1 ds s^2 \frac{\sin sK\sigma}{sK\sigma} (\alpha + \beta s + \gamma s^3). \quad (4)$$

The parameters α , β , and γ are functions of a packing-density parameter η , the fraction of total fluid volume occupied by the spheres:

$$\begin{aligned} \eta &= (\pi/6)n\sigma^3, \\ \alpha &= (1+2\eta)^2/(1-\eta)^4 \\ \beta &= -6\eta(1+\eta/2)^2/(1-\eta)^4, \\ \gamma &= (1/2)\eta(1+2\eta)^2/(1-\eta)^4 \end{aligned} \quad (5)$$

The evaluation of $c(K\sigma)$ is immediate so that the structure factor for a fluid of hard spheres is expressed in terms of elementary functions.

This structure factor is shown in Fig. 1 for three densities, where 30, 40 and 50% of the volume is occupied by the hard spheres. Although the Percus-Yevick equation shows no singularities for $\eta < 1$, the region beyond $\eta = \pi/3\sqrt{2} = 0.74$ is unphysical, since the fluid then has a packing density greater than that of the close-packed solid.

In Figs. 2 [(a)-(c)] the theory is compared with the experimental data of Gingrich and Heaton¹⁶ for the alkali metals, and in Figs. 3 and 4 with data for indium due to Ocken.¹⁷ It is apparent that up to and including the major diffraction peak, the structure factor is well reproduced by the model fluid.¹⁸ More remarkable is

¹⁶ N. S. Gingrich and LeRoy Heaton, J. Chem. Phys. 34, 873 (1961).

¹⁷ H. Ocken (private communication).

¹⁸ It is encouraging to note that the Rb data, considered by Gingrich and Heaton to be the most accurate, is in best agreement with the theory.

the fact that in this model the alkali metals are seen to be of essentially the same packing density, or that they are simply scaled versions of each other. With regard to other liquid metals, we have made rough comparisons of the hard-sphere fluid $a(K)$ with all the data reviewed by Furukawa.¹⁹ There is often lack of agreement between the various experiments, but in all the metals we shall consider²⁰ it is possible to obtain a good representation of the liquid structure by choosing a packing density of between 40 and 50%. Where no data exist, namely, for Be, Mg, Ca, Ba, Si, and As, we shall still assume this to be true. For the polyvalent metals the resistivity is not highly sensitive to variations in $a(K)$, while for the alkali metals rather accurate data is available, which further is well fitted by the theory. These two circumstances make it possible for us to compare the resistivities predicted by several model potentials for the ion-electron interaction in the metallic state.

Returning to the interpretation of the rather surprising agreement between experimental liquid structure and what amounts to the simplest nontrivial model fluid, we must conclude that the arrangement of ions in liquid metals can be taken to be determined largely by the ion-ion repulsions. For short-range correlations, corresponding to larger momentum transfers in scattering, the details of the ion-ion interaction become important, as can be seen by the progressively greater deviation between theory and experiment after the first peak. Concerning the "hard" cores, we know that they correspond to the combined effect of the repulsion due to overlap of core wavefunctions, and the ion-ion Coulomb repulsion. The latter is screened by the Fermi gas of electrons. Because of the sharpness of the Fermi surface, however, the screening is not complete and there is a long-range oscillatory component in the ion-

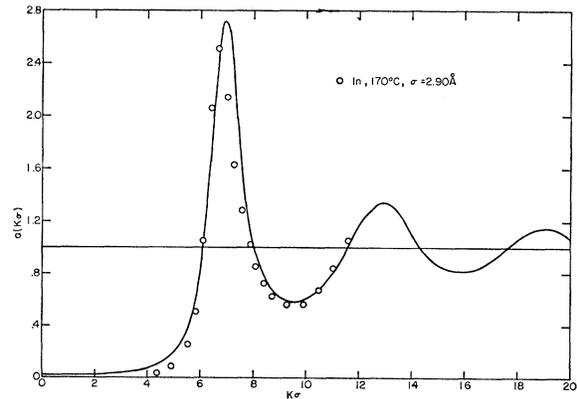


FIG. 4. The indium data of Fig. 3 compared with the theory for $\eta=0.47$. Slightly better agreement is apparent.

¹⁹ K. Furukawa, Rept. Progr. Phys. 25, 395 (1962).

