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# On the Electrical Conductivity of Metals by the Resolvent Method

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## Synopsis

Using the resolvent method previously developed by VAN HOVE and the author for describing dissipative quantum many-body systems, general expressions are derived for the asymptotic value of the time integral of operators which are diagonal at initial time (i. e. diagonal with respect to the eigenfunctions of the unperturbed Hamiltonian).

As illustrative example the formalism is applied to the calculation of the zeroth order electrical conductivity tensor for spherically symmetric impurity centres. Electron-electron interactions are however neglected. The result is compared with that derived by VERBOVEN for the same case, but using time-dependent perturbation. General agreement is found up to a non-Markoffian term which in fact should be omitted.

It is finally shown, how the same result can also be obtained from the Markoffian approximation of the general master equation.

## 1. Introduction

As CHESTER and THELLUNG<sup>1)</sup> have shown by their calculation on the electrical conductivity of metals, the evaluation of transport coefficients by means of the Kubo formula is a relatively easy matter if one knows the solutions of the master equation describing the time evolution of one of the factors involved in the correlation function. Actually, such a solution is explicitly known only in the weak coupling case ( $\lambda \rightarrow 0$ ,  $t \rightarrow \infty$ ;  $\lambda^2 t$  finite), for which the non-Markoffian general master equations derived by VAN HOVE<sup>2)</sup> and by the author<sup>3)</sup> reduce to the Markoffian Pauli master equation.

Higher order effects of various kinds can of course be taken into account by improving the various approximations made along the basic calculation. It is in this way, discussed in detail by CHESTER and THELLUNG<sup>1)</sup>, that VERBOVEN<sup>4)</sup> obtained explicit expressions for the conductivity tensor to zeroth order in the coupling constant. For getting corrections to higher order than this one, such a procedure is of course not suitable.

The aim of the present paper is to give a calculation performed, as far as possible, to general order in the perturbation, the various contributions being then obtained directly from the general expressions by power series expansion in the coupling constant. It was while looking for this goal that a general master equation for the interference term was derived one year ago<sup>3)</sup>. The general expressions mentioned above are here given in what we may call their spectral form, and in fact the last integration is performed only after having made the expansion in powers of  $\lambda$ . From this point of view we have not yet reached our final goal. Even so, there are general questions which can be discussed to all orders in the perturbation.

The present investigation is based on the fact that the solution of the general master equation represents a much too detailed information on the system, with respect to what is really needed, i.e. the asymptotic value ( $t \rightarrow \infty$ ) of the time integral of the solution. As shown in sections 2 to 5, this result can be better obtained directly from asymptotic equations. As illustrative example we apply in section 6 the formalism to the calculation of the zeroth order conductivity tensor for an electron scattered by spherically symmetric impurity centres. In section 7 the expressions obtained are compared with those derived by VERBOVEN<sup>4)</sup>, and in the last section we add some concluding remarks.

We know of other independent efforts<sup>5)6)</sup> performed along the same pattern of thoughts with a view to refining, by means of higher order corrections the basic formula for the conductivity. With the present approach we hope to give a contribution for a better knowledge of equations of the master type.

## 2. Outlines of VAN HOVE's resolvent method

We here briefly recall some general results of VAN HOVE's<sup>2)3)</sup> perturbative treatment based on the resolvent, which allows compact expressions to general order in the perturbation. The resolvent  $R_l$  is related to the operator of motion  $U_t$  by means of a complex Fourier transform:

$$U_t = \frac{-1}{2\pi i} \int_{\gamma} dl e^{-ilt} R_l, \quad (2.1)$$

where

$$R_l = (H_0 + \lambda V - l)^{-1}.$$

$l$  is a complex number and  $\gamma$  an integration contour encircling counter-clockwise a sufficient portion of the real axis.  $\lambda V$  represents the perturbation of  $H_0$ , the unperturbed hamiltonian whose eigenstates  $|\alpha\rangle$  are known and form a complete set, normalized (in the limit of an infinite system) to:

$$\langle \alpha | \alpha' \rangle = \delta(\alpha - \alpha'). \quad (2.2)$$

The matrix elements of an operator  $A_t$ , which for the initial time  $t = 0$  is diagonal in the  $\alpha$ -representation, may be written as:

$$A_t(\alpha \alpha') \equiv \langle \alpha | U_{-t} A U_t | \alpha' \rangle = \int d\alpha_0 A(\alpha_0) Z_t(\alpha_0 \alpha \alpha'), \quad (2.3)$$

where

$$Z_t(\alpha_0 \alpha \alpha') = P_t(\alpha_0 \alpha) \delta(\alpha - \alpha') + I_t(\alpha_0 \alpha \alpha'). \quad (2.4)$$

For  $A(\alpha_0)$  a smooth function of  $\alpha_0$ ,  $P_t(\alpha_0 \alpha)$  is not trivially zero for the systems we are considering here, and represents a coarse-grained transition probability.  $I_t(\alpha_0 \alpha \alpha')$  describes interference effects. The Fourier-transformed expressions corresponding to (2.3) and (2.4) are:

$$A_{ll'}(\alpha \alpha') \equiv \langle \alpha | R_l A R_{l'} | \alpha' \rangle = \int d\alpha_0 A(\alpha_0) Z_{ll'}(\alpha_0 \alpha \alpha'), \quad (2.5)$$

$$Z_{ll'}(\alpha_0 \alpha \alpha') = X_{ll'}(\alpha_0 \alpha) \delta(\alpha - \alpha') + Y_{ll'}(\alpha_0 \alpha \alpha'), \quad (2.6)$$

where

$$Z_t(\alpha_0 \alpha \alpha') = \frac{-1}{(2\pi)^2} \int_{\gamma} dl \int_{\gamma'} dl' e^{i(l-l')t} Z_{ll'}(\alpha_0 \alpha \alpha') \quad (2.7)$$

( $\gamma$  and  $\gamma'$  as above).  $Z_{ll'}$  obeys a general master equation which can be put into the following very convenient form:

$$Z_{ll'}(\alpha_0 \alpha \alpha') = D_l(\alpha_0) D_{l'}(\alpha_0) \left\{ \delta(\alpha_0 - \alpha) \delta(\alpha - \alpha') + V_{ll'}(\alpha_0 \alpha \alpha') + \lambda^2 \int d\alpha_1 W_{ll'}(\alpha_0 \alpha_1) Z_{ll'}(\alpha_1 \alpha \alpha') \right\} \quad (2.8)$$

which is expressed in terms of  $D_l$  (the diagonal part of  $R_l$ ), of  $V_{ll'}$  and of  $W_{ll'}$  whose definitions are:

$$D_l = R_l^d \quad D_l | \alpha \rangle = | \alpha \rangle D_l(\alpha), \quad (2.9)$$

$$\left. \begin{aligned} \langle \alpha | \{ (1 - \lambda D_l V + \lambda^2 D_l V D_l V - \dots) A (1 - \lambda V D_{l'} V D_{l'} - \dots) \}_{ind} | \alpha' \rangle \\ = \int d\alpha_0 A(\alpha_0) V_{ll'}(\alpha_0 \alpha \alpha') \end{aligned} \right\} \quad (2.10)$$

$$\{ (V - \lambda V D_l V + \dots) A (V - \lambda V D_{l'} V + \dots) \}_{id} | \alpha \rangle = | \alpha \rangle \int d\alpha_0 A(\alpha_0) W_{ll'}(\alpha_0 \alpha). \quad (2.11)$$

The suffixes "id" and "ind" mean "irreducible diagonal part" and "irreducible non-diagonal part" (for definitions, see rf. 3, p. 49). The singularities of  $Z_{ll'}$  are represented by cuts along the real axis in the complex  $l$  and  $l'$  planes and by a simple pseudo-pole (see  $H_2$  p. 465) for  $l = E \mp i0$ ,  $l' = E \pm i0$ , and  $E$  real, determining the asymptotic value of  $Z_t$ , which is given by:

$$\lim_{t \rightarrow \pm \infty} Z_t(\alpha_0 \alpha \alpha') = \int_{-\infty}^{+\infty} dE Z_E^{\pm}(\alpha_0 \alpha \alpha'), \quad (2.12)$$

$$Z_E^{\pm}(\alpha_0 \alpha \alpha') = \mp \frac{1}{2\pi i} \lim_{\substack{l \rightarrow E \mp i0 \\ l' \rightarrow E \pm i0}} (l - l') Z_{ll'}(\alpha_0 \alpha \alpha'). \quad (2.13)$$

Assuming interconnection of states with equal unperturbed energy (implying that the states  $|\alpha\rangle$  are dissipative) and the validity of a generalized microscopic reversibility ( $W_{ll'}(\alpha \alpha') = W_{l'l}(\alpha' \alpha)$ ), one obtains for  $Z_E^{\pm}$  the simple expression

$$Z_E^{\pm}(\alpha_0 \alpha \alpha') = \frac{A_E(\alpha) Q_E(\alpha \alpha')}{\int d\alpha_1 A_E(\alpha_1)} \quad (2.14)$$

where  $Q_E$  is defined by:

$$Q_E = \lim_{0 > \eta \rightarrow 0} \frac{1}{2\pi i} (R_{E+i\eta} - R_{E-i\eta}) \quad (2.15)$$

and  $A_E$  is its diagonal part. The hypothesis of a generalized microscopic reversibility is not an essential one, and can be dropped<sup>7)</sup>. In this case, however, one needs a more elaborated formulation than the one adopted here.

