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Multiple-scattering theory of electron transport in disordered metals in the muffin-tin potential model: II. Decomposition of the vector waves

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Abstract. The basic formulation of the EMA transport theory in disordered metals in the muffin-tin potential model is further investigated. We decompose the vector waves, which represent the vertex corrections, into longitudinal and transverse components. This leads us to the reduction of the Bethe–Salpeter equations into the one-dimensional form analogous to the case of the electronic structure calculations discussed previously by Huisman *et al*. Although the transverse component makes no direct contribution to the conduction, there exists a scattering mechanism that couples both components. Therefore the longitudinal component must be determined self-consistently with the transverse one, and the latter is thus shown to have a finite effect on the electron transport.

1. Introduction

In the previous paper of this series (Itoh *et al* 1989, hereafter referred to as I) we have reformulated the EMA transport theory due to Roth and Singh (1982) in a tractable form in the case of the muffin-tin potential model. By 'tractable' it is meant that the difficult off-shell corrections are suitably integrated into the formalism in such a way that the equations to be solved take practically the same form as that of the on-shell calculations (see equations (3.26) and (3.27) in I). The mathematical structure of these equations is very similar to that found in the case of the density-of-states (DOS) calculations (equations (3.13)–(3.16) in I), except that the former deals with vector quantities.

However, in applying the muffin-tin EMA to practical cases, whether to the DOS or to transport, one encounters some technical problems. The first is that one must solve the integral equations for matrices labelled by $L = (l, m)$. The number of matrix elements to be determined self-consistently becomes rather formidable when the higher-order phase shifts are taken into account. Secondly, the integration in the equations is three-dimensional. In the case of the DOS calculations the above problems have already been solved by considering the symmetry properties of the scalar quantities due to the isotropy of the system (Asano and Yonezawa 1980, Huisman *et al* 1981, hereafter referred to as AY and HNSB, respectively). The integral equations have been reduced by these authors to one-dimensional form. All the scalars in the new equations are labelled by three azimuthal quantum numbers l, l' and l'', thus reducing the number of independent elements.

In the present paper we re-examine the above idea and attempt to extend it to deal with transport. The basic equations derived in the previous paper (equations (3.26) and (3.27) in I) represent the propagation of vector waves, each component of which is a matrix with respect to the indices $L = (l, m)$. In this sense each component of a vector has the same form as for a scalar; its symmetry property is, however, quite different from that of the scalars and the simple expression for the latter by HNSM cannot be applied directly. Nevertheless, as we shall see later, similar arguments are made possible for each component of the vector if we decompose it into longitudinal and transverse parts. The result is that the angular dependence of each component is separated from the radial part and the integration is reduced to one-dimensional form. Also the magnetic quantum numbers m are eliminated from the labelling of the radial part. Thus the transport theory developed in I is reduced to the level of the DOS calculations both formally and technically.

At first sight it may appear that only the longitudinal component is the relevant quantity, since the transverse component does not contribute to conduction. This is indeed true as a whole, but the scattering amplitude between the longitudinal and transverse waves is finite and the former can be determined only self-consistently with the latter by the integral equations.

In order to proceed carefully we formulate the problem rather mathematically. In section 2 we rederive the results for the scalars obtained by HNSB on a rigorous background, emphasising the role of translational and rotational invariance of the system. There a simple algebra is introduced of the scalar quantities labelled by three l-values, with multiplication between them defined in a suitable way. This simplifies writing down the equations to a great extent, without which the appearance of the equations would become really formidable. Owing to this, our formalism becomes much more transparent; in particular the reduced integral equations preserve the original appearance. In section 3 we discuss the reduction of the vector quantities. Although the method of separating the matrix into its radial and angular parts is different for each of the three components, it is shown that in each case the radial part is labelled by three l-values and obeys similar algebra to that discussed in section 2. The explicit forms of the scattering kernels, which include the structure factor, are also given there. Although we have $3 \times 3 = 9$ combinations for the kernels for each value of l, only four of them are seen to be independent. The last section is devoted to some discussions.

We follow the notation used in I. Equations in I are quoted frequently. In that case the letter I will be attached to the equation numbers. For example equation (1.1) in I is quoted as (I.1.1).

2. Representation of scalars

2.1. Symmetry considerations

As formulated by Roth (1975, 1980; see also I) the EMA equations are written in terms of diagonal operators ($t_{\boldsymbol{R}}$, $\eta(\boldsymbol{R})$ and $Q_{\mathrm{d}}(\boldsymbol{R})$) and off-diagonal operators ($\tilde{G}(\boldsymbol{R}, \boldsymbol{R}')$ and $Q(\boldsymbol{R}, \boldsymbol{R}')$). The former become a special case of the latter if the delta function $\delta(\boldsymbol{R} - \boldsymbol{R}')$ is attached. In fact $Q(\boldsymbol{R}, \boldsymbol{R}')$ is the sum of the diagonal part $Q_{\mathrm{d}}(\boldsymbol{R}, \boldsymbol{R}')\delta(\boldsymbol{R} - \boldsymbol{R}')$ and the purely off-diagonal part.