²⁰ Two semi-metallic elements, Se and Te, will not be considered here because there is evidence (see Ref. 19) for the formation of rings or chains in their liquid state.

ion interaction, as discussed by Johnson, Hutchinson and March.²¹ These authors showed that the magnitude of this interaction is of the order of the thermal kinetic energy of the ions, so that its effect on the structure of the fluid is small compared to that of the short-range repulsion, which is of the order of rydbergs.

For long wavelengths (small momentum transfer) the structure factor is difficult to measure by diffraction experiments, but the limit is known thermodynamically: $a(0) = nkT\chi_T$, where χ_T is the isothermal compressibility. Measurements of χ_T are available for sodium,²² giving $nkT\chi_T = 0.024$ at 100°C. The theoretical hard-sphere value is readily found from Eqs. (3), (4), and (5):

$$a(0) = \alpha^{-1} = (1 - \eta)^4 / (1 + 2\eta)^2. \quad (6)$$

For $\eta = 0.45$, which is our fit to the sodium data, $a(0) = 0.025$. We can conclude that in this model the net contribution to the compressibility from the ion-ion oscillatory interaction and from the electron gas is surprisingly small in sodium. This is made the basis of the temperature-dependence calculations for sodium in Sec. III. The situation in the polyvalent metals (corresponding to much higher electron densities) is somewhat different. For example, lead at 327°C has $nkT\chi_T = 0.0086$ using the compressibility value of Gordon²³ (implying a value $\eta = 0.56$) while the neutron-diffraction data of Sharrah *et al.*²⁴ is better described by a curve with $\eta = 0.45$. The resistivity of the polyvalent metals is not sensitive to the long-wavelength region ($K \sim 0$) of the liquid structure factor and the discrepancy here introduces negligible error.

III. MODEL POTENTIALS AND LIQUID-METAL RESISTIVITIES

We now turn to the matrix element $v(K)$ appearing in the integrand of Eq. (2). As discussed by Ziman¹ and others² what we require is the Fourier transform of the total effective electron-ion interaction (including screening by the conduction electrons) for scattering of electrons on the Fermi surface. It is still an extremely difficult problem to calculate this quantity from first principles with any degree of precision. Consequently, the potential is generally, and conveniently, presented in a model form which includes in a simple parametric way all the salient features dictated by the physics of the situation. Thus, in the quantum defect method of Ham,²⁵ and Brooks and Ham,²⁶ information on the form

of the potential in the solid is obtained from spectroscopic data pertinent to the free atom. The method evolved from the observation of Kuhn and van Vleck²⁷ that all the information necessary for constructing the potential in a metal is contained in the logarithmic derivative of the radial wave function at the ion core. This quantity is closely connected with the phase shifts associated with the core and can also be related to the quantum defects in the Ritz energy formula which are determined from the spectroscopic energy levels. Heine and Abarenkov's approach is not dissimilar. The apparent cancellation of the potential in the core space which results from orthogonalizing the conduction-electron wave function to the metallic-core functions is replaced by a sequence of square wells (the pseudo wave functions now being plane-wave-like). Each well is labeled by an index l appropriate to the s, p , etc., shells of the core. Its strength as a function of energy is determined again by matching the first of its own level system to the observed levels of the free atom.

The over-all success of these methods depends to a large extent on the accuracy of the extrapolation and the choice of the core radius. For a single metal, Al, the possible errors were mostly eradicated by a further refinement imposed by the requirement that the model potential $v(K)$ pass through points on the curve determined by Fermi-surface studies.²⁸ For this particular case the resistivity of the liquid metal given by Eq. (2) [using the experimental $a(K)$] was in good agreement with experiment.²⁸ Heine and Abarenkov's model calculations of $v(K)$ gave reasonable agreement in Al, as they did in the alkali metals and Zn, Hg, Tl, Pb, and Bi.⁶ In some cases, the discrepancies were put down by Sundström to be due to experimental uncertainties in $a(K)$ particularly in the near-forward scattering region [see Fig. 2(b)].

In its original formulation, Heine and Abarenkov's model potential incorporated linear first-order screening of the bare electron-ion potential. A correction is made for exchange in Sham's²⁹ modification of Hubbard's approximation. More recently Animalu⁷ has included nonlocal dielectric screening of the model potential and has undertaken similar calculations of the resistivity of the liquid metals. For polyvalent metals there appears to be a slight improvement over Sundström's values, but the conclusions about the uncertainties in $a(K)$ remain.

We have evaluated the resistivity of the liquid metals listed in Table I with the Heine-Abarenkov potentials³⁰

²¹ M. D. Johnson, P. Hutchinson and N. H. March, Proc. Roy. Soc. (London) A282, 283 (1964).