### 3. Asymptotic time-integrated master equation

We consider the time integral of the operator  $A_t$  introduced above, and we suppose the existence of a corresponding asymptotic operator  $\tilde{A}_\pm$ :

$$\tilde{A}_\pm = \lim_{T \rightarrow \pm\infty} \int_0^T dt A_t. \quad (3.1)$$

This implies that:

$$\lim_{t \rightarrow \pm\infty} A_t = 0 \quad (3.2)$$

and together with (2.5), (2.12) and (2.13), that  $A_{ll'}$  is a bounded operator in the complex  $l, l'$ -planes. Interchanging the time integration with the complex ones, we get for  $\tilde{A}_\pm$ :

$$\tilde{A}_\pm = \lim_{T \rightarrow \pm\infty} \frac{-1}{(2\pi)^2} \int dl \int_{\gamma'} dl' \frac{e^{i(l-l')T}}{i(l-l')} A_{ll'}. \quad (3.3)$$

The term obtained from the limit  $t = 0$  in (3.1) vanishes because  $A_{ll'}$  approaches to zero as  $|ll'|^{-1}$  when  $l$  and  $l' \rightarrow \infty$ , and the integration paths can be deformed to infinity. Denoting the two partial contours above and below the real axis respectively by  $\gamma^+$  and  $\gamma^-$ , one verifies that in (3.3) for  $T > 0$  only  $\gamma^-$  and  $\gamma'^+$  give a non-vanishing contribution; for  $T < 0$  there only remain  $\gamma^+$  and  $\gamma'^-$ .

Using the asymptotic formula:

$$\frac{e^{i(E-E')T}}{E-E' \mp i0} = \pm 2\pi i \delta(E-E') \quad \text{for } T \rightarrow \pm\infty \quad (3.4)$$

where upper (and lower) signs are taken together, one finally obtains for (3.3):

$$A_\pm(\alpha\alpha') = \pm \frac{1}{2\pi} \lim_{0 < \eta \rightarrow 0} \int d\alpha_0 A(\alpha_0) \int_{-\infty}^{+\infty} dE Z_{E \mp i\eta, E \pm i\eta}(\alpha_0 \alpha \alpha'). \quad (3.5)$$

The limit  $\eta \rightarrow 0$  has to be taken only after integration over  $\alpha_0$ , because in this limit  $Z_{E \mp i\eta, E \pm i\eta}$  itself becomes singular.

Let us now look at the formal solution of the general master equation. We introduce a matrix formalism which allows a much shorter notation. We consider an “initial state”  $|\alpha\alpha'\rangle$  with the following two properties:

$$\langle \alpha_0 | 0 | \alpha\alpha' \rangle = 0 (\alpha_0 \alpha \alpha') \quad \text{for a general operator } 0 \quad (3.6)$$

and

$$\langle \alpha_0 | \alpha\alpha' \rangle = \delta(\alpha_0 - \alpha) \delta(\alpha - \alpha'). \quad (3.7)$$

In particular we have for a two-indice diagonal operator of the type of  $X_{ll'}$ :

$$X_{ll'}(\alpha_0 \alpha \alpha') \equiv X_{ll'}(\alpha_0 \alpha) \delta(\alpha - \alpha') \quad (3.8)$$

and for a one-indice diagonal operator of the type  $D_l$ :

$$D_l(\alpha_0 \alpha \alpha') \equiv D_l(\alpha_0) \delta(\alpha_0 - \alpha) \delta(\alpha - \alpha') \quad (3.9)$$

Multiplication from the left of a general operator by diagonal ones is defined according to the rules of matrix multiplication. So, for example:

$$Z_{ll'} = D_l D_{l'} \{1 + V_{ll'} + \lambda^2 W_{ll'} Z_{ll'}\} \quad (3.10)$$

gives (2.8) for the "final" state  $\langle \alpha_0 |$  and the "initial" one  $|| \alpha \alpha' \rangle^*$ .

Remembering that:

$$D_l = (H_0 - l - \lambda^2 G_l)^{-1} \quad (3.11)$$

where

$$G_l = (V - \lambda V D_l V + \lambda^2 V D_l V D_l V - \dots)_{id} \quad (3.12)$$

one finds

$$D_{E+i\eta} D_{E-i\eta} = \frac{D_{E+i\eta} - D_{E-i\eta}}{2\eta i + \lambda^2 (G_{E+i\eta} - G_{E-i\eta})}. \quad (3.13)$$

For further reference we recall that

$$\lim_{0 < \eta \rightarrow 0} G_{E \pm i\eta} = K_E \pm i J_E \quad (3.14)$$

where  $J_E \neq 0$  for a dissipative system. In this case (3.13) gives:

$$D_{E+i0} D_{E-i0} = \frac{\pi \Delta_E}{\lambda^2 J_E}. \quad (3.13a)$$

We define an operator  $\Omega_{E \mp i\eta}$  in the following way

$$\Omega_{E \mp i\eta} = \frac{\eta}{\lambda^2} + \frac{1}{2i} (G_{E+i\eta} - G_{E-i\eta}) - \frac{1}{2i} (D_{E+i\eta} - D_{E-i\eta}) W_{E \mp i\eta, E \pm i\eta} \quad (3.15)$$

giving for  $\eta \rightarrow 0$

$$\Omega_{E \mp i0} = J_E - \pi \Delta_E W_{E \mp i0, E \pm i0}. \quad (3.15a)$$

The general master equation (3.10) can now be written as:

$$\lambda^2 \Omega_{E \mp i\eta} Z_{E \mp i\eta, E \pm i\eta} = \frac{1}{2i} (D_{E+i\eta} - D_{E-i\eta}) (1 + V_{E \mp i\eta, E \pm i\eta}). \quad (3.16)$$

The corresponding formal solution is:

$$Z_{E \mp i\eta, E \pm i\eta} = (\lambda^2 \Omega_{E \mp i\eta})^{-1} \frac{1}{2i} (D_{E+i\eta} - D_{E-i\eta}) (1 + V_{E \mp i\eta, E \pm i\eta}) + Z_{E \mp i\eta, E \pm i\eta}^{(0)} \quad (3.17)$$

\*) These formal "bra" and "ket" are related to the physical states  $\alpha_0, \alpha$  and  $\alpha'$  in the following way:

$$\langle \alpha | \dots || \alpha \alpha' \rangle \leftrightarrow \langle \alpha | \dots | \alpha_0 \rangle \langle \alpha_0 | \dots | \alpha' \rangle.$$

$Z_{E \mp i\eta, E \pm i\eta}^{(0)}$  is a solution of the homogeneous equation:

$$\lambda^2 \Omega_{E \mp i\eta} Z_{E \mp i\eta, E \pm i\eta} = 0. \quad (3.18)$$

In the following we omit  $Z_{E \mp i\eta, E \pm i\eta}^{(0)}$  because it gives a vanishing contribution to  $\tilde{A}_\pm$ . In fact one verifies that:

$$\lim_{0 < \eta \rightarrow 0} Z_{E \mp i\eta, E \pm i\eta}^{(0)} = c Z_E^\pm, \quad (3.19)$$

where  $c$  is an arbitrary constant.