The translational invariance of the system allows for the relative coordinate representation (I.3.1). The isotropy of the system is expressed in this representation as

$$M(\boldsymbol{\rho}, \boldsymbol{\rho}'; X) = M(\mathcal{R}\boldsymbol{\rho}, \mathcal{R}\boldsymbol{\rho}'; \mathcal{R}X) \tag{2.1}$$

where $\mathcal{R}\boldsymbol{\rho}$, $\mathcal{R}\boldsymbol{\rho}'$ and $\mathcal{R}X$ represent the relative position vectors $\boldsymbol{\rho}$, $\boldsymbol{\rho}'$ and X in the coordinate system rotated by the rotation $\mathcal{R}$ and $M(\boldsymbol{\rho}, \boldsymbol{\rho}'; X)$ is the relative coordinate representation of an arbitrary scalar operator $M(\boldsymbol{R}, \boldsymbol{R}')$. From the definition (I.3.3) the matrix element of $M(\boldsymbol{R}, \boldsymbol{R}')$ is seen to be given by

$$M_{\boldsymbol{K}}^{LL'}(p, p') = \int \mathrm{d}X \int \mathrm{d}\boldsymbol{\rho}\, \mathrm{d}\boldsymbol{\rho}'\, Y_L(\boldsymbol{\rho}) j_l(p\rho) M(\boldsymbol{\rho}, \boldsymbol{\rho}'; X) j_{l'}(p'\rho') Y_{L'}^*(\boldsymbol{\rho}'). \tag{2.2}$$

Now we seek the result of the restriction (2.1) on the element (2.2). This is easily seen by applying the rotation to $M_{\boldsymbol{K}}$ in $\boldsymbol{K}$-space and using the transformation property of the spherical harmonics. The result is

$$M_{\mathcal{R}\boldsymbol{K}}^{LL'} = \sum_{\tilde{m}, \tilde{m}'} D_{\tilde{m}m}^{l}(\mathcal{R}) M_{\boldsymbol{K}}^{\tilde{L}\tilde{L}'} D_{\tilde{m}'m'}^{l'}(\mathcal{R})^* \tag{2.3}$$

where the matrix $D^l(\mathcal{R})$ is the lth irreducible representation of the rotational group corresponding to the rotation $\mathcal{R}$. In (2.3) we have also introduced the handy notations $\tilde{L} = (l, \tilde{m})$ and $\tilde{L}' = (l', \tilde{m}')$ associated with $L = (l, m)$ and $L' = (l', m')$; namely the angular momenta with and without tilde have a common l-value. We follow this convention hereafter. Note that the dependence on p and p' is assumed for M on both sides of (2.3), although it is not shown explicitly. Again we shall follow this hereafter. Of course only the κ-dependence needs to be assumed when the matrix is on-shell.

A special case of (2.3) is of particular importance. We set the Euler angles α, β and γ of the rotation $\mathcal{R} \equiv \mathcal{R}(\alpha, \beta, \gamma)$ equal to $\alpha = \varphi_k$, $\beta = \theta_k$ and $\gamma = 0$, where θ_k and φ_k are the direction angles of the $\boldsymbol{K}$-vector. Then (2.3) becomes

$$M_{\boldsymbol{K}}^{LL'}(p, p') = \sum_{\tilde{m}, \tilde{m}'} D_{m\tilde{m}}^{l}(\boldsymbol{K})^* M_{K}^{\tilde{L}\tilde{L}'}(p, p') D_{m'\tilde{m}'}^{l'}(\boldsymbol{K}) \tag{2.4}$$

where $D_{m\tilde{m}}^{l}(\boldsymbol{K})$ is the representation of $\mathcal{R}(\varphi_k, \theta_k, 0)$, the coordinate rotation that brings the z axis to the direction of the $\boldsymbol{K}$-vector. We shall call the coordinate system rotated by $\mathcal{R}(\varphi_k, \theta_k, 0)$ the '$\boldsymbol{K}$-system' hereafter. According to the convention the unit vectors along the x, y and z axes of the $\boldsymbol{K}$-system are denoted by $\hat{\boldsymbol{\theta}}_k$, $\hat{\boldsymbol{\varphi}}_k$ and $\hat{\boldsymbol{k}}$ respectively, bearing in mind that they are normal to the surfaces of $\theta_k = \text{const}$, $\varphi_k = \text{const}$ and $K = \text{const}$, respectively. The importance of (2.4) is that $M_K^{\tilde{L}\tilde{L}'}$ appearing on the RHS is dependent only on $K = |\boldsymbol{K}|$, since it is calculated in the $\boldsymbol{K}$-system, and therefore it shows that the angular dependence of the matrix element in the original coordinates is separated from the radial part.

It has been claimed by AY that (2.4) is equivalent to the following form

$$M_{\boldsymbol{K}}^{LL'} = \sum_{L''} C(ll''l'|mm''m')\, [M_K]_{l''}^{ll'}\, Y_{L''}(\boldsymbol{K}) \tag{2.5}$$

where we have used the Wigner coefficient instead of the Gaunt number used in I. The above representation is more suitable for practical calculations because the radial part $[M_K]$ is labelled by l-values only. It has also been used by HNSB. The EMA equations indeed allow for the above forms of the solution, as we shall see later. However, it seems to be dependent on the type of integral equation and (2.5) is not a general conclusion derived directly from (2.4). In this connection we note that the last equation in AY in the appendix, which connects (2.4) and (2.5), is found to be erroneous. The point becomes important in the next section.