²² *Liquid Metals Handbook* [Sodium (NaK) Supplement] (U. S. Office of Naval Research in cooperation with the Atomic Energy Commission, Washington, D. C., 1955).

²³ R. B. Gordon, Acta Met. 7, 1 (1959).

²⁴ P. C. Sharrah, J. I. Petz, and R. F. Kruh, J. Chem. Phys. 32, 241 (1960).

²⁵ F. S. Ham, Solid State Phys. 1, 127 (1955).

²⁶ H. Brooks and F. S. Ham, Phys. Rev. 112, 344 (1958).

²⁷ T. S. Kuhn and J. S. Van Vleck, Phys. Rev. 79, 382 (1950).

²⁸ N. W. Ashcroft and Lorna J. Guild, Phys. Letters 14, 23 (1965).

²⁹ L. J. Sham, Proc. Roy. Soc. (London) A283, 33 (1965).

³⁰ These are taken from Ref. 6, Table II. Although referred to by Sundström and by us as Heine-Abarenkov potentials, they were calculated by Animalu and Heine. Local screening was employed.

TABLE I. Comparison of liquid-metal resistivities: Twenty-three liquid metals are considered. Column 2 gives the temperatures (in °C) for which the calculations apply. The next seven columns are resistivities in $\mu\Omega$ cm. Here ρ_{expt} = the experimental resistivity at the temperature indicated, $\rho_S = \rho$ [Sundström (Ref. 6) with V_{HA} and the experimental $a(K)$], $\rho_A = \rho$ [Animalu (Refs. 7 and 31) with V_{HAA} and the experimental $a(K)$], $\rho_{\text{HA}} = \rho$ [V_{HA} with the theoretical $a(K)$, $\eta = 0.45$], $\rho_{\text{HAA}} = \rho$ [V_{HAA} with the theoretical $a(K)$, $\eta = 0.45$]. Δ_{HA} and Δ_{HAA} show the change in resistivity produced by a change in the theoretical $a(K)$. For the alkalis the change shown is for η increased from 0.45 to 0.46. In the polyvalent metals the change corresponds to η increasing to 0.50. Column 10 lists the hard core-radii (in atomic units) calculated using the known number density of the liquid and assuming a packing density of 45%. Column 11 lists the Heine-Abarenkov model potential radius (Ref. 31), and columns 12 and 13 give, respectively, the well depth A_0 (a.u.) and the change ΔA (a.u.) which will bring the HA-predicted resistivity into agreement with experiment.

Metal	Temp.	ρ_{expt}	ρ_S	ρ_A	ρ_{HA}	$\Delta\rho_{\text{HA}}$	ρ_{HAA}	$\Delta\rho_{\text{HAA}}$	$\sigma/2$	R_M	A_0	ΔA
Li	180	25	17.4	24.7	15.7	-0.7	17.1	-0.7	2.55	2.8	0.336	0.055
Na	100	9.6	9.4	7.9	9.5	-0.7	5.3	-0.4	3.10	3.4	0.305	-0.001
K	65	13.0	31.7	22.9	16.2	-1.1	7.5	-0.5	3.84	4.2	0.240	0.006
Rb	40	22.0	13.9	10.2	27.2	-1.6	8.1	-0.6	4.07	4.4	0.224	0.007
Cs	30	36.0	12.7	9.7	36.0	-2.1	9.1	-0.6	4.47	4.8	0.205	0.0
Be	1284	24.6	+2.4	1.87	2.0	1.01	...
Mg	650	27.4	25.1	+0.2	19.2	-0.4	2.65	2.6	0.78	0.01
Ca	851	15.5	+0.2	3.28	2.6	0.54	...
Ba	710	~134	15.4	-0.4	3.70	3.4	0.45	...
Zn	420	37.4	44.0	37.2	18.6	-0.3	16.6	-1.5	2.25	2.2	0.99	0.14
Cd	330	33.7	20.1	-3.2	2.56	2.6	0.88	...
Hg	-20	91	77.2	33.7	-5.7	2.61	2.6	0.97	...
Al	660	24.2	24.5	26.7	20.6	-3.9	19.2	-3.4	2.39	2.0	1.38	0.07
Ga	30	25.8	28.3	-5.4	2.40	2.4	1.44	...
In	156	33.1	30.4	-5.1	2.70	2.4	1.32	...
Tl	303	73.1	37.1	57.9	-2.8	2.77	2.4	1.44	...
Si	1410	~71	28.8	-3.4	2.50	2.0	2.08	...
Ge	937	~73	40.8	-2.2	2.61	2.0	2.10	...
Sn	410	48	34.8	-3.0	2.76	2.0	1.84	...
Pb	400	95	58.4	63.6	73.5	-1.4	69.8	-0.7	2.88	2.1	1.92	0.11
As	817	61.7	-2.5	2.53	2.0	2.71	...
Sb	640	113.5	58.2	-1.7	2.83	2.0	2.42	...
Bi	300	128	109	87.5	-1.0	2.93	2.0	2.38	...

