

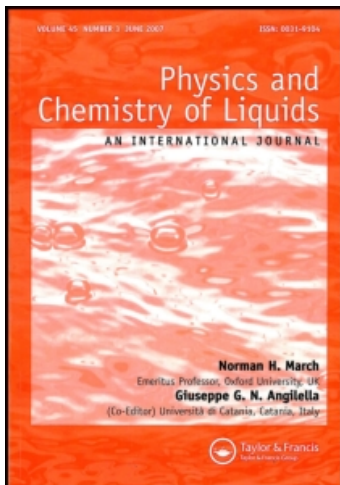
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Review Article

Electronic Transport in Short Mean-free Path Liquid Metals

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Recent work on the theory of electronic transport is reviewed. Attention is focused on liquid metals but contact is made with theories of localization due to disorder.

1 OUTLINE

The object of this review is to consider recent treatments of electronic transport in short mean-free path liquid metals.¹ In particular, the connection between the approach of Götze² on the one hand and that of Ferraz and March³ on the other is considered. It will be demonstrated that they are both theories of inverse transport coefficients.^{4,5}

In Section 2, we present physical arguments by means of which one can introduce a finite mean-free path into the Ziman theory of liquid metals. This establishes a general framework for the theory but leaves one with the task of establishing how the blurring of the Fermi surface in the liquid metal due to the disorder scattering is to be described quantitatively. This is treated in Section 3, where the specific theories of Fermi surface blurring presently available are reviewed. Section 4 treats some more general aspects of transport and spectra in the presence of disorder. The review concludes by focusing on some presently unanswered questions in the theory of electronic transport in disordered systems.

2 INTRODUCTION OF FINITE MEAN FREE PATH INTO ZIMAN THEORY OF LIQUID METALS

The Ziman formula¹ for the electrical resistivity

$$\rho_{nfe} = \frac{3\pi m^2}{4Ze^2\hbar^3nk_f^6} \int_0^\infty dq q^3 S(q) |V(q, k_f)|^2 \theta(2k_f - q) \quad (2.1)$$

has as the basic input information:

- i) The static liquid structure factor $S(q)$, accessible through X-ray or neutron scattering experiments and
- ii) The screened electron-ion pseudopotential form factor $V(q, k_f)$ for elastic scattering on the Fermi sphere of radius k_f .

In Eq. (2.1), the conduction electron density n is related to k_f by $k_f = (3\pi^2 n)^{1/3}$, θ is the unit step function, m and e are as usual the electron mass and charge respectively while Z is the number of conduction electrons per ion.

It is immediately clear that while Eq. (2.1) is of course correct to second order in the form factor $V(q, k_f)$, it is not self-consistent in that it leads to a finite resistivity ρ and hence to a finite transport mean-free path

$$l_v = \frac{\hbar k_f}{ne^2 \rho} \quad (2.2)$$

whereas on the right-hand side of Eq. (2.1) the Heaviside function θ cuts off the q integration at $2k_f$ corresponding to a perfectly sharp Fermi surface. But the Heisenberg uncertainty principle requires that the blurring of the Fermi surface, Δq say, is directly related to the mean-free path l by

$$l\Delta q \sim 1 \quad (2.3)$$

and hence one ought to determine the mean-free path self-consistently.

Ferraz and March³ therefore replace Eq. (2.1) by

$$\rho = \frac{\hbar k_f}{ne^2 l} = \int_0^\infty q^4 S(q) |V(q, k_f)|^2 \Gamma(q, k_f, l) dq \quad (2.4)$$

Evidently the new feature of the theory beyond the nearly free electron approximation (2.1) is the way in which Γ depends on the mean-free path l . Once this question can be settled, Eq. (2.4) provides an equation which must be solved self-consistently for the mean-free path. This feature is essential to the discussion of the present review. It is quite clear that as the mean-free path l becomes longer and longer the function Γ in Eq. (2.4) must cut off more and more sharply at $q = 2k_f$. In this limit when the mean-free path

tends to infinity, comparison of Eqs. (2.4) and (2.1) shows that, apart from a multiplying constant we need not write out here, $\Gamma = q^{-1}\theta(2k_f - q)$.