The diagonal operator has a very simple matrix representation. Denoting an arbitrary diagonal operator by $M_{\rm d}(\boldsymbol{R})$, its matrix representation is written as

$$M_{\rm d}^{LL'}(p,p') = M_{\rm d}^{l}\delta_{LL'}. \tag{2.6}$$

That is, a diagonal operator is diagonal with respect to the L-indices and, furthermore, the element is dependent only on l. The above result is obtained by a symmetry argument only. Recalling that both Ms in equation (2.3) become independent of $\boldsymbol{K}$ for a diagonal operator, the RHS of the same equation is seen to be independent of the Euler angles of the rotation $\mathcal{R}$. We can then take the average over the Euler angles and, making use of the orthogonal property of $D^{l}_{m\bar{m}}$, equation (2.3) turns into (2.6). The property (2.6) has already been used in I in deriving (I.3.13)–(I.3.16) from (I.2.1)–(I.2.4). It is also seen to be a special case of (2.5) when $[M_K]^{ll'}_{l''}$ is independent of K and only the $l''=0$ component is non-zero:

$$[M_{\rm d}]^{ll'}_{l''} = (4\pi)^{1/2}M_{\rm d}^{l}\delta_{ll'}\delta_{l''0}. \tag{2.7}$$

2.2. *Algebra for $[M_K]^{ll'}_{l''}$ and the reduction of the* EMA *equation*

Since we shall rely on the representation (2.5) rather than on (2.4), we must deal with the quantities labelled by the three azimuthal numbers. We will therefore introduce a new algebra for the 'cubic matrices' $[M_K]^{ll'}_{l''}$ in such a way that the relation between the ordinary 'square matrices' $M_{\boldsymbol{K}}^{LL'}$ are properly mapped through (2.5). We use the same alphabet for both quantities. When the indices are suppressed they are distinguished only by $\boldsymbol{K}$ or K (a cubic matrix is dependent on $K=|\boldsymbol{K}|$ only).

First multiplication is examined. We show that the product between two square matrices

$$M_{\boldsymbol{K}} = S_{\boldsymbol{K}}\cdot T_{\boldsymbol{K}} \tag{2.8a}$$

is cast into the form

$$M_K = S_K\otimes T_K \tag{2.8b}$$

by defining multiplication $\otimes$ by

$$[S_K\otimes T_K]^{ll'}_{l''} = \sum_{l_1,l_2,l_3}\left(\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}\right)^{1/2} W(l\,l_1\,l'\,l_2;l_3\,l'')$$
$$\times\, C(l_1\,l_2\,l''|0\,0\,0)[S_K]^{ll_3}_{l_1}[T_K]^{l_3l'}_{l_2}. \tag{2.9}$$

In the above equation $W(l\,l_1\,l'\,l_2;\,l_3\,l'')$ is the Racah coefficient. The equivalence between (2.8a) and (2.8b) can be proved by substituting the representations (2.5) for $M_{\boldsymbol{K}}$, $S_{\boldsymbol{K}}$ and $T_{\boldsymbol{K}}$ in (2.8a) and then using the formula (see e.g. Rose 1957)

$$\sum_{m_1,m_2,m_3} C(l\,l_2\,l_3|m\,m_2\,m_3)C(l_3\,l_1l'|m_3\,m_1\,m')C(l_2\,l_1\,l''|m_2\,m_1\,m'')$$
$$= [(2l_3+1)(2l''+1)]^{1/2}W(l\,l_2\,l'\,l_1;l_3\,l'')C(l\,l'\,l''|m\,m'\,m''). \tag{2.10}$$

Essentially the same result as (2.8a) and (2.9) is used in HNSB. So far we have tacitly assumed that the product of two square matrices of the form (2.5) can be written in the same form, i.e. the group of square matrices of the form (2.5) is closed with respect to multiplication. In fact the formula (2.10) guarantees this important aspect. In other words the group of cubic matrices $[M_K]_{l''}^{ll'}$ has shown to be isomorphic to the group of square matrices $M_K^{LL'}$ written in the form (2.5), under the multiplication (2.9).

The above definition of multiplication satisfies the associative law, i.e.

$$S_K \otimes (T_K \otimes U_K) = (S_K \otimes T_K) \otimes U_K. \tag{2.11}$$

Although the direct proof of (2.11) is formidable, it is rather trivial if we note that both sides of (2.11) are the mapping of the same quantity $S_K(T_K \cdot U_K) = (S_K \cdot T_K)U_K$. It is also trivial that the distributive law holds:

$$S_K \otimes (T_K + U_K) = S_K \otimes T_K + S_K \otimes U_K. \tag{2.12}$$

The product between the diagonal and off-diagonal matrices becomes particularly simple:

$$[M_K \otimes M_\mathrm{d}]_{l''}^{ll'} = [M_K]_{l''}^{ll'} \cdot M_\mathrm{d}^{l'} \tag{2.13}$$

and

$$[M_\mathrm{d} \otimes M_K]_{l''}^{ll'} = M_\mathrm{d}^{l} \cdot [M_K]_{l''}^{ll'} \tag{2.14}$$

which can be proved directly by using (2.7), (2.8*b*) and (2.9). We note in passing that the unit element I for our multiplication is given by

$$[I]_{l''}^{ll'} = (4\pi)^{1/2} \delta_{ll'} \delta_{l''0}. \tag{2.15}$$

We are now in a position to prove that the EMA equations (I.3.13)–(I.3.16) allow for the solution of the form (2.5). In order to do so we first show that if a matrix U_K is of the form (2.5), so is the following convolution:

$$M_K = \int_{K'} h(\boldsymbol{K} - \boldsymbol{K}') U_{K'} \tag{2.16a}$$

and that its mapped relation is given by

$$[M_K]_{l''}^{ll'} = \int_0^\infty \frac{\mathrm{d}K'\, K'^2}{(2\pi)^2} h^{l''}(K, K') [U_{K'}]_{l''}^{ll'} \tag{2.16b}$$

where

$$h^l(K, K') = \int_{-1}^{1} \mathrm{d}(\cos\theta) h((K^2 + K'^2 - 2KK' \cos\theta)^{1/2}) P_l(\cos\theta). \tag{2.17}$$