(ρ_{HA}) and the Animalu-Heine modification³¹ of this potential (ρ_{HAA}). Examples of these potentials are given in Fig. 5. It is apparent from the differences between ρ_{HA} and ρ_{HAA} that the resistivity is very sensitive to changes in the potential $v(K)$ near $K = 2k_F$, especially in metals of low valence. In all cases we have used a theoretical $a(K)$ corresponding to a packing density of 45% and have indicated the change $\Delta\rho$ obtained when this density is varied. For the special case of aluminum, the resistivity is evaluated with Ashcroft's³² potential, which is known from Fermi-surface studies to be correct near $K = 2k_F$. We have taken the effective mass to be unity for all metals. To sufficient accuracy, the resistivity corresponding to an effective mass of m^* can be obtained from the values in Table I by multiplication by $(m^*/m)^2$. For comparison, we have also listed the published results of Sundström⁶ and Animalu,⁷ which were obtained with the experimental liquid structure factors.

Table I also lists a series of hard-core radii for the liquid metals, obtained from $\eta = (\pi/6)n\sigma^3 = 0.45$. These

³¹ A. O. E. Animalu, Solid State Theory Group, Cavendish Laboratory, Cambridge, England, Technical Report No. 3, 1965 (unpublished), and A. O. E. Animalu and V. Heine, Phil. Mag. **12**, 1249 (1965). These potentials are tabulated for volumes appropriate to the solid. Although we have converted them to the volume and k_F corresponding to the liquid, we have not allowed for small variations in the potential parameters due to their energy dependence. The Cd figures given in Table I refer to a corrected potential taken from Solid State Theory Group, Cavendish Laboratory, Cambridge, England, Technical Report No. 4, 1965 (unpublished).

³² See Ref. 28.

radii are generally slightly larger than nearest neighbor distances in the solid. They correspond to the distance at which the ion-ion interaction becomes large in comparison with the thermal kinetic energy of the ions. Thus "hard" in this context is on the scale of kT rather than of rydbergs. The values of $\sigma/2$ agree well with the radii at which the ion-ion potentials deduced by Johnson, Hutchinson and March²¹ become large and repulsive.

In Table II we present the alkali-metal resistivities calculated with the Cohen⁴ potential

$$v_C(r) = -A, \quad r < R_M \\ = -Ze^2/r, \quad r > R_M.$$

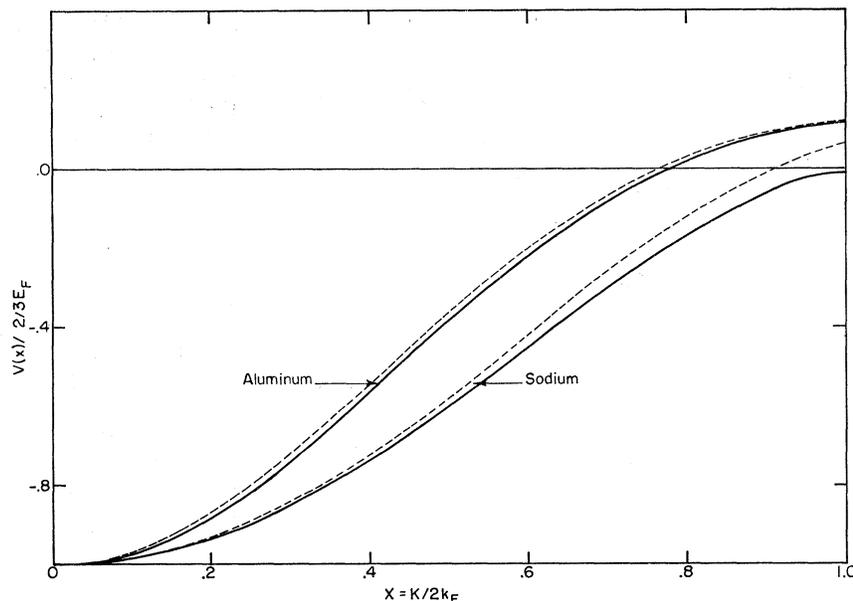
The parameters A and R_M were calculated by N. Wisner by fitting the lowest s and p levels of the single valence electron to those determined from atomic spectra. We have screened this potential in the way suggested by Heine and Abarenkov. The effective mass for the liquid metals is again taken to be unity.