For the same reason also, the residue of the pole in  $1/\eta$  of  $Z_{E \mp i\eta, E \pm i\eta}(\alpha_0 \alpha \alpha')$  vanishes in (3.5) after integration over  $\alpha_0$ . This pole is related to the existence of a zero eigenvalue  $\omega^{(1)} = 0$  of  $\Omega_{E \mp i\eta}$  in the limit of  $\eta \rightarrow 0$ . We assume that there is only one such vanishing eigenvalue in the spectrum of  $\Omega_{E \mp i\eta}$ . For a dissipative system, the assumption is physically reasonable as can be seen by looking at the corresponding weak coupling limit. It then follows that there exists an eigenvector  $x^{(1)}$ , with component  $x^{(1)}(\alpha)$  which fulfil the equation:

$$\lim_{0 < \eta \rightarrow 0} \int d\alpha' \Omega_{E \mp i\eta}(\alpha \alpha') x^{(1)}(\alpha') = \omega^{(1)} x^{(1)}(\alpha) = 0. \quad (3.20)$$

In fact, using the property:

$$\int d\alpha' \Omega_{E \mp i\eta}(\alpha \alpha') = \int d\alpha' \Omega_{E \pm i\eta}(\alpha' \alpha) = \frac{\eta}{\lambda^2} \quad (3.21)$$

one finds a solution of (3.20); namely,

$$x^{(1)}(\alpha) = \text{const.} \quad (3.22)$$

In (3.5), therefore, one may take the limit  $\eta \rightarrow 0$  before integrating over  $\alpha_0$  if one excludes from  $\Omega_{E \mp i\eta}$  ist zero eigenvalue. Indicating this by a tilda, we obtain:

$$\tilde{A}_\pm(\alpha \alpha') = \int d\alpha_0 A(\alpha_0) \tilde{Z}_\pm(\alpha_0 \alpha \alpha'), \quad (3.23)$$

where

$$\begin{aligned} \tilde{Z}_\pm &= \pm \frac{1}{2\pi} \int_{-\infty}^{+\infty} dE \tilde{Z}_{E \mp i0, E \pm i0} \\ &= \pm \frac{1}{2\lambda^2} \int_{-\infty}^{+\infty} dE \tilde{\Omega}_{E \mp i0}^{-1} \mathcal{A}_E (1 + V_{E \mp i0, E \pm i0}). \end{aligned} \quad \left. \right\} (3.24)$$

In the following, however, we omit for simplicity the tilda on  $\tilde{\Omega}_{E \mp i0}^{-1}$ ; of course, the expressions derived are then only meaningful after integration over  $\alpha_0$ . The various contributions to  $\tilde{A}_\pm$  are obtained by integration over  $E$  of the expansion in  $\lambda^n$  of  $\tilde{Z}_{E \mp i0, E \pm i0}$ . The point discussed in section 1 is that we have not been able to perform the integration over  $E$  without expanding first.

#### 4. Perturbative expansion in powers of $\lambda$

From now on we restrict our considerations to  $\tilde{A}_+$  (one easily obtains from it the corresponding results for  $\tilde{A}_-$ ). Before calculating explicitly the various contributions to  $\tilde{Z}_{E-i0, E+i0}$ , we indicate for further reference the series expansions in power of  $\lambda$  of the most important operators occurring in (3.17). We introduce first two new types of functions defined by:

$$\left. \begin{aligned} \{V A_1 V A_2 V \dots A_n V\}_{id} |\alpha\rangle &\equiv |\alpha\rangle \int d\alpha_1 d\alpha_2 \dots d\alpha_n A_1(\alpha_1) A_2(\alpha_2) \dots A_n(\alpha_n) \\ &\quad \times W(\alpha_1 \alpha_2 \dots \alpha_n \alpha) \end{aligned} \right\} \quad (4.1)$$

and

$$\left. \begin{aligned} \langle \alpha | \{V A_1 V A_2 V \dots A_n V\}_{ind} | \alpha' \rangle & \\ &\equiv \int d\alpha_1 d\alpha_2 \dots d\alpha_n A_1(\alpha_1) A_2(\alpha_2) \dots A_n(\alpha_n) V(\alpha_1 \alpha_2 \dots \alpha_n \alpha \alpha') \end{aligned} \right\} \quad (4.2)$$

We call  $V$ -irreducible those contributions in which only sums of  $W$  and  $V$ -functions respectively occur. By  $V$ -reducible are denoted the terms where products of such functions appear. The term of order  $\lambda^n$  in the expansion is indicated by the suffix  $n$  put on the corresponding operator.

In particular looking at (3.11) and (3.12) we find for  $D_{n,l}$  and  $G_{n,l}$  the system of recurrent relations:

$$D_{n,l}(\alpha) = \frac{\lambda^2}{(\varepsilon - l)^2} G_{n-2,l}(\alpha) + \frac{\lambda^4}{(\varepsilon - l)^3} \sum_{m=0}^{n-4} G_{n-m-4,l}(\alpha) G_{m,l}(\alpha) + \dots, \quad (4.3)$$

$$\left. \begin{aligned} G_{n,l}(\alpha) &= \int d\alpha_0 D_{n,l}(\alpha_0) W(\alpha_0 \alpha) - \lambda \sum_{m=0}^{n-1} \int d\alpha_0 d\alpha_1 D_{n-m-1,l}(\alpha_0) \\ &\quad \times D_{m,l}(\alpha_1) W(\alpha_0 \alpha_1 \alpha) + \dots \end{aligned} \right\} \quad (4.4)$$

$\varepsilon_k$  always means  $\varepsilon(\alpha_k)$  and represents the unperturbed energy of the state  $|\alpha_k\rangle$ . The  $V$ -irreducible contribution to  $G_{n,l}$  is:

$$G_{n,l}^v(\alpha) = (-\lambda)^n \int \frac{d\alpha_0 d\alpha_1 \dots d\alpha_n W(\alpha_0 \alpha_1 \dots \alpha_n \alpha)}{(\varepsilon_0 - l)(\varepsilon_1 - l) \dots (\varepsilon_n - l)}. \quad (4.5)$$

From (4.3) and (4.4) the explicit evaluation of the lower terms yields:

$$D_{0,l}(\alpha) = (\varepsilon - l)^{-1}, \quad D_{1,l}(\alpha) = 0, \quad D_{2,l}(\alpha) = \lambda^2 (\varepsilon - l)^{-2} \int \frac{d\alpha_1 W(\alpha_1 \alpha)}{\varepsilon_1 - l} \quad (4.6)$$

and

$$\left. \begin{aligned} G_{0,l}(\alpha) &= \int \frac{d\alpha_1 W(\alpha_1 \alpha)}{\varepsilon_1 - l}, \quad G_{1,l}(\alpha) = -\lambda \int \frac{d\alpha_1 d\alpha_2 W(\alpha_1 \alpha_2 \alpha)}{(\varepsilon_1 - l)(\varepsilon_2 - l)}, \\ G_{2,l}(\alpha) &= \lambda^2 \int \frac{d\alpha_1 d\alpha_2 d\alpha_3 W(\alpha_1 \alpha_2 \alpha_3 \alpha)}{(\varepsilon_1 - l)(\varepsilon_2 - l)(\varepsilon_3 - l)} + \lambda^2 \int \frac{d\alpha_1 d\alpha_2 W(\alpha_2 \alpha_1) W(\alpha_1 \alpha)}{(\varepsilon_1 - l)^2 (\varepsilon_2 - l)} \end{aligned} \right\} \quad (4.7)$$

where the second right-hand side term of the last relation represents the  $V$ -reducible contributions to  $G_{2,l}$ . In the same way one gets from (2.10) the general term  $V_{n,l,l'}$ :

$$\left. \begin{aligned} V_{n,l,l'}(\alpha_0 \alpha \alpha') &= -\lambda V(\alpha \alpha') \{D_{n-1,l}(\alpha) \delta(\alpha_0 - \alpha') + D_{n-1,l'}(\alpha') \delta(\alpha_0 - \alpha)\} \\ &+ \lambda^2 \sum_{m=0}^{n-2} \left\{ V(\alpha_0 \alpha \alpha') D_{n-m-2,l}(\alpha) D_{m,l'}(\alpha') + \int d\alpha_1 V(\alpha_1 \alpha \alpha') \right. \\ &\times [D_{n-m-2,l}(\alpha_1) D_{m,l}(\alpha) \delta(\alpha_0 - \alpha') + D_{n-m-2,l'}(\alpha_1) D_{m,l'}(\alpha') \delta(\alpha_0 - \alpha)] - \dots \left. \right\} \end{aligned} \right\} \quad (4.8)$$

and in particular:

$$V_{1,l,l'}(\alpha_0 \alpha \alpha') = -\lambda V(\alpha \alpha') \left\{ \frac{\delta(\alpha_0 - \alpha')}{\varepsilon - l} + \frac{\delta(\alpha_0 - \alpha)}{\varepsilon' - l'} \right\}. \quad (4.9)$$