Equation (2.16*b*) is proved if we substitute the expression (2.5) for $U_{K'}$ in (2.16*a*) and perform the angular integration in the $\boldsymbol{K}$-system. In doing so, we make use of the following relations:

$$Y_L(\boldsymbol{K}') = \sum_{\bar m} D_{m\bar m}^l(\boldsymbol{K})^* Y_{\bar L}(\mathcal{R}(\varphi_k, \theta_k, 0) \cdot \boldsymbol{K}') = \sum_{\bar m} D_{m\bar m}^l(\boldsymbol{K})^* Y_{\bar L}(\theta, \varphi) \tag{2.18}$$

where θ and φ are the direction angles of $\boldsymbol{K}'$ in the $\boldsymbol{K}$-system, and

$$Y_L(\boldsymbol{K}) = [(2l+1)/4\pi]^{1/2} D_{m0}^l(\boldsymbol{K})^*. \tag{2.19}$$

It is essential that the function $h(\boldsymbol{K} - \boldsymbol{K}')$ depends only on K, K' and θ, i.e. that the system is isotropic. The above proof is not the simplest one but is instructive for the later argument.

If the total correlation function $h(\boldsymbol{K}-\boldsymbol{K}')$ is replaced by unity, then $h^{l''}(K, K')$ is replaced by $2\delta_{l''0}$ in (2.16*b*). According to (2.5) there is no possibility that $l''=0$ and yet $l \neq l'$; M_K defined by (2.16*a*) therefore becomes diagonal in that case:

$$M_{\mathrm{d}}^{l}\delta_{LL'} = \int_{K} U_{K}^{LL'} \tag{2.20a}$$

$$M_{\mathrm{d}}^{l} = \frac{1}{\pi^{1/2}}\int_{0}^{\infty}\frac{\mathrm{d}K\,K^{2}}{(2\pi)^{2}}[U_{K}]_{0}^{ll}. \tag{2.20b}$$

We have derived all the necessary relations to map the EMA equations (I.3.13)–(I.3.16) onto the cubic matrix space. By way of (2.8*b*), (2.16*b*) and (2.20*b*) they become

$$Q_K = Q_{\mathrm{d}} + Q_{\mathrm{d}}\otimes\tilde{G}\otimes Q_K \tag{2.21}$$

$$[\tilde{G}_K]_{l''}^{ll'} = [B_K]_{l''}^{ll'} + \int_{0}^{\infty}\frac{\mathrm{d}k'\,k'^{2}}{(2\pi)^{2}}h^{l''}(K, K')[\tilde{G}_{K'}\otimes Q_{K'}\otimes\tilde{G}_{K'}]_{l''}^{ll'} \tag{2.22}$$

$$Q_{\mathrm{d}} = \tau + \tau\otimes\eta\otimes Q_{\mathrm{d}} \tag{2.23}$$

$$\eta^{l} = \frac{1}{\pi^{1/2}}\int_{0}^{\infty}\frac{\mathrm{d}K\,K^{2}}{(2\pi)^{2}}[\tilde{G}_K\otimes Q_K\otimes B_K]_{0}^{ll} \tag{2.24}$$

where τ and η are the diagonal cubic matrices, with M_{d}^{l} being replaced by τ^{l} and η^{l} respectively in (2.7).

The EMA equations for the DOS calculation have thus been rewritten in terms of a smaller number of elements. Finally we note that the number of independent elements is further reduced by the selection rules for a scalar, i.e. $[M_K]_{l''}^{ll'}$ is non-zero only when (i) $l+l'+l''$ is an even integer, and (ii) l, l' and l'' satisfy the triangular relation.

The first condition is proved by noting that the inhomogeneous terms satisfy this condition, and that our definition (2.9) of multiplication preserves the same property (when l_1+l_2+l'', $l+l_2+l_3$ and l_3+l_1+l' are all even, so is $l+l'+l''$). The second condition states that the three segments of length l, l' and l'' can form a triangle. It is also satisfied because the Racah coefficient in (2.9) is non-zero only when l, l', l'', l_1, l_2 and l_3 take the configuration of a tetrahedron.

3. Representation of vectors: the transport calculation

We proceed to the vector operators to discuss transport. As in the case of the scalars we distinguish between the off-diagonal vectors (e.g. $\delta\tilde{G}(\boldsymbol{R}, \boldsymbol{R}')$) and the diagonal vectors (e.g. $\delta\eta(\boldsymbol{R})$). Therefore $\boldsymbol{W}_K$ is off-diagonal and $\boldsymbol{K}_{\mathrm{d}}$ is diagonal. The possible forms of the matrices for these operators are also restricted by the isotropy of the system. We first show that when an arbitrary off-diagonal vector $\boldsymbol{\Gamma}(\boldsymbol{R}, \boldsymbol{R}')$ is decomposed as

$$\boldsymbol{\Gamma}_K = \hat{\boldsymbol{k}}\cdot\Gamma_K^{\parallel} + \hat{\boldsymbol{\theta}}_k\cdot\Gamma_K^{\theta} + \hat{\boldsymbol{\varphi}}_k\cdot\Gamma_K^{\varphi} \tag{3.1}$$

where $\hat{\boldsymbol{k}}$, $\hat{\boldsymbol{\theta}}_k$ and $\hat{\boldsymbol{\varphi}}_k$ are defined in the last section, then each of the components

$\Gamma_K^{\parallel}$, Γ_K^{θ} and Γ_K^{φ} is written in the form (2.4). We start from the expression (2.2) for a vector:

$$\Gamma_K^{LL'}(p,p') = \int \mathrm{d}X \exp(\mathrm{i}K \cdot X) \int \mathrm{d}\rho\, \mathrm{d}\rho'\, Y_L(\rho) j_l(p\rho) \Gamma(\rho,\rho';X) j_{l'}(p'\rho') Y_{L'}^*(\rho'). \tag{3.2}$$