In the calculation of the temperature dependence, we have followed different procedures for sodium and

TABLE II. Liquid-metal resistivities for the Cohen potential.

Metal	A (Ry)	R_M (a_0)	$\sigma/2$ (a_0)	ρ_{expt}	ρ_C
Na	0.424	2.1	3.10	9.6	7.9
K	0.435	3.2	3.84	13.0	8.8
Rb	0.451	4.6	4.07	22.0	9.4
Cs	0.410	5.5	4.47	36.0	11.3

FIG. 5. Model potential for sodium and aluminum as function of the momentum transfer K . The full lines are the original Heine-Abarenkov (Ref. 6) potentials and the dashed lines are the same potentials as modified by Animalu (Refs. 7 and 31). All of the curves drawn are appropriate to atomic volumes just above the melting point.



rubidium. For Na the variation of compressibility with temperature is known experimentally,²² and we have determined the parameter η by fitting $a(0)=\alpha^{-1}$ to $nkT\chi_T$. The results are given in Table III and Fig. 6.

TABLE III. Temperature dependence of the resistivity of liquid sodium.

$T(^{\circ}\text{C})$	$n(\text{\AA}^{-3})$	$nkT\chi_T$	$\eta = (\pi/6)n\sigma^3$	$\sigma(\text{\AA})$	ρ_{expt}	ρ_C	ρ_{HA}	ρ_{HAA}
100	0.0243	0.0240	0.456	3.30	9.6	7.6	9.0	5.0
160	0.0239	0.0289	0.437	3.27	11.7	9.1	10.7	5.9
200	0.0237	0.0323	0.424	3.25	13.1	10.3	12.1	6.6
240	0.0234	0.0359	0.413	3.23	14.5	11.4	13.3	7.2
300	0.0231	0.0414	0.396	3.20	16.6	13.6	15.4	8.3

We note that the hard-core diameter decreases by only about 3% as the temperature increases almost by a factor of 2. For Rb, compressibility data is not available. The neutron-diffraction experiments were performed at four temperatures, however, and we have determined the parameter η by fitting $a(K)$ to give the correct height, a_{MAX} , of the structure factor. The results are given in Table IV and Fig. 7.³³ The variation of σ with temperature is similar to that obtained for Na, being such as to keep the screened Coulomb repulsion

TABLE IV. Temperature dependence of the resistivity of liquid rubidium. The variation of liquid-metal density with temperature is taken from the *International Critical Tables* (McGraw-Hill Book Company, Inc., New York, 1933), Vol. I, p. 102.

$T(^{\circ}\text{C})$	$n(\text{\AA}^{-3})$	a_{max}	$\eta = (\pi/6)n\sigma^3$	$\sigma(\text{\AA})$	ρ_{expt}	ρ_C	ρ_{HA}	ρ_{HAA}
40	0.0108	2.61	0.459	4.33	22.0	8.7	25.4	7.5
160	0.0103	2.13	0.412	4.24	33.0	13.9	36.1	11.7
240	0.0100	2.01	0.395	4.22	40.5	16.8	41.1	13.8
360	0.0096	1.82	0.365	4.17	52.0	22.8	50.9	18.1

³³ *Liquid Metals Handbook* (U. S. Office of Naval Research in cooperation with the Atomic Energy Commission, Washington, D. C., 1952).

between the ions separated by a distance σ of the order of kT .