But there are other points to be made when we pass to the regime of strong scattering, or short mean-free path. The first is that even in the regime where there is still good metallic conductivity, one cannot expect the pair function, which is the Fourier transform of $S(q) - 1$, to contain adequate structural information concerning the liquid metal. Therefore one must recognize that, in the final theory of electronic transport in short mean-free path liquid metals, it may be necessary to derive a formula for $\Gamma(q, k_f, l)$ which is an average over configurations into which is built the higher-order ionic correlation functions g_3, g_4 , etc., for 3, 4, etc., particle correlations.

Though some attention has been given to this point in earlier theories of electronic states in liquid metals,^{7,8} progress to date has resulted, as we shall clarify below, from regarding this information as approximately subsumed into the electrical resistivity ρ through the dependence of Γ on the mean-free path l . Clearly, this is an approximation, but as already stressed, the idea behind the two basic approaches reviewed in Section 3 below is to solve self-consistently for the mean-free path. The final point we must make before turning to discuss these two treatments is that we know from the pioneering work of Anderson⁹ that under conditions of sufficient disorder there will be a (one-electron) transition from extended to localized electron states. If, as seems possible from both experiment and theory, there is a critical mean-free path, l_c say, below which the system becomes insulating at $T = 0$ due to disorder scattering, then it is obvious that the calculation of the function Γ near $l = l_c$ is a matter of considerable complexity. Therefore, in Section 3 below, we shall first discuss the case of liquid simple metals, where Γ can be calculated essentially by rather elementary kinetic methods.³ Following that, we shall turn to Götze's work which appears to contain within itself a procedure which will work, at least semiquantitatively, near the critical mean-free path l_c .

3 THEORIES OF FERMI SURFACE BLURRING IN LIQUID METALS

Accepting that the self-consistent solution of Eq. (2.4) for the mean-free path l is the basic approach presently available to us, we shall now outline below the two theories proposed to date which allow explicit approximations to the function $\Gamma(q, k_f, l)$ to be set up. We start with the work of Ferraz and March³ which has been refined and also applied numerically to liquid simple metals by Leavens *et al.*⁶ Then we shall review the alternative approach of Götze.²

3.1 Force-force correlation function and average density matrix

In Refs. 3 and 6, the problem of the higher order ionic correlation functions referred to above, which will arise in the presence of strong scattering, is circumvented by arguing that what is important in the theory of the electrical resistivity of liquid metals is that the density matrix describing the electron states has built into it knowledge of the electronic mean-free path. Ferraz and March³ accomplish this by starting from the theory of inverse transport coefficients,^{4,5} which yields ρ , apart from a multiplying constant, in terms of the force-force correlation function, denoted by F below:

$$\rho \propto F = \int d\mathbf{r}_1 d\mathbf{r}_2 \frac{\partial V(\mathbf{r}_1)}{\partial \mathbf{r}_1} \cdot \frac{\partial V(\mathbf{r}_2)}{\partial \mathbf{r}_2} |\sigma(\mathbf{r}_1, \mathbf{r}_2, E_f)|^2 \quad (3.1)$$

where V is the total scattering potential energy while σ denotes the energy derivative of the Dirac density matrix evaluated at the Fermi energy E_f .[†] In the work of Ferraz and March,³ the very simplest choice

$$\sigma(\mathbf{r}_1, \mathbf{r}_2, E_f) = \sigma_0(\mathbf{r}_1, \mathbf{r}_2, E_f) \exp\left(-\frac{|\mathbf{r}_1 - \mathbf{r}_2|}{2l}\right) \quad (3.2)$$

is made, in which only the off-diagonal elements of the density matrix are altered from the Ziman nearly free electron theory, these off-diagonal elements being damped with a factor which is essentially coming from the kinetic theory formula for the probability of a path of a given length, which is proportional to $\exp(-r/l)$.

In the treatment of Ferraz and March,³ and also that in Ref. 6, the screened electron-ion pseudopotential was also taken to depend on the mean-free path through the dependence of the q -dependent dielectric function on l . This point is discussed fully in Ref. 6.

Without going into the intricate details, we record in Table I the results of Leavens *et al.*⁶ for liquid simple metals, together with the values obtained from the Ziman formula (2.1) and with the experimental results.

It is clear from Table I that while the self-consistent results could not be claimed to afford a systematic improvement on those of the Ziman theory, in cases where there is a large discrepancy between that theory and experiment, namely Li and Cs, a distinct improvement is found. The other point concerning Table I is that the self-consistent results are in the cases studied all greater than the Ziman values.

What seems more important to stress than the above points of detail is that the approach based on Eq. (2.4) allows a self-consistent completion of

[†] See Appendix 1 for the use of Eq. (3.1) to treat impurity scattering.