The isotropy of the system is such that

$$\mathcal{R}\Gamma(\rho,\rho';X) = \Gamma(\mathcal{R}\rho,\mathcal{R}\rho';\mathcal{R}X) \tag{3.3}$$

and therefore, by rotating the K-vector in (3.2) by $\mathcal{R}$, it becomes

$$\Gamma_{\mathcal{R}K}^{LL'} = \sum_{\bar m,\bar m'} D_{\bar m m}^{l}(\mathcal{R}) \cdot \mathcal{R}\Gamma_K^{\bar L\bar L'} \cdot D_{\bar m' m'}^{l'}(\mathcal{R})^*. \tag{3.4}$$

By choosing again $\alpha = \varphi_k, \beta = \theta_k$ and $\gamma = 0$ for the Euler angles of rotation $\mathcal{R}$, the above equation can be written as

$$\Gamma_K^{LL'} = \sum_{\bar m,\bar m'} D_{m\bar m}^{l}(K)^* \cdot \mathcal{R}(\varphi_k,\theta_k,0)^{-1} \cdot \Gamma_K^{\bar L\bar L'} \cdot D_{m'\bar m'}^{l'}(K) \tag{3.5}$$

where in the RHS $\Gamma_K^{\bar L\bar L'}$ is dependent on $K = |K|$ only. Noting that $\mathcal{R}^{-1}\hat{x} = \hat{\theta}_k$, $\mathcal{R}^{-1}\hat{y} = \hat{\varphi}_k$ and $\mathcal{R}^{-1}\hat{z} = \hat{k}$, where $\hat{x}, \hat{y}$ and $\hat{z}$ are the unit vectors along x, y and z axes, we can identify the x, y and z components of Γ_K with $\Gamma_k^{\theta}, \Gamma_k^{\varphi}$ and $\Gamma_k^{\parallel}$ respectively. Therefore $\Gamma_k^{\parallel}$, Γ_k^{θ} and Γ_k^{φ} in (3.1) become scalars in the sense of (2.4).

It does not, however, mean that these quantities can be written in the form of (2.5), as pointed out in the last section. The precise forms of $\Gamma_k^{\parallel}$, Γ_k^{θ} and Γ_k^{φ} are dependent on the equations governing them and they can be found out only by trial and error. We present the result here and then prove it.

It is best presented by choosing a different recombination of the transverse components. We define two independent transverse unit vectors

$$\hat{\varepsilon}_+ = -(\hat{\theta}_k + \mathrm{i}\hat{\varphi}_k)/2 \tag{3.6}$$

and

$$\hat{\varepsilon}_- = +(\hat{\theta}_k - \mathrm{i}\hat{\varphi}_k)/2 \tag{3.7}$$

and make the corresponding decomposition of a vector Γ_K

$$\Gamma_K = \hat{k} \cdot \Gamma_K^{(0)} + \hat{\varepsilon}_+ \cdot \Gamma_K^{(+)} + \hat{\varepsilon}_- \cdot \Gamma_K^{(-)}. \tag{3.8}$$

Then it is shown that our equations (I.3.26) and (I.3.27) allow for the following solution:

$$\Gamma_K^{(\mu)LL'} = \sum_{L''} C(l\, l''\, l' | m\, m''\, m') [\Gamma_K^{(\mu)}]_{l''}^{ll'} Y_{L''}^{\mu}(K) \tag{3.9}$$

where $\mu = 0$, $+1$ or -1 and $Y_L^{\mu}(K)$ is defined by extending the relation (2.19):

$$Y_L^{\mu}(K) = [(2l+1)/4\pi]^{1/2} D_{m\mu}^{l}(K)^*. \tag{3.10}$$

That is, although each component of a vector Γ_K has the same symmetry as that of a scalar (2.4), the simpler form (2.5) is allowed only for the longitudinal component $\Gamma_K^{(0)} \equiv \Gamma_K^{\parallel}$ (note that $Y_L^{\mu}(K) \equiv Y_L(K)$ for $\mu = 0$). The representation (3.9) for $\mu = \pm 1$ is incompatible with the form (2.5); the expansion in terms of the $Y_L(K)$ does not lead to the labelling by l-values only.

For a proof, we start by showing that if an arbitrary vector V_K has the expression (3.8) and (3.9), so has the convolution

$$\Gamma_K = \int_{K'} h(K - K')V_{K'} \tag{3.11a}$$

and that its components are given by

$$[\Gamma_K^{(\mu)}]_{l''}^{ll'} = \sum_\nu \int_0^\infty \frac{dK'\,K'^2}{(2\pi)^2} h_{\mu\nu}^{l''}(K, K')[V_{K'}^{(\nu)}]_{l''}^{ll'} \tag{3.11b}$$

with suitable kernel functions $h_{\mu\nu}^l(K, K')$ (μ, $\nu = 0, \pm 1$). The proof of the above statement proceeds as follows. First we decompose $V_{K'}$ in (3.11a) into $\hat{k}$, $\hat{\varepsilon}_+$ and $\hat{\varepsilon}_-$ components by using

$$\hat{k}' = \hat{k}\cos\theta + \hat{\varepsilon}_+[-(\sin\theta)/\surd 2]\,e^{-i\varphi} + \hat{\varepsilon}_-[+(\sin\theta)/\surd 2]\,e^{i\varphi} \tag{3.12}$$

$$\hat{\varepsilon}'_+ = \hat{k}[+(\sin\theta)/\surd 2] + \hat{\varepsilon}_+[(1+\cos\theta)/2]\,e^{-i\varphi} + \hat{\varepsilon}_-[(1-\cos\theta)/2]\,e^{i\varphi} \tag{3.13}$$

$$\hat{\varepsilon}'_- = \hat{k}[-(\sin\theta)/\surd 2] + \hat{\varepsilon}_+[(1-\cos\theta)/2]\,e^{-i\varphi} + \hat{\varepsilon}_-[(1+\cos\theta)/2]\,e^{i\varphi}. \tag{3.14}$$