Finally, we have calculated the change in well depth

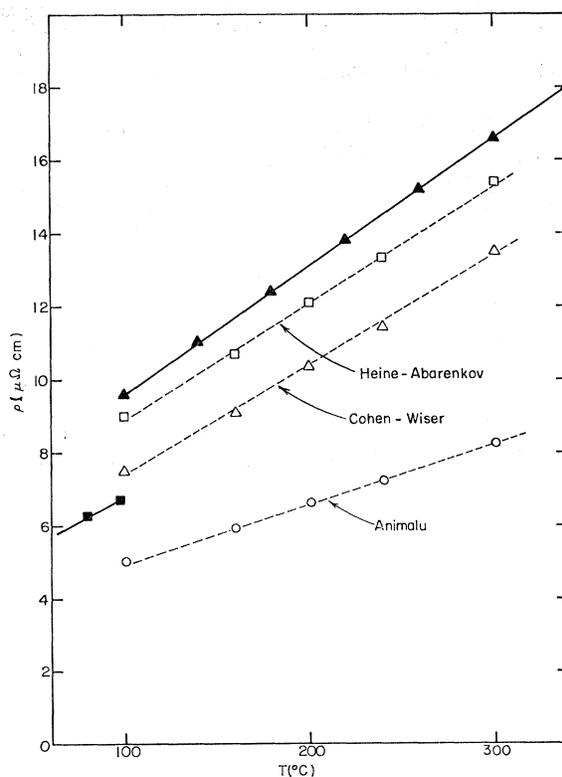


FIG. 6. Temperature dependence of the resistivity of liquid sodium. The experimental points (solid squares and triangles) are taken from the *Liquid Metals Handbook*, NaK Supplement (Ref. 22). The resistivities for the various model potentials are evaluated from compressibility data, as described in the text.

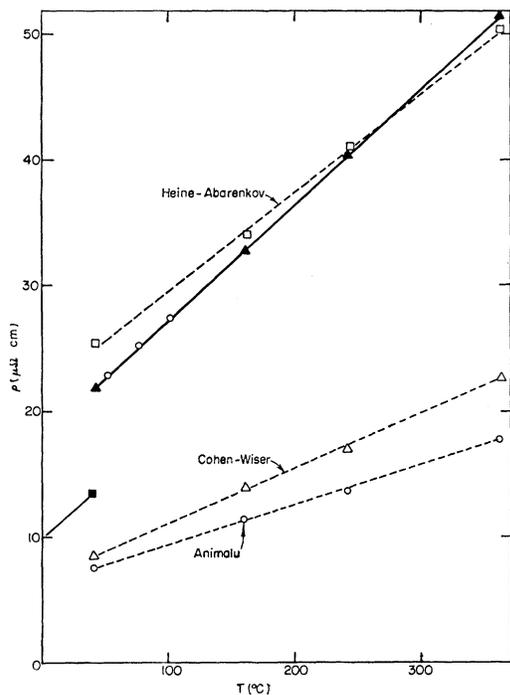


FIG. 7. The temperature dependence of the resistivity of liquid rubidium. The experimental points (solid squares and triangles) are taken from the Liquid Metals Handbook (Ref. 33) and from Sundström (Ref. 6). The resistivities for the model potentials are calculated from neutron-diffraction data as described in the text.

of the Heine-Abarenkov potential required to reproduce the experimental resistivity. This serves the double purpose of indicating the sensitivity of resistivity to the well depth, and, possibly, of being made the basis of a correction of the HA potential in conjunction with a calculation of the effective mass. The unscreened HA potential has the form

$$v_{\text{HA}}(r) = -A_2 - (A_0 - A_2)\hat{P}_0 - (A_1 - A_2)\hat{P}_1, \quad r < R_M$$

$$= -Ze^2/r, \quad r > R_M.$$

Here \hat{P}_l is a projection operator selecting out the l th partial wave from the electron wave function. We have

added to this potential a term $-\Delta A (r < R_M)$, screened in the manner described by HA, and adjusted ΔA so as to give the correct resistivity. The results are given in the last column of Table I. The changes are significant only in the case of Li and Zn.

IV. SUMMARY

We have seen that a simple expression for the structure factor of the hard-sphere fluid follows immediately from the known solution of the Percus-Yevick equation. Agreement with experimental determinations of liquid metal structure is satisfactory. Assuming similar structure in metals for which data does not as yet exist, we are able to calculate and compare resistivities of metals for which the electron-ion interaction has been estimated. The results indicate that, both in magnitude and in temperature dependence, the resistivities predicted by the Ziman theory and employing Heine-Abarenkov potentials are close to experiment. With the exception of Li and Zn, the resistivities calculated with $m^* = m$ are all correct to better than 25%. The correction of the potentials for nonlinear screening (HAA) destroys this good agreement, and indicates the extreme sensitivity of the resistivity to small changes in the potential—a point which has recently been stressed by Wiser.³⁴

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³⁴ N. Wiser, Phys. Rev. (to be published).