TABLE I

Electrical resistivities calculated from the Ziman formula (2.1) and from the self-consistent treatment of Leavens *et al.*⁶ Units of ρ are $\mu\Omega$ cm

Liquid metal	Exp.	Ziman	Self-cons.
Li (463 K)	25.1	13.9	17.7
Na (378 K)	9.7	10.2	10.9
K (343 K)	14.3	15.9	16.9
Rb (313 K)	22.6	28.2	29.9
Cs (303 K)	37.1	29.2	33.3
Mg (953 K)	25.5	21.5	22.4
Al (943 K)	24.4	19.5	20.5

the Ziman theory without affecting the overall success of that theory for the liquid simple metals.

Of course, none of the metals treated above is a really short mean-free path metal. It is not at all clear that the use of the approach of Ferraz and March would give equally satisfactory results for short mean-free path metals. However, it seems entirely possible that the work of Götze² may be applicable to such situations and we therefore turn next to consider his method.

3.2 Mode coupling approach of Götze

Götze's work was primarily motivated by the desire to discuss both really short mean-free path situations and also to treat the transition to localization induced by disorder. To this end, he did not explicitly consider the short-range order, so vital to obtain quantitative results for transport coefficients in liquid metals. Nevertheless, his treatment is readily extended to incorporate the pair correlation function, or its q -space transform, the liquid structure factor $S(q)$.

It should also be emphasized that, unlike the treatment of Ferraz and March which dealt solely with the the d.c. resistivity, Götze from the outset regarded the d.c. conductivity as the zero frequency limit of the frequency dependent conductivity $\sigma(\omega)$. Following the ideas of Drude theory, which expresses $\sigma(\omega)$ in the form

$$\sigma(\omega) = \frac{\sigma(0)}{1 + i\omega\tau}, \quad (3.3)$$

τ being the Drude relaxation time, Götze chose to work with a quantity $M(z)$ introduced by writing

$$\sigma(z) = \frac{i}{z + M(z)} \quad (3.4)$$

with z viewed as a complex variable. Taking the limit of zero frequency, which is equivalent to letting z tend to zero in Eq. (3.4), it is clear that

$$\sigma(0) = \frac{i}{M(0)}. \quad (3.5)$$

Therefore it becomes evident that (a) the theory, being based on M , is that for an inverse transport coefficient and (b) the quantity M in the zero frequency limit is pure imaginary.

If at this stage we extend Götze's work by introducing the structure factor $S(q)$, we can write his mode-coupling approximation for $M(0)$ in terms of the screened electron-ion pseudopotential $V(q, k_f)$ as

$$M(0) = \frac{1}{3nm} \sum_q q^2 S(q) |V(q, k_f)|^2 \phi(q, 0). \quad (3.6)$$

Equation (3.6) is evidently of the same form as Eq. (2.4) when we replace the summation over q by an integration. Unlike the treatment of Ferraz and March³ however, Götze regards $\phi(q, 0)$ as the zero frequency limit of the particle density correlation function $\phi(q, z)$ which he then approximates in terms of the Lindhard function $\phi^0(q, z)$ and wavenumber dependent compressibility $g(q)$ through

$$\phi(q, z) = \frac{\phi^0(q, z + M(z))}{1 + M(z)\phi^0(q, z + M(z))/g(q)}. \quad (3.7)$$

Since from Eqs. (3.5)–(3.7), one can solve self-consistently for $M(0)$ (actually Götze solves more generally for $M(z)$), one can see that though the detail of the theory differs importantly from that of Ferraz and March,³ it fits into the form represented by Eq. (2.4). In other words, it affords another way of introducing the Fermi surface blurring through the function $\Gamma(q, k_f, l)$. That this method will reduce correctly to the Ziman theory in the limit of very long mean-free path has already been emphasized by Götze.

In spite of the differences in the form of $\Gamma(q, k_f, l)$ in the two approaches, it seems clear that for simple liquid metals they should yield rather similar results (cf Section 4 and Appendix 2 also). However, by making some further approximations, Götze has been able to solve the self-consistent problem he has posed, for random scattering centres, by analytical methods in the two limits of weak and of strong coupling. It is an appealing feature of his

approach that he can demonstrate in the strong coupling limit that his approximate Eqs. (3.6) and (3.7) can lead to localization due to disorder. We shall discuss this point, though by more elementary methods than those of Götze, a little further in the following section. However, to conclude the present section, the final comment we must make on the relation between the the two different methods surveyed above is that in each case the function Γ representing the blurring of the Fermi surface in Eq. (2.4) is, essentially, constructed from quantities characteristic of the uniform electron gas.