The general term  $W_{n,l,l'}$  also looks very similar. We indicate here only the first three terms:

$$\left. \begin{aligned} W_{0,l,l'}(\alpha_0 \alpha) &= W(\alpha_0 \alpha), \\ W_{1,l,l'}(\alpha_0 \alpha) &= -\lambda \int d\alpha_1 \left[ \frac{W(\alpha_1 \alpha_0 \alpha)}{(\varepsilon_1 - l)} + \frac{W(\alpha_0 \alpha_1 \alpha)}{(\varepsilon_1 - l')} \right], \\ W_{2,l,l'}(\alpha_0 \alpha) &= \lambda^2 \int d\alpha_1 d\alpha_2 \left[ \frac{W(\alpha_1 \alpha_2 \alpha_0 \alpha)}{(\varepsilon_1 - l)(\varepsilon_2 - l)} + \frac{W(\alpha_1 \alpha_0 \alpha_2 \alpha)}{(\varepsilon_1 - l)(\varepsilon_2 - l')} + \frac{W(\alpha_0 \alpha_1 \alpha_2 \alpha)}{(\varepsilon_1 - l')( \varepsilon_2 - l')} \right]. \end{aligned} \right\} \quad (4.10)$$

All these are  $V$ -irreducible contributions. The development of  $J_E$  is best obtained from (3.15a) together with (3.21). We have:

$$\left. \begin{aligned} J_{0,E}(\alpha) &= \pi \int d\alpha_0 \delta(\varepsilon_0 - E) W(\alpha_0 \alpha), \\ J_{1,E}(\alpha) &= \pi \int d\alpha_0 \delta(\varepsilon_0 - E) W_{1,E-i_0,E+i_0}(\alpha_0 \alpha), \\ J_{2,E}(\alpha) &= J_{2,E}^v(\alpha) + J_{2,E}'(\alpha) \end{aligned} \right\} \quad (4.11)$$

with

$$J_{2,E}^v(\alpha) = \pi \int d\alpha_0 \delta(\varepsilon_0 - E) W_{2,E-i_0,E+i_0}(\alpha_0 \alpha)$$

and

$$J_{2,E}'(\alpha) = \pi \int d\alpha_0 \Delta_{2,E}(\alpha_0) W(\alpha_0 \alpha)$$

where  $J_{2,E}'$  is the  $V$ -reducible contribution.

$\Delta_{n,E}$  follows directly from  $D_{n,E \pm i_0}$ . The first terms are:

$$\left. \begin{aligned} \Delta_{0,E}(\alpha) &= \delta_E(\alpha) \equiv \delta(\varepsilon - E), & \Delta_{1,E}(\alpha) &= 0 \\ \text{and} \quad \Delta_{2,E}(\alpha) &= \frac{\lambda^2}{2 \pi i} \left\{ (\varepsilon - E - i_0)^{-2} \int \frac{d\alpha_1 W(\alpha_1 \alpha)}{(\varepsilon_1 - E - i_0)} - c.c. \right\}. \end{aligned} \right\} \quad (4.12)$$

As operator in an integral over  $\alpha$ ,  $\Delta_{2,E}(\alpha)$  takes the form:

$$\left. \begin{aligned} \Delta_{2,E}(\alpha) &= \lambda^2 \left[ \left\{ \left( \frac{1}{\varepsilon - E} \right)_P \right\} \left\{ \frac{\partial}{\partial \varepsilon} \right\} \int d\alpha_1 \delta(\varepsilon_1 - E) W(\alpha_1 \alpha) \right. \\ &\quad \left. + \left\{ \delta(\varepsilon - E) \right\} \left\{ \frac{\partial}{\partial \varepsilon} \right\} \int d\alpha_1 \left( \frac{1}{\varepsilon_1 - E} \right)_P W(\alpha_1 \alpha) \right]. \end{aligned} \right\} \quad (4.12a)$$

$\{\partial/\partial\varepsilon\}$  is a differential operator due to a partial integration and acts therefore on all the functions depending on  $\varepsilon$  (and also on  $\alpha$  because  $\alpha = \alpha(\varepsilon)$ ), in the  $\alpha$ -integral, not included in the other  $\{\dots\}$  bracket.

It is also useful to consider the  $V$ -irreducible contribution to  $\Omega_{n, E-i0}$ :

$$\Omega_{n, E-i0}^v = J_{n, E}^v - \pi \delta_E W_{n, E-i0, E+i0}^v. \quad (4.13)$$

The inverse of  $\Omega_{n, E-i0}^v$  obeys the following equations:

$$\left. \begin{aligned} (\Omega_{n, E-i0}^v)^{-1} &= (J_{n, E}^v)^{-1} [1 + \pi \delta_E W_{n, E-i0, E+i0}^v (\Omega_{n, E-i0}^v)^{-1}] \\ &= [1 + (\Omega_{n, E-i0}^v)^{-1} \pi \delta_E W_{n, E-i0, E+i0}^v] (J_{n, E}^v)^{-1}. \end{aligned} \right\} \quad (4.14)$$

One verifies (4.14) by developing  $\Omega_{n, E-i0}^v$  in powers of  $\pi \delta_E W_{n, E-i0, E+i0}^v$ .  $E = \varepsilon$  represents an important particular case for  $\Omega_{E-i0}^v(\alpha_0 \alpha)$ . Let us therefore introduce for it a new symbol  $\Omega$ .

$$\Omega(\alpha_0 \alpha) = \Omega_{\varepsilon-i0}^v(\alpha_0 \alpha). \quad (4.15)$$

Together with

$$\tilde{W}(\alpha_0 \alpha) = \pi \delta(\varepsilon_0 - \varepsilon) W_{\varepsilon-i0, \varepsilon+i0}^v(\alpha_0 \alpha) \quad (4.16)$$

and

$$\Gamma(\alpha) = \int d\alpha_0 \tilde{W}(\alpha_0 \alpha) \quad (4.17)$$

we have

$$\Omega = \Gamma - \tilde{W} \quad (4.18)$$

so that its inverse obeys the relations:

$$\Omega^{-1} = \Gamma^{-1} (1 + \tilde{W} \Omega^{-1}) = (1 + \Omega^{-1} \tilde{W}) \Gamma^{-1}. \quad (4.19)$$

The following properties have to be noted:

$$J_E^v \delta_E = \Gamma \delta_E; \quad (J_E^v)^{-1} \delta_E = \Gamma^{-1} \delta_E, \quad (4.20)$$

$$\begin{aligned} \pi \delta_E W_{E-i0, E+i0}^v \delta_E &= \tilde{W} \delta_E, \\ \Omega_{E-i0}^v \delta_E &= \Omega \delta_E, \\ (\Omega_{E-i0}^v)^{-1} \delta_E &= \Omega^{-1} \delta_E. \end{aligned} \quad (4.21)$$

This last relation (4.21) together with (4.14) allows us to write:

$$(\Omega_{E-i0}^v)^{-1} = [1 + \Omega^{-1} \pi \delta_E W_{E-i0, E+i0}^v] (J_E^v)^{-1}. \quad (4.22)$$

Relations (4.15) to (4.22) are of course also true for the respective  $\lambda^n$ -component.

## 5. Zeroth order contributions to the kernel $\tilde{Z}_+$

We consider separately the diagonal contributions  $\tilde{X}_+$  and the non-diagonal ones  $\tilde{Y}_+$  to  $\tilde{Z}_+$ . The first contributions up to the order  $\lambda^0$ , the second ones up to  $\lambda^{-1}$  only. In the following we omit the explicit indication that our considerations are restricted to positive time.