Here $\hat{\varepsilon}'_\pm = (\hat{\theta}_{k'} \pm i\hat{\varphi}_{k'})/\surd 2$ and θ and φ are the direction angles of K' in the K-system. Note that the coefficients in (3.12)–(3.14) are the components of $D_{m\tilde{m}}^l(\varphi, \theta, 0)$ for $l = 1$. By this procedure we obtain the expressions for $\Gamma_K^{(0)}$, $\Gamma_K^{(+)}$ and $\Gamma_K^{(-)}$ in terms of $V_{K'}^{(0)}$, $V_{K'}^{(+)}$ and $V_{K'}^{(-)}$. Next we perform the angular integrations of these equations in the K-system, assuming that the expression (3.9) holds for $V_{K'}^{(\mu)}$. In doing so we recall that the functions $Y_L^\mu(K)$ have the same transformation property as (2.18); this is easily derived from (3.10) by using the formula

$$D_{m\mu}^l(K') = \sum_{\tilde{m}} D_{m\tilde{m}}^l(K) D_{\tilde{m}\mu}^l(\mathcal{R}(\varphi_k, \theta_k, 0)\cdot K'). \tag{3.15}$$

We also note that the rotational matrix is written as

$$D_{m\tilde{m}}^l(K) = \exp(-im\varphi_k)\,d_{m\tilde{m}}^l(\theta_k) \tag{3.16}$$

with

$$d_{m\tilde{m}}^l(\theta) = \sum_s \frac{(-1)^s[(l+m)!(l-m)!(l+\tilde{m})!(l-\tilde{m})!]^{1/2}}{(l-m-s)!(l+\tilde{m}-s)!(s+m-\tilde{m})!s!} \times \left(\cos\frac{\theta}{2}\right)^{2l-m+\tilde{m}-2s}\left(-\sin\frac{\theta}{2}\right)^{m-\tilde{m}+2s} \tag{3.17}$$

and therefore the φ integration is carried out separately. We thus obtain (3.11b) with the kernel functions being given by

$$h_{\mu\nu}^l(K, K') = \int_{-1}^1 d(\cos\theta)\,h((K^2 + K'^2 - 2KK'\cos\theta)^{1/2})\,d_{\nu\mu}^1(\theta)\,d_{\mu\nu}^l(\theta). \tag{3.18}$$

The above function has the following symmetry properties:

$$h_{\mu\nu}^l(K, K') = h_{\nu\mu}^l(K, K') \tag{3.19}$$

and

$$h_{-\mu,-\nu}^l(K, K') = h_{\mu\nu}^l(K, K') \tag{3.20}$$

which are derived from $d_{\nu\mu}^l(\theta) = (-1)^{\nu-\mu}d_{\mu\nu}^l(\theta) = d_{-\mu,-\nu}^l(\theta)$.

We have not considered the diagonal vector. It appears in the form

$$\Gamma_{\mathrm{d}} = \int_{K} V_{K}. \tag{3.21a}$$

Since it is a special case of (3.11a) in which $h(\boldsymbol{K} - \boldsymbol{K}')$ is replaced by unity, its decomposition is readily obtained from (3.11b) and (3.18). Only $l = 1$ components are non-vanishing ($d^{l}_{\mu\nu}(\theta)$ forms a complete set for given μ and ν values) and we obtain $h^{l}_{00} = h^{l}_{11} = h^{l}_{1,-1} = h^{l}_{-1,1} = h^{l}_{-1,-1} = \frac{2}{3}\delta_{l1}$ and $h^{l}_{01} = h^{l}_{0,-1} = h^{l}_{10} = h^{l}_{-1,0} = -\frac{2}{3}\delta_{l1}$ for the kernel functions. It therefore becomes

$$[\Gamma^{(0)}_{\mathrm{d}}]^{ll'}_{l''} = -[\Gamma^{(\pm)}_{\mathrm{d}}]^{ll'}_{l''} = \delta_{l''1}\tfrac{2}{3}\int_{0}^{\infty}\frac{\mathrm{d}K\,K^{2}}{(2\pi)^{2}}\{[V^{(0)}_{K}]^{ll'}_{l''} - [V^{(+)}_{K}]^{ll'}_{l''} - [V^{(-)}_{K}]^{ll'}_{l''}\}. \tag{3.21b}$$

Note that Γ_{d} is decomposed into a sum of $\boldsymbol{K}$-dependent components:

$$\Gamma_{\mathrm{d}} = \hat{\boldsymbol{k}}\cdot\Gamma^{(0)}_{\mathrm{d}}(\boldsymbol{K}) + \hat{\boldsymbol{\varepsilon}}_{+}\cdot\Gamma^{(+)}_{\mathrm{d}}(\boldsymbol{K}) + \hat{\boldsymbol{\varepsilon}}_{-}\cdot\Gamma^{(-)}_{\mathrm{d}}(\boldsymbol{K}) \tag{3.22}$$

where

$$\Gamma^{(\mu)}_{\mathrm{d}}(\boldsymbol{K})^{LL'} = \sum_{L''} C(l\,l''\,l'|m\,m''\,m')[\Gamma^{(\mu)}_{\mathrm{d}}]^{ll'}_{l''}Y^{\mu}_{L''}(\boldsymbol{K}). \tag{3.23}$$

The first line of (3.21b) assures the $\boldsymbol{K}$ *independence* of the RHS of (3.22) after summation.