4 TRANSPORT AND SPECTRA IN DISORDERED SYSTEMS

In this section we shall be concerned with the relation between the theory of electronic transport in short mean-free path liquid metals, treated at some length above, and electronic level spectra. In calculating the average density of states, or more generally the average Green function, no clear distinction is drawn between the closely spaced sequence of delta functions and the continuum when the former are averaged over the disordered structures.^{10,11} The Ferraz-March assumption in Eq. (3.2) has the structure of an average Green function and in the light of the preceding comment it is hard, at first sight to see how it can contain information about localization. However, by a standard mean field theory of the resulting self-consistent equation we demonstrate in Section 4.1 that this is in fact the case. In this way we forge a link which enables a comparison to be made with Götze's theory.

4.1 Relation between self-consistent theory and electron localization

To examine whether the simple kinetic approach of Ferraz and March can have any link with localization, we show in Table II below the ratio of the self-consistent resistivity to the Ziman value for the liquid metals listed in Table I.

TABLE II
Ratio R of self-consistently calculated resistivity to Ziman value for liquid metals considered in Table I

Liquid metal	Li	Ma	K	Rb	Cs	Mg	Al
Ratio R							
$= \frac{\rho \text{ self-cons.}}{\rho \text{ Ziman}}$	1.27	1.07	1.06	1.06	1.14	1.04	1.05

What is seen to be rather striking is that the ratio for all the liquid metals except for the two with the largest deviation from the Ziman resistivity is rather constant, ranging only from 1.04–1.07. If, additionally, we argue that the Ziman theory is best for those liquid metals with the weakest electron-ion interaction, that would immediately reduce the discussion to Na, K and Rb, the polyvalent metals having a stronger electron-ion coupling. For these three liquid metals the ratio in Table II is essentially constant at the value 1.06.

To see the significance of this consequence $R = \text{constant}$ of the approach embodied in Eqs. (3.1) and (3.2), let us expand in powers of $1/l$ and write to first order

$$\rho = \rho_{nfe} + \Delta\rho \quad (4.1)$$

and for all the cases in Table II we see that $\Delta\rho(l^{-1})$ is positive. If we now write

$$\frac{\Delta\rho}{\rho_{nfe}} = \frac{l^*}{l} \quad (4.2)$$

then in the treatment of Ferraz and March it follows that l^* is precisely defined as

$$l^* = - \frac{\int \frac{\partial V(\mathbf{r}_1)}{\partial \mathbf{r}_1} \cdot \frac{\partial V(\mathbf{r}_2)}{\partial \mathbf{r}_2} |\mathbf{r}_1 - \mathbf{r}_2| |\sigma_0(\mathbf{r}_1 \mathbf{r}_2 E_f)|^2 d\mathbf{r}_1 d\mathbf{r}_2}{\int \frac{\partial V(\mathbf{r}_1)}{\partial \mathbf{r}_1} \cdot \frac{\partial V(\mathbf{r}_2)}{\partial \mathbf{r}_2} |\sigma^0(\mathbf{r}_1 \mathbf{r}_2 E_f)|^2 d\mathbf{r}_1 d\mathbf{r}_2} \quad (4.3)$$

the denominator of Eq. (4.3) being, essentially, the Ziman resistivity. Writing Eqs. (4.1) and (4.2) as

$$R = \frac{\rho}{\rho_{nfe}} = 1 + \frac{l^*}{l} \quad (4.4)$$

it follows immediately from the result $R = \text{constant}$ that for the three nearly free electron alkali metals

$$\frac{l^*}{l_{\text{melting point}}} = \text{constant} \doteq 0.06. \quad (4.5)$$

