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TRANSPORT PROPERTIES IN LIQUID AND AMORPHOUS METALS

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We have obtained a result for the conductivity of a liquid metal in the effective medium approximation (EMA), which reduces to Velicky's coherent potential approximation (CPA) result for the crystalline alloy case. We use a method similar to that which Popielawski used to obtain the Gyorffy-Korringa-Millis (GKM) result. This variational derivative technique is general enough to allow us to derive expressions for the conductivity for all the approximation schemes proposed to deal with the one electron properties of liquid metals. However, those schemes which do not renormalize the electron propagator lead to singularities, and we shall specifically consider only the GKM and EMA theories here.

The theory is based on the Kubo formula for the conductivity

$$\sigma_{xx} = \frac{n}{\pi} \int_{-\infty}^{\infty} \mathrm{d} \omega \left\{ -\frac{g}{\omega} + \tau \tau \mathcal{G}(\omega) \mathcal{G}^\dagger(\omega) \right\} \rangle_c$$

(1)

where \( j \) is a current operator, and \( \mathcal{G}(\omega) \) is the one electron Greens function before configuration averaging -- the latter is denoted by \( \langle \rangle_c \). The other transport coefficients obey similar equations. We need to calculate the quantity

$$\pi_\nu(z,z') = \langle \mathcal{G}(z) \mathcal{J}_\nu \mathcal{G}(z') \rangle_c$$

(2)

The most interesting case will be \( z = z' = \omega + i\epsilon \). The object is to obtain an approximation to

$$\pi_\nu = \delta G$$

(3)

This ordered variation is obtained by letting

$$\mathcal{G}_0' + \delta \mathcal{G}_0$$

where \( \mathcal{G}_0' \) is the free electron Greens function and where \( \delta \mathcal{G}_0 = \mathcal{G}_0 \mathcal{J}_\nu \mathcal{G}_0' \), and finding the change in \( \mathcal{G} \) to first order, but putting primes on all quantities to the right of \( \mathcal{G}_0 \). Here we write \( \mathcal{G}_0(z') = \mathcal{G}_0' \), etc. Eq. (3) follows from the Greens function equation

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \mathcal{V} \mathcal{G}_0$$

(4)

where \( \mathcal{V} = \frac{1}{\Lambda} \mathcal{V}_1 \) is the potential due to the ions. Introducing the self-energy \( \Sigma \), which from its definition obeys,

$$\mathcal{G} = \mathcal{G}_0 + \mathcal{G}_0 \Sigma \mathcal{G}_0$$

(5)

we find

$$\pi_\nu = \delta \mathcal{G} = \mathcal{G}_0 \mathcal{J}_\nu \mathcal{G}_0' + \mathcal{G}_0 \delta \mathcal{G}_0$$

(6)

This will be our fundamental equation.

To evaluate \( \delta \mathcal{G} \) we use the several liquid metal theories. In what follows we will rely heavily on a recent article on the problem of analyticity for the multiple scattering theories, which gives much of the needed formalism. We defined in that article a self-energy path operator \( \sigma \rangle \).
which has the property that the self energy operator in Eq. (5) is given by,
\[ \mathcal{Z}(r, r') = \int_0^\infty \sigma(\mathbf{r}, \mathbf{r}', \mathbf{R}, \mathbf{R}') \, d\mathbf{r}' d\mathbf{R}' \]  
(7)

Here \( r \) and \( r' \) are electron coordinates and \( R \) and \( R' \) are ion coordinates corresponding to the first and last scatterings in each sequence contributing to \( \sigma \). We also make use of a relative coordinate description which is most conveniently given in \( k \)-space:
\[ \hat{G}_{kk} = \hat{A} \]
(8)

For several liquid metal theories, \( \sigma \) has an integral equation form
\[ \hat{G}_{kk} = \sigma_{kk} = \frac{1}{n} \int \exp \left[-ip \cdot (\mathbf{r} - \mathbf{R}) + ip' \cdot (\mathbf{r}' - \mathbf{R}') \right] \sigma(\mathbf{r}, \mathbf{r}', \mathbf{R}, \mathbf{R}') \, d\mathbf{r} d\mathbf{r}' d\mathbf{R} d\mathbf{R}' \]  
(9)

The first form for \( \hat{G}_o \) and \( \hat{G}_{2k} \) depends on the medium path operator which obeys
\[ \hat{G}_o = \frac{1}{n} \left\{ \hat{G}_{kk} + \hat{G}_{k} + \hat{G}_{k} \right\} \]  
(10)

The second form of Eq. (10) depends on the coherent \( T \)-matrix which obeys the integral equation
\[ t_c = \frac{1}{n} \int \hat{G}_{kk} \, d\mathbf{k} \]  
(11)

The second equalities in Eq. (15) involve \( G \) rather than \( G_0 \). In the definition of \( \hat{G}_o \) the integrands can be written in reverse order of factors. We can define \( \hat{G}_{1k} \) as the integrand, but it is not unique for the EMA.