(a) *Diagonal contributions*

(3.24) yields:

$$\tilde{X} = \frac{1}{2\lambda^2} \int_{-\infty}^{+\infty} dE \Omega_{E-i0}^{-1} \Delta_E. \quad (5.1)$$

The lowest order of (5.1) is in  $\lambda^{-2}$ . Using (4.21) we get for it:

$$\tilde{X}_{-2} = \frac{1}{2\lambda^2} \Omega_0^{-1}. \quad (5.2)$$

The next term  $\tilde{X}_{-1}$  is readily obtained as:

$$\tilde{X}_{-1} = \frac{-1}{2\lambda^2} \Omega_0^{-1} \Omega_1 \Omega_0^{-1}. \quad (5.3)$$

The evaluation of  $\tilde{X}_0$  is a more elaborate one. The zeroth order terms of  $\tilde{X}_{E-i0, E+i0}$  are:

$$\left. \begin{aligned} \tilde{X}_{0, E-i0, E+i0} = \pi \lambda^{-2} \{ & -\Omega_{0, E-i0}^{-1} \Omega_{2, E-i0}^v \Omega_{0, E-i0}^{-1} \\ & + \Omega_{0, E-i0}^{-1} [\Omega_{1, E-i0} \Omega_{0, E-i0}^{-1}]^2 - \Omega_{0, E-i0}^{-1} J_{2, E}^r \Omega_{0, E-i0}^{-1} \\ & + \pi \Omega_{0, E-i0}^{-1} \Delta_{2, E} W \Omega_{0, E-i0}^{-1} \} \Delta_{0, E} + \pi \lambda^{-2} \Omega_{0, E-i0}^{-1} \Delta_{2, E}. \end{aligned} \right\} \quad (5.4)$$

For clarity, the various contributions to  $\tilde{X}_0$  obtained from (5.4) by integration over  $E$  are indicated already in their  $\alpha$ -representation. They are:

$$\tilde{X}_{0,1}(\alpha_0 \alpha) = -\frac{1}{2\lambda^2} \int d\alpha_1 d\alpha_2 \Omega_0^{-1}(\alpha_0 \alpha_1) \Omega_2(\alpha_1 \alpha_2) \Omega_0^{-1}(\alpha_2 \alpha), \quad (5.5)$$

$$\left. \begin{aligned} \tilde{X}_{0,2}(\alpha_0 \alpha) = \frac{1}{2\lambda^2} \int d\alpha_1 d\alpha_2 d\alpha_3 d\alpha_4 \Omega_0^{-1}(\alpha_0 \alpha_1) \Omega_1(\alpha_1 \alpha_2) \\ \times \Omega_0^{-1}(\alpha_2 \alpha_3) \Omega_1(\alpha_3 \alpha_4) \Omega_0^{-1}(\alpha_4 \alpha), \end{aligned} \right\} \quad (5.6)$$

$$\left. \begin{aligned} \tilde{X}_{0,3}(\alpha_0 \alpha) = -\frac{\pi}{2} \int d\alpha_1 d\alpha_2 d\alpha_3 \Omega_0^{-1}(\alpha_0 \alpha_1) \Omega_0^{-1}(\alpha_1 \alpha) \\ \times \left[ \left( \frac{1}{\varepsilon_3 - \varepsilon_1} \right)_P \delta(\varepsilon_2 - \varepsilon_1) + \delta(\varepsilon_3 - \varepsilon_1) \left( \frac{1}{\varepsilon_2 - \varepsilon_1} \right)_P \right] \frac{\partial W(\alpha_3 \alpha_2) W(\alpha_2 \alpha_1)}{\partial \varepsilon_2}, \end{aligned} \right\} \quad (5.7)$$

$$\left. \begin{aligned} \tilde{X}_{0,4}(\alpha_0 \alpha) = \frac{\pi}{2\lambda^2} \int d\alpha_1 d\alpha_2 \Omega_{0, \varepsilon-i0}^{-1}(\alpha_0 \alpha_1) \Delta_{2, \varepsilon}(\alpha_1) W(\alpha_1 \alpha_2) \Omega_0^{-1}(\alpha_2 \alpha) \\ = \frac{\pi}{2} \int d\alpha_1 d\alpha_2 \delta(\varepsilon_1 - \varepsilon) \frac{\partial}{\partial \varepsilon_1} (\Omega_{0, \varepsilon-i0}^{-1}(\alpha_0 \alpha_1) K_{0, \varepsilon}(\alpha_1) W(\alpha_1 \alpha_2)) \Omega_0^{-1}(\alpha_2 \alpha) \\ + \frac{1}{2} \operatorname{Re} \int \frac{d\alpha_1 W(\alpha_0 \alpha_1) \Omega_0^{-1}(\alpha_1 \alpha)}{(\varepsilon_0 - \varepsilon_1 - i0)^2} + \frac{1}{2} \operatorname{Re} \int d\alpha_1 d\alpha_2 d\alpha_3 \Omega_0^{-1}(\alpha_0 \alpha_1) \\ \times \frac{\pi \delta(\varepsilon_1 - \varepsilon) W(\alpha_1 \alpha_2) W(\alpha_2 \alpha_3) \Omega_0^{-1}(\alpha_3 \alpha)}{(\varepsilon_2 - \varepsilon_3 - i0)^2}. \end{aligned} \right\} \quad (5.8)$$

This last result was obtained by using (3.14) and (4.22). Analogously we evaluate the last contribution:

$$\left. \begin{aligned} \tilde{X}_{0,5}(\alpha_0 \alpha) &= \frac{1}{2 \lambda^2} \int_{-\infty}^{+\infty} dE \Omega_{0,E-i0}^{-1}(\alpha_0 \alpha) \Delta_{2,E}(\alpha) \\ &= -\frac{1}{2} \left\{ \frac{\partial}{\partial E} (\Omega_{0,E-i0}^{-1}(\alpha_0 \alpha) K_{0,E}(\alpha)) \right\}_{E=\varepsilon} + \frac{1}{2} \operatorname{Re} \int \frac{d\alpha_1 \Omega_0^{-1}(\alpha_0 \alpha_1) W(\alpha_1 \alpha)}{(\varepsilon - \varepsilon_1 - i0)^2}. \end{aligned} \right\} \quad (5.9)$$

Now:

$$\left. \begin{aligned} \frac{\partial \Omega_{0,E-i0}^{-1}(\alpha_0 \alpha)}{\partial E} &= \int d\alpha_1 d\alpha_2 \pi \delta(\varepsilon_1 - E) \frac{\partial}{\partial \varepsilon_1} (\Omega_{0,E-i0}^{-1}(\alpha_0 \alpha_1) W(\alpha_1 \alpha_2)) \\ &\times \Omega_{0,E-i0}^{-1}(\alpha_2 \alpha) - \int d\alpha_1 d\alpha_2 \Omega_{0,E-i0}^{-1}(\alpha_0 \alpha_1) \Omega_{0,E-i0}^{-1}(\alpha_1 \alpha) \pi \delta(\varepsilon_2 - E) \frac{\partial W(\alpha_2 \alpha_1)}{\partial \varepsilon_2} \end{aligned} \right\} \quad (5.10)$$

and

$$\frac{\partial K_{0,E}(\alpha)}{\partial E} = \operatorname{Re} \int \frac{d\alpha_1 W(\alpha_1 \alpha)}{(\varepsilon_1 - E + i0)^2} \quad (5.11)$$

so that for (5.9) we get:

$$\left. \begin{aligned} \tilde{X}_{0,5}(\alpha_0 \alpha) &= \frac{\pi}{2} \int d\alpha_1 d\alpha_2 \Omega_0^{-1}(\alpha_0 \alpha_1) \Omega_0^{-1}(\alpha_1 \alpha) \delta(\varepsilon_2 - \varepsilon_1) \frac{\partial W(\alpha_2 \alpha_1)}{\partial \varepsilon_2} \\ &\times \int \frac{d\alpha_3 W(\alpha_3 \alpha)}{(\varepsilon_3 - \varepsilon)_P} - \frac{\pi}{2} \int d\alpha_1 d\alpha_2 \delta(\varepsilon_1 - \varepsilon) \frac{\partial}{\partial \varepsilon_1} (\Omega_{0,E-i0}^{-1}(\alpha_0 \alpha_1) W(\alpha_1 \alpha_2)) \\ &\times \Omega_0^{-1}(\alpha_2 \alpha) K_{0,\varepsilon}(\alpha) - \frac{1}{2} \Omega_0^{-1}(\alpha_0 \alpha) \operatorname{Re} \int \frac{d\alpha_1 W(\alpha_1 \alpha)}{(\varepsilon_1 - \varepsilon + i0)^2} \\ &+ \frac{1}{2} \operatorname{Re} \int \frac{d\alpha_1 \Omega_0^{-1}(\alpha_0 \alpha_1) W(\alpha_1 \alpha)}{(\varepsilon - \varepsilon_1 + i0)^2}. \end{aligned} \right\} \quad (5.12)$$

### (b) Non-diagonal contributions

The lowest order contribution is already of order  $\lambda^{-1}$ :

$$\left. \begin{aligned} \tilde{Y}_{-1}(\alpha_0 \alpha \alpha') \\ &= \frac{1}{2 \lambda} V(\alpha \alpha') \left\{ [\Omega_0^{-1}(\alpha_0 \alpha) - \Omega_0^{-1}(\alpha_0 \alpha')] \left[ \left( \frac{1}{\varepsilon - \varepsilon'} \right)_P - i \pi \delta(\varepsilon - \varepsilon') \right] \right\}. \end{aligned} \right\} \quad (5.13)$$

The results obtained so far can be applied to a large number of physical cases. We show how this can be done by using these results for the evaluation of the electrical conductivity in metals.