If, following arguments given by Götze,² but now in the context of the approach of Ferraz and March,³ we argue that mean field theory can be used to discuss the transition to a localized regime, then this theory would replace $1 + x$ in Eq. (4.4), valid for small $x = l^*/l$ by $1/(1 - x)$ and write

$$R = \frac{1}{1 - (l^*/l)}. \quad (4.6)$$

Thus, this corresponds to infinite resistivity when the mean-free path l becomes equal to l^* . The prediction of this treatment would be then

$$l_{\text{critical}} = l^* = 0.06 l_{\text{melting point}} \quad (4.7)$$

for the three alkali metals. We do not, in fact, expect there will be any real liquid metal which will behave precisely in accord with Eq. (4.7). However, what all this does suggest is that, in addition to the mean-free path obtained from the Ziman theory, a further important length for electronic transport theory is that introduced in Eq. (4.3). This equation is readily written in Fourier transform as shown in Appendix 2, just as is the Ziman formula. We expect that this precisely defined length, once $S(q)$ and $V(q, k_f)$ are given, will play an important role in the theory of electron localization due to disorder. This is confirmed if we form $l^*/(2\pi/k_f)$, i.e. the ratio of l^* to the de Broglie wavelength for an electron at the Fermi energy. This ratio is found from Eq. (4.5) to be nearly unity for Na, being 0.6 for K and Rb.

Of course, though we think the length l^* is therefore of considerable importance for electron localization, one will eventually need a fuller discussion, perhaps along lines similar to those laid down by Götze,² to give a first-principles relation between l^* and the metal-insulator transition induced by disorder. It should be stressed in this context that the evaluation of l^* from Eq. (4.3) requires merely the input information needed to calculate the Ziman resistivity from Eq. (2.1).

Before turning to discuss the transport information contained in averages of single-particle quantities, we want to add here that further confirmation of the usefulness of the force-force correlation function formula for the electrical resistivity is presented in Appendix 1. There we use it to provide an independent derivation of the Dawber-Turner result for the resistivity of a binary metallic alloy in the Koster-Slater model.

4.2 Transport information contained in the single-particle average

Having thus formed a clearer picture of the ability of the self-consistent theories to describe a phase with localized electron states in addition to the short mean-free path liquid metal phase, and the likely limitations of this description, we refer again to the dilemma posed at the beginning of this section; namely how can single-particle averages know about electron localization? We shall discuss this from two standpoints:

- i) the optical theorem and
- ii) the character of the Bardeen approximation to the density matrix, reflected in Eq. (3.2).

First of all, the optical theorem establishes a relationship between the spherically symmetric part of the resistivity formula involving a sum of the squares of T -matrix elements and an average force formula involving the imaginary part of the T -matrix, namely

$$\sum_{\mathbf{k}'} T_{\mathbf{k}\mathbf{k}'}(E) T_{\mathbf{k}'\mathbf{k}}(E) \delta(\varepsilon_{\mathbf{k}'} - E) = \frac{\hbar}{2\pi} \text{Im} T_{\mathbf{k}\mathbf{k}}(E - i\delta) \quad (4.8)$$

where the states \mathbf{k} are a complete basis, with energies $\varepsilon_{\mathbf{k}}$. Thus in cases where the $\cos \theta$ factor in the Ziman formula could be ignored, as for example in s -wave scattering, the resistivity is exactly expressible in the form of the average of a single-particle property.

Secondly, half of the resulting mean-free path is the length which enters into the modification of the Green function to an average Green function, as in the work of Edwards.¹² This then leads to the interpretation of the Ferraz-March method as decoupling $\langle G^2 \rangle$ to $\langle G \rangle^2$. However, the mean-free path which is calculated in this latter theory is not the above spherically symmetrical dependent quantity from the optical theorem, but a self-consistently determined one from a theory which includes the $\cos \theta$ factor in zeroth order. Thus the approximation amounts to

$$\langle G^2 \rangle = \langle G \rangle^2 \exp \left\{ -r \left(\frac{1}{l} - \frac{1}{l_0} \right) \right\} \quad (4.9)$$

where l_0 is the coherence length appearing in the average Green function.

It is clear however that for the case of a band with spherical scattering, the difference in (4.9) would not appear and that the arguments of Section 4.1 would still indicate the possibility of a transition. Thus the clear separation of single-particle properties from a discussion of the metal-insulator transition needs modification in cases where the optical theorem is applicable.

5 OUTSTANDING QUESTIONS FOR FUTURE STUDY

We have shown in the body of this article and in Appendix 1 that a statistical decoupling of averages, or a mode coupling approximation, lead independently to a structure of the force-force correlation type for the electrical resistivity. A feedback of the calculated mean-free path into the average square of the density matrix, or of the calculated zero frequency memory kernel into the density-density correlation function, then leads to self-consistent equations capable of demonstrating localization behaviour and the transition to an insulating phase from the short mean-free path liquid metal.