As a consequence of the integral equation (Eq. 10) for \( \sigma \), we can readily prove the important result
\[ \partial \mathcal{G}_k = \hat{A}_k G_0 \]  
(12)

Using this and Eqs. (9) and (6) we can express \( \tau_k \) in the form
\[ \tau_k = G_k \left\{ \hat{A}_k G_0 + \hat{G}_k \right\} \]  
(13)
For the GKM we have simply
\[ \delta K_{kk'} = 8\pi^3 \delta(p-p') \frac{1}{n} S(k-p) \delta G'_{p} \] (21)
where \( S(k-k') = 1 + nh(k-k') \) is the x-ray interference function since \( \delta G'_{p} \) is just \( \pi \mu p' \), this results in an integral equation for \( \pi_{kk'} \)
\[ \pi_{kk'} = G_k \left[ \int_{\mu p'} W(k,k',z,z') \delta k' \right] G_k' \] (22)
where for GKM
\[ \pi_{kk'} = G_k' G_k = [(1 + G_k' G_k) \tau]_{kk'} \] (23)
This equation has the Bethe-Salpeter form proposed by Rubio. \( W \) is the vertex function and \( V \) is an effective potential. This result was obtained by Popielowski who observed that it is the same as that used by Ashcroft and Schaich. Actually Ashcroft and Schaich replace \( G \) by \( G_0 \) in Eq. (13).

Provided the level width is small compared to the Fermi energy, the effective potential \( V_{kk'} \) replaces the ordinary potential \( v_{kk'} \) in the Ziman formula. Otherwise, the integral equation, Eq. (22) is not difficult to solve iteratively.

For the EMA, we have obtained the following set of integral equations for \( \delta \kappa_{kk'} = \delta K_{kk'} + \delta W_{kk'} \)
\[ \delta K_{kk'} = \frac{1}{n} \int \left\{ (1 + \omega_{kk'}\omega_{kk'}) \dot{\tau}_{0k'} (1 + \omega_{kk'}\omega_{kk'}) \right. \]
\[ + \left[ (G_{2k'} c \delta \kappa_{kk'} + \omega_{kk'} \omega_{kk'} \dot{\tau}_{0k'}) \right] \delta k' \] (24)
\[ \delta W_{kk'} = \int (G_{k'} c \delta \kappa_{kk'} \dot{\tau}_{0k}) \left\{ (1 + \omega_{kk'}\omega_{kk'}) \dot{\tau}_{0k'} (1 + \omega_{kk'}\omega_{kk'}) \right. \]
\[ + \left[ (G_{k'} c \delta \kappa_{kk'} + \omega_{kk'} \omega_{kk'} \dot{\tau}_{0k'}) \right] \delta k' \] (25)
Here \( \tau_{0k} = G_k \dot{\pi}_{kk'} \). The proof of this result will be published elsewhere, but we note that the result for \( K_0 \) was easier to perform in real space, using the result that \( K_0 (RR') = \delta(0-R')G^R \), where \( G^R \) corresponds to removing an ion at \( R \). In the second term of Eq. (24) we have used the identity
\[ \delta \kappa_{kk'} = \int (G_{k'} c \delta \kappa_{kk'} \dot{\tau}_{0k}) \delta k' \] (26)
and the unsymmetrical form occurs because we must avoid overmultiplying certain terms by the pair distribution function \( g(R-R') \). We can express all quantities in terms of \( W, \sigma, \) and \( G_k \) by writing
\[ \delta \kappa_{kk'} = \left\{ \left[ \omega_{kk'} + (1 + \omega_{kk'}\omega_{kk'}) \dot{\tau}_{0k'} \right] \right\} \delta k' \] (27)
and the analogous result in reverse.

We have shown that in the case of the random alloy the EMA result reduces to that of Velicky for the alloy CPA. This is as it should be because the EMA reduces to the CPA for this case. The result expressed in Eqs. (24) and (25) is somewhat complicated because \( K_0 \) and \( W_k \) have upper indices, and because there are two coupled equations. A simplification which may be useful is related to an approximation introduced by Schwartz. If we allow \( g^2 \) in Eq. (24) and neglect the last two terms in Eq. (26), we find
\[ \delta K_{kk'} = \frac{1}{n} \int \left\{ (1 + \omega_{kk'}\omega_{kk'}) \dot{\tau}_{0k'} \right. \]
\[ + \left[ (G_{2k'} c \delta \kappa_{kk'} + \omega_{kk'} \omega_{kk'} \dot{\tau}_{0k'}) \right] \delta k' \] (28)
If in addition we neglect the first term in Eq. (27), our result reduced to the form used by Rubio, Eq. (22), and now the effective potential is given by
\[ \pi_{kk'} = \left\{ (1 + \omega_{kk'}\omega_{kk'}) \tau \right\}_{kk'} \] (29)
Comparing this with the GKM result, we see that the latter omits the last factor and is not symmetrical in \( k \) and \( k' \), as it should be. Actually if we omit both factors we would take as the effective potential the coherent T-matrix \( \tau \).
We are investigating these various approximations using a simple model with a separable potential. We hope to use our EMA result to investigate vertex corrections, saturation effects, and deviations from the Ziman formula for conductivity.

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