## 6. Electrical conductivity tensor for spherically symmetric elastic scattering by impurities

The electrical conductivity tensor of metals has already been calculated by CHESTER and THELLUNG<sup>1)</sup> to the lowest order in the perturbation, and by VERBOVEN<sup>4)</sup> to the zeroth one. In both papers time-dependent perturbation has been used. To illustrate the alternative approach represented by the resolvent method, we apply to the same problem the formalism developed here, which is better suited for further

calculations to higher order corrections. Comparison between the results already published and the present ones is made only in the next section, as it requires some supplementary calculations.

We start by considering the symmetrized Kubo formula for the conductivity ((2.4 of CHESTER and THELLUNG's<sup>1</sup>) and (2.24) of VERBOVEN's<sup>4</sup>) papers), which is already reduced to the one-electron approximation.

$$\sigma^{\mu\nu} = -t r_e \left\{ \lim_{T \rightarrow \infty} \int_0^T dt \frac{1}{2} [j_t^\mu j_0^\nu + j_0^\mu j_t^\nu] \frac{\partial f}{\partial H} \right\}. \quad (6.1)$$

The trace is taken over a complete set of one-electron wave functions. Considered here are the eigenfunctions  $|\mathbf{k}\rangle$  of  $H_0$ , where  $\mathbf{k}$  is the electron wave vector with energy  $\varepsilon(\mathbf{k})$ . For contributions restricted to a single band,  $j_0^\nu$  is diagonal with respect to  $|\mathbf{k}\rangle$ . In this representation, (6.1) becomes:

$$\sigma^{\mu\nu} = -\frac{1}{2} \int d\mathbf{k}_0 d\mathbf{k} d\mathbf{k}' \{j_0^\mu(\mathbf{k}_0) j_0^\nu(\mathbf{k}') + j_0^\nu(\mathbf{k}) j_0^\mu(\mathbf{k}_0)\} \tilde{Z}(\mathbf{k}_0 \mathbf{k} \mathbf{k}') \frac{\partial f}{\partial H}(\mathbf{k}' \mathbf{k}), \quad (6.2)$$

where  $\tilde{Z}$  represents the dynamical and  $\partial f/\partial H \equiv S$  the statistical factor.

Clearly the expression (6.2) contains a factor  $\langle \mathbf{k} | \mathbf{k} \rangle$  which diverges in the limit of an infinite system. This is however not a significant difficulty, and it can be eliminated by an appropriate definition of the trace<sup>8</sup>) or by using reduced expressions<sup>7)9</sup>). In the one-electron case it is sufficient to divide by  $\langle \mathbf{k} | \mathbf{k} \rangle$  on the right-hand side of (6.2).

We consider  $\sigma^{\mu\nu}$  developed in powers of  $\lambda$ :

$$\sigma^{\mu\nu} = \sigma_{-2}^{\mu\nu} + \sigma_{-1}^{\mu\nu} + \sigma_0^{\mu\nu} + \dots \quad (6.3)$$

i.e. we expand the dynamical and the statistical factors respectively. Observing that to the lowest order two factors are diagonal, whereas to the first order the statistical factor is non-diagonal, we obtain:

$$\left. \begin{aligned} \sigma^{\mu\nu} = & -\frac{1}{2} \int d\mathbf{k}_0 d\mathbf{k} d\mathbf{k}' \{j_0^\mu(\mathbf{k}_0) j_0^\nu(\mathbf{k}') + j_0^\nu(\mathbf{k}) j_0^\mu(\mathbf{k}_0)\} \\ & \times \{[\tilde{X}_{-2}(\mathbf{k}_0 \mathbf{k}) + \tilde{X}_{-1}(\mathbf{k}_0 \mathbf{k}) + \tilde{X}_0(\mathbf{k}_0 \mathbf{k})] S_0(\mathbf{k} \mathbf{k}) \delta(\mathbf{k} - \mathbf{k}') \\ & + \tilde{X}_{-2}(\mathbf{k}_0 \mathbf{k}) S_2(\mathbf{k} \mathbf{k}) \delta(\mathbf{k} - \mathbf{k}') + \tilde{Y}_{-1}(\mathbf{k}_0 \mathbf{k} \mathbf{k}') S_1(\mathbf{k}' \mathbf{k}) + \dots\} / \langle \mathbf{k} | \mathbf{k} \rangle. \end{aligned} \right\} \quad (6.4)$$

With the formula derived in section 5, (6.4) already gives the conductivity tensor to the zeroth order for the general case of elastic scattering by impurities. For the particularly simple case of spherically symmetric scattering centres, (6.4) can be further simplified. From now on we therefore restrict our considerations to this case, for which we derive first some general relations.

One sees from (4.17) that  $\Gamma(\mathbf{k})$  becomes a function of the energy  $\varepsilon$  only and does not depend more on the direction of  $\mathbf{k}$ ; the same is true for  $\Gamma^1(\mathbf{k})$  which is defined by the relation:

$$\int d\mathbf{k}_0 j_0^\mu(\mathbf{k}_0) \tilde{W}(\mathbf{k}_0 \mathbf{k}) = \int d\mathbf{k}_0 \tilde{W}(\mathbf{k} \mathbf{k}_0) j_0^\mu(\mathbf{k}_0) = \Gamma^1(\mathbf{k}) j_0^\mu(\mathbf{k}) = \Gamma^1(\varepsilon) j_0^\mu(\mathbf{k}). \quad (6.5)$$

Introducing a general relaxation time  $\tau(\varepsilon)$  by:

$$\frac{1}{\tau(\varepsilon)} = 2\lambda^2 [\Gamma(\varepsilon) - \Gamma^1(\varepsilon)], \quad (6.6)$$

together with (6.5) we get:

$$\int d\mathbf{k}_0 j_0^\mu(\mathbf{k}_0) \Omega(\mathbf{k}_0 \mathbf{k}) = \int d\mathbf{k}_0 \Omega(\mathbf{k} \mathbf{k}_0) j_0^\mu(\mathbf{k}_0) = \frac{1}{2\lambda^2 \tau(\varepsilon)} j_0^\mu(\mathbf{k}) \quad (6.7)$$

and also:

$$\int d\mathbf{k}_0 j_0^\mu(\mathbf{k}_0) \Omega^{-1}(\mathbf{k}_0 \mathbf{k}) = \int d\mathbf{k}_0 \Omega^{-1}(\mathbf{k} \mathbf{k}_0) j_0^\mu(\mathbf{k}_0) = 2\lambda^2 \tau(\varepsilon) j_0^\mu(\mathbf{k}). \quad (6.8)$$

This last equation can be verified, according to (4.18), by expansion of  $\Omega^{-1}$  in powers of  $\tilde{W}$  and integration over  $\mathbf{k}_0$  of its  $(\mathbf{k}_0 \mathbf{k})$ -matrix elements. The relations given above are of course also valid between corresponding  $\lambda^n$ -terms.

Finally, we note that:

$$j_0^\mu(-\mathbf{k}) = -j_0^\mu(\mathbf{k}) \quad (6.9)$$

and therefore:

$$\int d\mathbf{k} j_0^\mu(\mathbf{k}) f(\varepsilon) = 0 \quad (6.10)$$

for every function  $f(\varepsilon)$  independent of the direction of  $\mathbf{k}$ . This property, together with  $\Delta_E(\mathbf{k}) = \Delta_E(\varepsilon)$ , ensures that

$$\lim_{t \rightarrow \infty} j_t^\mu(\mathbf{k} \mathbf{k}') = \int_{-\infty}^{+\infty} dE \int d\mathbf{k}_0 j_0^\mu(\mathbf{k}_0) \Delta_E(\mathbf{k}_0) \frac{\Omega_E(\mathbf{k} \mathbf{k}')}{\int d\mathbf{k}_1 \Delta_E(\mathbf{k}_1)} = 0 \quad (6.11)$$

which is a necessary condition for the existence of (3.1) for  $A_t = j_t^\mu$ .