But this discussion leads us to raise the following questions:

i) Is there a natural basis consisting of localized and extended states in terms of which the dynamics can be understood as involving statistically independent transitions governed by a Boltzmann equation, or is some fundamentally new structure required? The above analysis would suggest that a mode coupling approximation and self-consistency are successful more in renormalizing the Boltzmann dynamics.

ii) To what extent does a renormalization of the scattering potential from a single-centre one to a multicentre form extend the applicability of the force-force correlation function formula. This extension was envisaged in the work of Rousseau, Stoddart and March¹³ and was further discussed by Jones.¹⁴

Since it is clear that electron correlation plays an essential role in defining the character of a metal-insulator transition, the ultimate applicability of an orbital description of the random electron liquid in terms of energy dependent localization lengths and radial distribution functions is brought into question for the short mean-free path liquid metal. However the goal of a kinetic approach to the description of the transport as a functional of the single-particle spectrum remains a worthwhile challenge.

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Appendix 1

RELATION TO IMPURITY SCATTERING

In this Appendix we shall review two limiting cases of the transport theory based on Eq. (3.1). In the first example treated below, plane waves are scattered by a spherical potential energy $V(r)$ of arbitrary strength. For this case, as Huang¹⁵ was the first to show, the excess resistivity is exactly calculable in terms of the phase shifts η_l of the l -th partial wave at the Fermi level, the result for the resistivity increment being, apart from a multiplying constant,

$$\Delta\rho \propto \sum_{l=1}^{\infty} \sin^2(\eta_{l-1} - \eta_l) \quad (\text{A1.1})$$

Plane waves scattered by spherical potential of arbitrary strength

As one of us has shown elsewhere,¹⁶ Eq. (3.1) can be rewritten by expressing $\sigma(\mathbf{r}_1, \mathbf{r}_2, E_f)$ in terms of the radial wave functions $R_l(r, E_f)$ of electrons in the potential $V(r)$. To relate the resulting formula to Huang's result (A1.1), one needs to appeal to a result due to Gerjuoy,¹⁷ which was rediscovered by Gaspari and Gyorffy,¹⁸ namely

$$\int_0^{\infty} dr r^2 R_l \frac{dV}{dr} R_{l+1} = \sin(\eta_{l+1} - \eta_l) \quad (\text{A1.2})$$

when one readily regains Eq. (A1.1).

To date, this is the sole example we are aware of in which the (energy derivative of the) density matrix, σ in Eq. (3.1) can be evaluated exactly without very restrictive conditions being imposed on V (in this case, solely the spherical symmetry). The above example makes it clear that in this impurity

scattering case, the starting point (3.1) of the argument of Ferraz and March contains within itself the exact Huang formula (A1.1). Naturally, one must no longer make the approximation (3.2). Götze's mode coupling approximation does not allow this limit of strong single centre impurity scattering to be regained exactly but it is more powerful than the approach of Ferraz and March for multicentre problems with strong scattering and therefore short mean-free path.

Koster-Slater impurity model: scattering cross-section

There is a further case, first treated by Dawber and Turner¹⁹ using the Golden Rule, in connection with metallic alloys, in which the scattering cross-section can be precisely evaluated from Eq (3.1). This is for the simplest version of the Koster-Slater²⁰ model of an impurity centre. In the case of a perfect crystalline host material, this is the model in which the impurity potential V is assumed to have non-zero matrix elements only between Wannier fuctions on the impurity site.

The way progress can be made in this case is via the T -matrix already discussed in Section 4.2. As shown in Ref. 21, the force-force correlation function (3.1) can be rewritten as, with the appropriate multiplying factors inserted,

$$\rho = -\frac{\hbar n_i}{e^2 \Omega n^4 (2\pi)^5} \int d\mathbf{k}_1 d\mathbf{k}_2 (\mathbf{k}_1 - \mathbf{k}_2)^{2\frac{1}{3}} \langle |T^+(\mathbf{k}_1 \mathbf{k}_2)|^2 \rangle \times \delta\left(E_f - \frac{\hbar k_1^2}{2m}\right) \delta\left(E_f - \frac{\hbar k_2^2}{2m}\right) \tag{A1.3}$$

where n_i is the density of ions.