We still need to examine the product between a vector and a scalar. It is shown to yield a vector in the same form. For this purpose we slightly extend the algebra in the last section, which has been introduced to deal with the case $\mu = 0$ only, to the product between square matrices with different μ-values. Let us call μ the rank of a matrix. We first show that the product between ranks μ and ν yields a matrix of rank $\mu + \nu$. This is readily confirmed by using the following formula:

$$Y^{\mu}_{L}(\boldsymbol{K})Y^{\mu'}_{L'}(\boldsymbol{K}) = \sum_{L''}\left(\frac{(2l+1)(2l'+1)}{4\pi(2l''+1)}\right)^{1/2} \times C(l\,l'\,l''|m\,m'\,m'')C(l\,l'\,l''|\mu\,\mu'\,\mu+\mu')Y^{\mu+\mu'}_{L''}(\boldsymbol{K}) \tag{3.24}$$

which is obtained by using the formula concerning the integration of the product of three rotational matrices, and noting that the functions $Y^{\mu}_{L}(\boldsymbol{K})$ form a complete orthonormal set for each value of μ. By this we can see that the product of the square matrices

$$\Gamma^{(\mu+\nu)}_{K} = M^{(\mu)}_{K}\cdot U^{(\nu)}_{K} \tag{3.25a}$$

is cast into the form

$$\Gamma^{(\mu+\nu)}_{K} = M^{(\mu)}_{K}\otimes U^{(\nu)}_{K} \tag{3.25b}$$

where the multiplication $\otimes$ is extended as

$$[M^{(\mu)}_{K}\otimes U^{(\nu)}_{K}]^{ll'}_{l''} = \sum_{l_1,l_2,l_3}\left(\frac{(2l_1+1)(2l_2+1)(2l_3+1)}{4\pi}\right)^{1/2} W(l\,l_1\,l'\,l_2;l_3\,l'') \times C(l_1\,l_2\,l''|\mu\,\nu\,\mu+\nu)[M^{(\mu)}_{K}]^{ll_3}_{l_1}[U^{(\nu)}_{K}]^{l_3l'}_{l_2}. \tag{3.26}$$

In the EMA equations for transport we need only the case of $\mu = 0, \pm 1$. This is because the matrices of rank ± 1 are multiplied by rank -0 matrices only, so that no higher ranks appear in the equations. In this respect the current vertex is rather special.

By using equations (3.8), (3.9), (3.11), (3.21)–(3.23) and (3.25) we are now able to rewrite (I.3.26) and (I.3.27) in terms of cubic matrices. Making use of the symmetry of $\boldsymbol{K}_{\mathrm{d}}$ shown in (3.21b) it becomes

$$[W_K^{(\mu)}]_{l''}^{ll'} = [W_{0K}^{(\mu)}]_{l''}^{ll'} + \sum_{\nu} \int_0^\infty \frac{\mathrm{d}K'\, K'^2}{(2\pi)^2} h_{\mu\nu}^{l''}(K, K')[\tilde{G}_{K'} \otimes Q_{K'} \otimes W_{K'}^{(\nu)} + W_{K'}^{(\nu)} \otimes Q'_{K'} \otimes \tilde{G}'_{K'} + \tilde{G}_{K'} \otimes Q_{K'} \otimes (W_{K'}^{(\nu)} + K_{\mathrm{d}}^{(\nu)}) \otimes Q'_{K'} \otimes \tilde{G}'_{K'}]_{l''}^{ll'} \tag{3.27}$$

$$[K_{\mathrm{d}}]_{l''}^{ll'} = [K_{0\mathrm{d}}]_{l''}^{ll'} + \delta_{l''1} \int_0^\infty \frac{\mathrm{d}K\, K^2}{2\pi^2} [W_K \otimes Q'_K \otimes B'_K + \tilde{G}_K \otimes Q_K \otimes (W_K + K_{\mathrm{d}}) \otimes Q'_K \otimes B'_K]_{l''}^{ll'}. \tag{3.28}$$

Here in the second equation we have introduced

$$W_K \equiv W_K^{(0)} - W_K^{(+)} - W_K^{(-)} \tag{3.29}$$

and

$$K_{\mathrm{d}} \equiv K_{\mathrm{d}}^{(0)} - K_{\mathrm{d}}^{(+)} - K_{\mathrm{d}}^{(-)} = 3K_{\mathrm{d}}^{(0)}. \tag{3.30}$$

In the practical calculation we need only four kernel functions h_{00}^l, h_{01}^l, h_{11}^l and $h_{1,-1}^l$ for each l-value, owing to the symmetry shown in (3.19) and (3.20). The inhomogeneous terms $W_{0K}^{(\mu)}$ and $K_{0\mathrm{d}}$ are not to be confused with the longitudinal components $W_K^{(0)}$ and $K_{\mathrm{d}}^{(0)}$, and given from (I.3.28) and (I.3.29) as

$$[W_{0K}^{(\mu)}]_{l''}^{ll'} = \int_0^\infty \frac{\mathrm{d}K'\, K'^2}{(2\pi)^2} h_{\mu 0}^{l''}(K, K')[(I + \tilde{G}_{K'} \otimes Q_{K'}) \otimes \tilde{f}_{K'} \otimes \pi_{K'} \otimes f'_{K'} \otimes (I + Q'_{K'} \otimes \tilde{G}'_{K'})]_{l''}^{ll'} \tag{3.31}$$

and

$$[K_{0\mathrm{d}}]_{l''}^{ll'} = \delta_{l''1} \int_0^\infty \frac{\mathrm{d}K K^2}{2\pi^2} [(I + \tilde{G}_K \otimes Q_K) \otimes \tilde{f}_K \otimes \Pi_K \otimes f'_K \otimes (I + Q'_K \otimes B'_K)]_{l''}^{ll'}. \tag{3.32}$$