It is now very easy to write down the various contributions to the conductivity tensor. To the lowest order, using (5.2) and (6.6), we get the known result:

$$\sigma_{-2}^{\mu\nu} = - \int d\mathbf{k} \tau_0(\varepsilon) j_0^\mu(\mathbf{k}) j_0^\nu(\mathbf{k}) \frac{\partial f}{\partial \varepsilon} \quad (6.12)$$

where

$$\frac{\partial f}{\partial H_0} |\mathbf{k}\rangle = |\mathbf{k}\rangle \frac{\partial f}{\partial \varepsilon}.$$

In (6.12), and in the following corrections as well,  $\tau_n(\varepsilon)$  is defined by (6.6) if one replaces  $\Gamma(\varepsilon)$  and  $\Gamma^1(\varepsilon)$  by the corresponding  $\lambda^n$ -terms. In the same manner, (5.3) gives us the first order correction.

$$\sigma_{-1}^{\mu\nu} = \int d\mathbf{k} \tau_0^2(\varepsilon) \tau_1^{-1}(\varepsilon) j_0^\mu(\mathbf{k}) j_0^\nu(\mathbf{k}) \frac{\partial f}{\partial \varepsilon}. \quad (6.13)$$

A number of zero order corrections arises from the various  $\tilde{X}_{0,\nu}$  terms. The first three are directly obtained by putting (5.5), (5.6) and (5.7) in (6.4), and by making use of the symmetry properties indicated above. We get:

$$\sigma_{0,1}^{\mu\nu} = \int d\mathbf{k} \tau_0^2(\varepsilon) \tau_2^{-1}(\varepsilon) j_0^\mu(\mathbf{k}) j_0^\nu(\mathbf{k}) \frac{\partial f}{\partial \varepsilon}, \quad (6.14)$$

$$\sigma_{0,2}^{\mu\nu} = - \int d\mathbf{k} \tau_0^3(\varepsilon) \tau_1^{-2}(\varepsilon) j_0^\mu(\mathbf{k}) j_0^\nu(\mathbf{k}) \frac{\partial f}{\partial \varepsilon}, \quad (6.15)$$

$$\left. \begin{aligned} \sigma_{0,3}^{\mu} &= 2 \lambda^4 \int d\mathbf{k} \tau_0^2(\varepsilon) j_0^{\mu}(\mathbf{k}) j_0^{\nu}(\mathbf{k}) \frac{\partial f}{\partial \varepsilon} \\ &\times \int d\mathbf{k}_0 d\mathbf{k}_1 \left[ \left( \frac{1}{\varepsilon_1 - \varepsilon} \right)_P \pi \delta(\varepsilon_0 - \varepsilon) + \pi \delta(\varepsilon_1 - \varepsilon) \left( \frac{1}{\varepsilon_0 - \varepsilon} \right)_P \right] \frac{\partial W(\mathbf{k}_1 \mathbf{k}_0) W(\mathbf{k}_0 \mathbf{k})}{\partial \varepsilon_0} . \end{aligned} \right\} \quad (6.16)$$

For the next group of terms it is worthwhile to take  $\tilde{X}_{0,4}$  and  $\tilde{X}_{0,5}$  together, i. e. (5.8) and (5.12). Before indicating the result, we consider the partial contribution:

$$\begin{aligned} I &= \frac{1}{2} \pi^* \int d\mathbf{k}_0 d\mathbf{k}_1 d\mathbf{k}_2 j_0^{\mu}(\mathbf{k}_0) \delta(\varepsilon_1 - \varepsilon) \frac{\partial}{\partial \varepsilon_1} \\ &\times \{ \Omega_{0,\varepsilon-i0}^{-1}(\mathbf{k}_0 \mathbf{k}_1) W(\mathbf{k}_1 \mathbf{k}_2) \Omega_0^{-1}(\mathbf{k}_2 \mathbf{k}) [K_{0,\varepsilon}(\mathbf{k}_1) - K_{0,\varepsilon}(\mathbf{k})] \} \end{aligned}$$

giving, after Taylor-expansion of  $K_{0,\varepsilon}(\varepsilon_1)$  in the neighbourhood of  $K_{0,\varepsilon}(\varepsilon)$ , the result

$$I = 2 \lambda^4 \int \frac{d\mathbf{k}_1}{(\varepsilon_1 - \varepsilon)_P} \frac{\partial W(\mathbf{k}_1 \mathbf{k})}{\partial \varepsilon} \tau_0^2(\varepsilon) \Gamma_0^1(\varepsilon) j_0^{\mu}(\mathbf{k}) . \quad (6.17)$$

Making use of (6.17) and regrouping the terms in such a way as to facilitate a comparison with Verboven's result, we obtain for

$$\sigma_{0,(4,5)}^{\mu\nu} = \sigma_{0,4}^{\mu\nu} + \sigma_{0,5}^{\mu\nu} + \sigma_{0,6}^{\mu\nu} + \sigma_{0,7}^{\mu\nu}$$

the following contributions:

$$\sigma_{0,4}^{\mu\nu} = - \frac{\lambda^2}{2} \text{Re} \int \frac{d\mathbf{k}_0 d\mathbf{k} W(\mathbf{k}_0 \mathbf{k})}{(\varepsilon_0 - \varepsilon - i0)^2} [\tau_0(\varepsilon) + \tau_0(\varepsilon_0)] [j_0^{\mu}(\mathbf{k}_0) j_0^{\nu}(\mathbf{k}) + j_0^{\mu}(\mathbf{k}) j_0^{\nu}(\mathbf{k}_0)] \frac{\partial f}{\partial \varepsilon} , \quad (6.18)$$

$$\sigma_{0,5}^{\mu\nu} = - 2 \lambda^4 \text{Re} \int d\mathbf{k}_0 d\mathbf{k} d\mathbf{k}_1 \tau_0^2(\varepsilon_0) j_0^{\mu}(\mathbf{k}_0) j_0^{\nu}(\mathbf{k}) \frac{\partial f}{\partial \varepsilon} \pi \delta(\varepsilon_0 - \varepsilon) \frac{W(\mathbf{k}_0 \mathbf{k}_1) W(\mathbf{k}_1 \mathbf{k})}{(\varepsilon_1 - \varepsilon - i0)^2} , \quad (6.19)$$

$$\left. \begin{aligned} \sigma_{0,6}^{\mu\nu} &= - 2 \lambda^4 \int d\mathbf{k}_0 d\mathbf{k} \tau_0^2(\varepsilon) j_0^{\mu}(\mathbf{k}) j_0^{\nu}(\mathbf{k}) \frac{\partial f}{\partial \varepsilon} \pi \delta(\varepsilon - \varepsilon_0) \frac{\partial W(\mathbf{k}_0 \mathbf{k})}{\partial \varepsilon_0} \\ &\times \int \frac{d\mathbf{k}_1 W(\mathbf{k}_1 \mathbf{k})}{(\varepsilon_1 - \varepsilon)_P} + \lambda^2 \text{Re} \int d\mathbf{k}_0 d\mathbf{k} \tau_0(\varepsilon) j_0^{\mu}(\mathbf{k}) j_0^{\nu}(\mathbf{k}) \frac{\partial f}{\partial \varepsilon} \frac{W(\mathbf{k}_0 \mathbf{k})}{(\varepsilon_0 - \varepsilon + i0)^2} , \end{aligned} \right\} \quad (6.20)$$

$$\sigma_{0,7}^{\mu\nu} = - 2 \lambda^4 \int d\mathbf{k} \tau_0^2(\varepsilon) \Gamma_0^1(\varepsilon) j_0^{\mu}(\mathbf{k}) j_0^{\nu}(\mathbf{k}) \frac{\partial f}{\partial \varepsilon} \int \frac{d\mathbf{k}_1}{(\varepsilon_1 - \varepsilon)_P} \frac{\partial W(\mathbf{k}_1 \mathbf{k})}{\partial \varepsilon} . \quad (6.21)$$

The remaining two zero-order corrections are those related to the higher order terms of the statistical factor. They have already been indicated by CHESTER and THELLUNG<sup>1</sup>:

$$S_1(\mathbf{k}' \mathbf{k}) = \lambda V(\mathbf{k}' \mathbf{k}) \frac{f'(\varepsilon') - f'(\varepsilon)}{\varepsilon' - \varepsilon} , \quad (6.22)$$

$$S_2(\mathbf{k} \mathbf{k}) = \lambda^2 \int d\mathbf{k}_0 \langle \mathbf{k} | \mathbf{k} \rangle W(\mathbf{k}_0 \mathbf{k}) \left\{ \frac{f''(\varepsilon)}{\varepsilon - \varepsilon_0} - \frac{f'(\varepsilon) - f'(\varepsilon_0)}{(\varepsilon - \varepsilon_0)^2} \right\} . \quad (6.23)$$