We shall now write down the integral equation for the T -matrix as

$$T^+(\mathbf{k}_2, \mathbf{k}_1) = V_{k_2, k_1} + \sum_{\mathbf{k}} V_{k_2, \mathbf{k}} G_0^+(\mathbf{k}, \mathbf{k}) T^+(\mathbf{k}, \mathbf{k}_1) \tag{A1.4}$$

where the plane wave matrix elements of the impurity potential in the Koster-Slater model are

$$V_{\mathbf{k}\mathbf{k}'} = V = \text{constant.} \tag{A1.5}$$

Then it is straightforward to iterate out Eq. (A1.4) and to sum the resulting series to obtain

$$T^+(k_2, k_1) = \frac{V}{1 - V \sum_{\mathbf{k}} G_{\mathbf{k}\mathbf{k}}^0} \equiv V^*. \tag{A1.6}$$

In this expression, the sum in the denominator can be evaluated in terms of the density of states $n(E)$ and its Hilbert transform $P(E)$ to yield

$$\sum_{\mathbf{k}} G_{\mathbf{k}\mathbf{k}}^{+0} = P(E) - i\pi n(E). \tag{A1.7}$$

Into this we can incorporate Dawber and Turner's consistency condition for V (see their Eq. (4.6)) in the form

$$\begin{aligned} \sin^2(\frac{1}{2}\alpha\pi Z') &= \frac{\pi^2 V^2 n_0^2(E_f) N^{-2}}{(1 - VP(E_f))^2 + \pi^2 V^2 n_0^2(E_f) N^{-2}} \\ &= V^{*2} \pi^2 n_0^2(E_f) N^{-2}. \end{aligned} \quad (\text{A1.8})$$

Thus in Eq. (A1.3) we have

$$|T^*(\mathbf{k}_1, \mathbf{k}_2)|^2 = \frac{N^2}{\pi^2 n_0(E_f)^2} \sin^2(\frac{1}{2}\alpha\pi Z') \quad (\text{A1.9})$$

and

$$\int d\mathbf{k}_1 d\mathbf{k}_2 (\mathbf{k}_1 + \mathbf{k}_2)^2 \delta\left(E - \frac{\hbar k_1^2}{2m}\right) \delta\left(E - \frac{\hbar^2 k_2^2}{2m}\right) = -(2\pi)^2 4k_f^4 (2m/\hbar^2)^2 \quad (\text{A1.10})$$

where we have used the property

$$\delta\left(E_f - \frac{\hbar^2 k^2}{2m}\right) = \left(\frac{\hbar^2 k}{2m}\right)^{-1} \delta(k_f - k) \quad (\text{A1.11})$$

We then find

$$\rho = \frac{n_i}{N} \frac{4\hbar k_f^4}{3e^2 (2\pi)^3} \frac{1}{n^3} \frac{\rho e^2}{\pi^2 (n_0(F_f)\Omega)^2} \left(\frac{2n}{\hbar^2}\right)^2 \sin^2(\frac{1}{2}\alpha\pi Z'). \quad (\text{A1.12})$$

Although it is physically appealing to retain $n(E_f)$ in the denominator, let us finally substitute the free electron expressions

$$\Omega^{-1} n(E_f) = \frac{4mk_f}{(2\pi\hbar)^2}, \quad n(E_f) = \frac{k_f^3}{3\pi^2}, \quad (\text{A1.13})$$

and putting the impurity concentration c as the ratio of the number of impurities to the total number of atoms N we find the Dawber-Turner result

$$\rho = c \frac{2\hbar}{e^2} \left(\frac{\pi}{3n}\right)^{1/3} \sin^2(\frac{1}{2}\alpha\pi Z') \quad (\text{A1.14})$$

from the inverse transport result (3.1).

We anticipate that the above examples will prove relevant to the discussion of the excess resistivity of appropriate dilute liquid metal alloys but it would take us outside the scope of the present review to go into further details here.

Appendix 2

FORM OF CORRECTIONS TO ZIMAN FORMULA IN LIMIT OF LONG MEAN FREE PATH

In this Appendix, we write in q space the appropriate approximations for the resistivity in:

- a) the approach of Ferraz and March³
- b) the mode coupling approximation of Götze,²

demonstrating the reliance on the free electron gas reference system that underlies both approaches. The lowest order deviation from the Ziman formula is then calculated using the Lindhard dielectric function and the two results for l^* in Eq. (4.3) compared.