The necessary input quantities in the above equations are

$$[f_K]_{l''}^{ll'} = (4\pi)^{1/2} t^l(K, \kappa) \tau^l(\kappa)^{-1} \delta_{ll'} \delta_{l''0} \tag{3.33}$$

$$[\tilde{f}_K]_{l''}^{ll'} = (4\pi)^{1/2} \tau^l(\kappa)^{-1} t^l(\kappa, K) \delta_{ll'} \delta_{l''0} \tag{3.34}$$

$$[B_K]_{l''}^{ll'} = \left(\frac{(2l+1)(2l'+1)}{4\pi(2l''+1)}\right)^{1/2} C(l\, l''\, l'|0\,0\,0) \frac{4\pi(K/\kappa)^{l''}}{E - \kappa^2} \tag{3.35}$$

and

$$[\Pi_K]_{l''}^{ll'} = \left(\frac{(2l+1)(2l'+1)}{4\pi(2l''+1)}\right)^{1/2} C(l\, l''\, l'|0\,0\,0) \frac{4\pi J_K}{(E - K^2)(E' - K^2)}. \tag{3.36}$$

Here Π_K is the unperturbed current vertex, which has longitudinal component only (so that it is a rank-0 matrix).

Equations (3.27)–(3.36), together with the kernel function (3.18), are the principal results. The three-dimensional integral equations have thus been reduced to one-dimensional form. After having solved (3.29) and (3.30) self-consistently, the vertex correction is calculated by using the longitudinal component only:

$$\Xi_{\mathrm{c}}(E, E') = \sum_{l} \frac{(2l+1)}{\pi^{1/2}} \int_0^\infty \frac{\mathrm{d}K\, K^2}{(2\pi)^2} [\Pi_K \otimes f_K \otimes Q_K \otimes (W_K^{(0)} + \tfrac{1}{3}K_{\mathrm{d}}) \otimes Q'_K \otimes \tilde{f}'_K]_0^{\parallel} \tag{3.37}$$

and this completes the solution to our problem.

4. Discussion

One of the remarkable features of the problem is that the transverse components are non-vanishing and affect the conduction through the coupling with the longitudinal component. This fact appears to be at variance with the following simple argument. The two-particle Green function of the system is written in the form

$$\langle G(\boldsymbol{K}, \boldsymbol{K}')G'(\boldsymbol{K}', \boldsymbol{K})\rangle \equiv F(K, K'; \theta) = \sum_L Y_L(\boldsymbol{K}) Y_L^*(\boldsymbol{K}') F_l(K, K') \tag{4.1}$$

where θ is the angle between $\boldsymbol{K}$ and $\boldsymbol{K}'$, because our system is isotropic. Then, by using the first line of the above equation, we have

$$\int_{K'} \hat{\boldsymbol{K}}' \langle G(\boldsymbol{K}, \boldsymbol{K}')G'(\boldsymbol{K}', \boldsymbol{K})\rangle = \hat{\boldsymbol{K}} \int_{K'} F(K, K'; \theta) \cos\theta. \tag{4.2}$$

The key quantity for the transport calculation is therefore purely longitudinal and, no doubt, so is the vertex function. The answer to the above puzzle is that the same argument cannot be applied to each component in the second line of (4.1). Namely the quantity

$$Y_L(\boldsymbol{K}) \int \mathrm{d}\Omega_{K'} \hat{\boldsymbol{K}}' \, Y_L(\boldsymbol{K}')$$

becomes proportional to $\hat{\boldsymbol{K}}$ only when the summation over m is carried out. The spurious transverse components of the vertex corrections have come out because we have adopted the angular-momentum decomposition of the ionic momentum. This is the price we must pay for having reduced the integral equations to one-dimensional form. It is also related to the existence of the diagonal vertex corrections, which are independent of $\boldsymbol{K}$-vector and therefore inevitably have transverse amplitudes. Indeed, if the system has only s scatterers, we have only one component ($l = 0$ and $m = 0$) and our vertex function $\boldsymbol{W}_K$ becomes purely longitudinal. The diagonal vertex function $\boldsymbol{K}_{\mathrm{d}}$ is then shown to disappear.

In our representation in terms of cubic matrices the scattering amplitudes between the longitudinal and transverse waves appear to be symmetric. However, it implies neither $W_K^{(+)} = W_K^{(-)}$ nor $|W_K^{(0)}| = |W_K^{(\pm)}|$. Note that we have not defined the cubic matrices in a symmetric way with respect to the positive and negative ranks. In particular, we need a different definition of multiplication for a different combination of the ranks. For the same reason the first selection rule discussed in section 2 for scalars does not hold in the case of vectors, whereas the second rule is still valid for vectors. This asymmetry of the definition is unavoidable; or the magnetic quantum numbers would be included in the labelling. Nevertheless we find the introduction of our multiplication very useful, without which our equations would have had tremendous length. The original forms of the EMA equations are most clearly seen by using the notation $\otimes$, both for the DOS and the transport calculations. It will also serve as a useful tool for simpler computer programming.

We have applied the present formalism to a system with s scatterers to see the multiple-scattering corrections to the Ziman formula. The corrections are seen to be *very* large when the scattering is strong (Fresard *et al* 1989). We further plan to include higher-order phase shifts to deal with realistic non-simple systems.

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