Firstly, the Ziman formula in the two notations appears as

$$\rho_z = \int_0^\infty q^4 S(q) |V(q, k_f)|^2 \Gamma_0(q, k_f) dq \quad (\text{A2.1})$$

where Γ_0 is the Fourier transform of $|\sigma(r_1, r_2, E_f)|^2$ in the Ferraz–March notation and $\phi_0(q, 0)$ in that of Götze. Going beyond this, Götze replaces Γ_0 by ϕ given in Eq. (3.7) and Ferraz and March by

$$\Gamma(q, k_f, l) = \int_0^\infty \frac{dq'}{2\pi} \Gamma_0(q - q', k_f) \frac{q'}{q'^2 + l^{-2}} \quad (\text{A2.2})$$

which contains the $\exp(-r/l)$ factor as a Lorentzian in convolution with ϕ_0 expressed in q -space. Both Eqs. (3.7) and (A2.2) are seen directly then as introducing Fermi surface blurring.

Despite the apparent difference in structure of these two equations and the fact that Eq. (3.7) exploits the frequency dependence of the free electron gas response function directly, the results for the lowest order deviation from the Ziman formula are similar when the (Lindhard) free electron characteristics are made explicit. Defining

$$\Lambda(q, k_f) = \lim_{l^{-1} \rightarrow 0} \frac{d}{dl^{-1}} \Gamma(q, k_f, l) \quad (\text{A2.3})$$

consistently with the kernel required for l^* in Eqs. (4.1) and (4.2)

$$\frac{l^*}{l} = \int_0^\infty q^4 S(q) |V(q, k_f)|^2 \Lambda(q, k_f). \quad (\text{A2.4})$$

With the aid of Eq. (2.2) the Ferraz-March approach gives

$$\begin{aligned}\Lambda(q, k_f) &= \lim_{l^{-1} \rightarrow 0} \int_0^\infty \frac{dq}{2\pi} \Gamma_0(q', k_f) \frac{d}{dq'} \left\{ - \frac{l^{-1}}{(q - q')^2 + l^{-2}} \right\} \\ &= \frac{1}{2} \int_0^\infty -dq' \Gamma_0(q', k_f) \frac{\partial}{\partial q'} \delta(q - q') \\ &= -\frac{1}{2} \frac{\partial \Gamma_0(q, k_f)}{\partial q} = -\frac{1}{2} \frac{\partial \phi''(q, 0)}{\partial q}\end{aligned}\quad (\text{A2.5})$$

and using Eq. (3.7) of Götze we find

$$\Lambda(q, k_f) = \frac{1}{g(q)} \phi_0''(q, 0)^2 + \left. \frac{\partial \phi_0''(q, z)}{\partial z} \right|_{z=0} \quad (\text{A2.6})$$

of which the first term stems from the static and the second term from the dynamic properties of the free electron gas.

A simple non-interacting free electron characteristic (Lindhard) yields:

$$|\sigma_0(r_1, r_2, E_f)|^2 = \frac{1}{2} \frac{\sin^2 k_f |\mathbf{r}_1 - \mathbf{r}_2|}{|\mathbf{r}_1 - \mathbf{r}_2|^2} \quad (\text{A2.7})$$

$$\Gamma_0(q, k_f) = \phi_0''(q, 0) = \frac{1}{q} \theta(q - 2k_f) \quad (\text{A2.8})$$

$$\left. \frac{\partial \phi_0''(q, z)}{\partial z} \right|_{z=0} = \frac{1}{8q^2} \left(\frac{16}{q^2 - 1} + \frac{2}{q} \ln \left| \frac{q - 1}{q + 1} \right| \right) \quad (\text{A2.9})$$

Hence the following results for $\Lambda(q, k_f)$ can be readily obtained:

a) In the Ferraz-March method

$$\Lambda(q, k_f) = \frac{1}{2} \left[\frac{1}{q^2} \theta(q - 2k_f) + \frac{1}{q} \delta(q - 2k_f) \right] \quad (\text{A2.10})$$

b) In the theory of Götze

$$\Lambda(q, k_f) = \frac{1}{2} \left[\frac{1}{q^2} \theta(q - 2k_f) + 2 \left. \frac{\partial \phi_0''(q, z)}{\partial z} \right|_{z=0} \right]. \quad (\text{A2.11})$$

which for $q \ll k_f$ becomes

$$\Lambda(q, k_f) = \frac{1}{2} \left(1 - \frac{4}{\pi^2} \right) \frac{1}{q^2} \quad (\text{A2.12})$$

We stress, in conclusion, the fact that both the methods lead to $1/q^2$ at small q while non-analyticity at the Fermi sphere diameter $q = 2k_f$ is exhibited in both treatments.