(6.22) together with (5.13) yield the next correction: only the principal value term in (5.13) gives a non-vanishing contribution:

$$\left. \begin{aligned} \sigma_{0,8}^{\mu\nu} &= \frac{1}{2} \lambda^2 \int d\mathbf{k}_0 d\mathbf{k} W(\mathbf{k}_0 \mathbf{k}) \frac{f'(\varepsilon_0) - f'(\varepsilon)}{\varepsilon_0 - \varepsilon} \left( \frac{1}{\varepsilon_0 - \varepsilon} \right)_P \\ &\times \{ j_0^{\mu}(\mathbf{k}) [j_0^{\nu}(\mathbf{k}) + j_0^{\nu}(\mathbf{k}_0)] \tau_0(\varepsilon) - j_0^{\nu}(\mathbf{k}_0) [j_0^{\mu}(\mathbf{k}) + j_0^{\mu}(\mathbf{k}_0)] \tau_0(\varepsilon_0) \} . \end{aligned} \right\} \quad (6.24)$$

The last correction is essentially the same as (6.12) with the only difference that now  $S_2(\mathbf{k} \mathbf{k})$  replaces  $S_0(\mathbf{k} \mathbf{k})$ :

$$\sigma_{0,9}^{\mu\nu} = -\lambda^2 \int d\mathbf{k}_0 d\mathbf{k} \tau_0(\varepsilon) j_0^\mu(\mathbf{k}) j_0^\nu(\mathbf{k}) W(\mathbf{k}_0 \mathbf{k}) \left\{ \frac{f''(\varepsilon)}{\varepsilon - \varepsilon_0} - \frac{f'(\varepsilon) - f'(\varepsilon_0)}{(\varepsilon - \varepsilon_0)^2} \right\}. \quad (6.25)$$

### 7. Comparison with Verboven's result

We here consider VERBOVEN's<sup>4)</sup> calculation of the conductivity tensor as in his paper he already discussed that of CHESTER and THELLUNG. The present comparison requires some small changes in the notation and a few additional calculations. To avoid confusion, we label VERBOVEN's equations as in his paper, but with the numbers in square brackets, and we keep to his notation at least partially.

One immediately verifies that [3.24] and (6.12) represent the same result

$$[3.24] \quad \sigma_{\mu\nu}^{(-2)} = \sigma_{-2}^{\mu\nu}. \quad (6.12)$$

Also [4.6] and (6.13) give the same result:

$$[4.6] \quad \delta\sigma_{\mu\nu}^{(-1)} = \sigma_{-1}^{\mu\nu} \quad (6.13)$$

and

$$\Gamma'(\varepsilon) - \Gamma'_1(\varepsilon) = \Gamma_1(\varepsilon) - \Gamma_1^1(\varepsilon) = (2\lambda^2 \tau_1(\varepsilon))^{-1}.$$

Inspection of [4.8] shows that in fact  $\delta\sigma_{\mu\nu}^{(0,1)}$  has the wrong sign. With the correct one it gives the same result as (6.24):

$$[4.8] \quad -\delta\sigma_{\mu\nu}^{0,1} = \sigma_{0,8}^{\mu\nu}. \quad (6.24)$$

There are a number of zero order corrections which are evidently equal and need no further comments. Let us only indicate the correspondance:

$$[4.10] \quad \delta\sigma_{\mu\nu}^{(0,2)} = \sigma_{0,9}^{\mu\nu}, \quad (6.25)$$

$$[4.12] \quad \delta\sigma_{\mu\nu}^{(0,3)} = \sigma_{0,2}^{\mu\nu}, \quad (6.15)$$

$$[4.15] \quad \delta\sigma_{\mu\nu}^{(0,4)} = \sigma_{0,1}^{\mu\nu}, \quad (6.14)$$

$$[4.24] \quad \delta\sigma_{\mu\nu}^{(0,5)} = \sigma_{0,3}^{\mu\nu}. \quad (6.16)$$

For the check of this last relation one simply verifies that:

$$[4.22] \quad \lambda^2 \bar{\Gamma}(\varepsilon) = J_{2,\varepsilon}^r(\mathbf{k}). \quad (4.11)$$

Further

$$[5.20] \quad \delta\sigma_{\mu\nu}^{(0,8)} = \sigma_{0,4}^{\mu\nu}, \quad (6.18)$$

$$[5.21] \quad \delta\sigma_{\mu\nu}^{(0,9)} = \sigma_{0,5}^{\mu\nu}. \quad (6.19)$$

Comparison between the remaining corrections requires some simplifications. We may write VERBOVEN's definitions of  $A$ ,  $\Gamma$  and  $\bar{\Gamma}$  in our notation as follows:

$$[5.6] \quad A(\varepsilon) = \int \frac{d\mathbf{k}_1 W(\mathbf{k} \mathbf{k}_1)}{(\varepsilon_1 - \varepsilon - i 0)^2},$$

$$[3.12], [3.13] \quad \Gamma(\varepsilon) + i \Delta(\varepsilon) = -i \int \frac{d\mathbf{k}_1 W(\mathbf{k}_1 \mathbf{k})}{(\varepsilon_1 - \varepsilon - i 0)}$$

and therefore

$$[5.7] \quad \bar{\Gamma}(\varepsilon) + i \bar{\Delta}(\varepsilon) = i \int \frac{d\mathbf{k}_1 W(\mathbf{k} \mathbf{k}_1)}{(\varepsilon_1 - \varepsilon - i 0)^2} \int \frac{d\mathbf{k}_2 W(\mathbf{k}_2 \mathbf{k})}{(\varepsilon_2 - \varepsilon - i 0)}, \quad (7.1)$$

so that

$$\bar{\Gamma}(\varepsilon) + \Gamma(\varepsilon) (A + A^*) = \text{Im} \int \frac{d\mathbf{k}_1 W(\mathbf{k}_1 \mathbf{k})}{(\varepsilon_1 - \varepsilon - i 0)} \int \frac{d\mathbf{k}_2 W(\mathbf{k} \mathbf{k}_2)}{(\varepsilon_2 - \varepsilon + i 0)^2}$$

where  $\text{Im}$  means imaginary part. In this way we obtain for  $\delta\sigma_{\mu\nu}^{(0,6)}$ :

$$\delta\sigma_{\mu\nu}^{(0,6)} = \lambda^2 \int d\mathbf{k} j_0^\mu(\mathbf{k}) j_0^\nu(\mathbf{k}) \left. \frac{\partial f}{\partial \varepsilon} \tau_0(\varepsilon) \left\{ \text{Re} \int \frac{d\mathbf{k}_2 W(\mathbf{k} \mathbf{k}_2)}{(\varepsilon_2 - \varepsilon + i 0)^2} \right. \right. \\ \left. \left. - 2 \lambda^2 \tau_0(\varepsilon) \int \frac{d\mathbf{k}_1 W(\mathbf{k}_1 \mathbf{k})}{(\varepsilon_1 - \varepsilon)_P} \int d\mathbf{k}_2 \pi \delta(\varepsilon_2 - \varepsilon) \frac{\partial W(\mathbf{k} \mathbf{k}_2)}{\partial \varepsilon_2} \right\} \right. \\ \left. + 2 \lambda^2 \tau_0(\varepsilon) \Gamma_1(\varepsilon) \text{Re} \int \frac{d\mathbf{k}_2 W(\mathbf{k} \mathbf{k}_2)}{(\varepsilon_2 - \varepsilon + i 0)^2} \right\}. \quad (7.2)$$

Observing that:

$$[3.13] \quad \Delta(\varepsilon) = -\text{Re} \int \frac{d\mathbf{k}_1 W(\mathbf{k}_1 \mathbf{k})}{(\varepsilon_1 - \varepsilon - i 0)},$$

for VERBOVEN's  $\Delta'_E(E)$  we get:

$$\frac{\partial \Delta(\varepsilon)}{\partial \varepsilon} = -\text{Re} \int \frac{d\mathbf{k}_1 W(\mathbf{k}_1 \mathbf{k})}{(\varepsilon_1 - \varepsilon - i 0)^2} - \int \frac{d\mathbf{k}_1}{(\varepsilon_1 - \varepsilon)_P} \frac{\partial W(\mathbf{k}_1 \mathbf{k})}{\partial \varepsilon}. \quad (7.3)$$

Keeping this result in mind, and adding  $\delta\sigma_{\mu\nu}^{(0,6)}$  and  $\delta\sigma_{\mu\nu}^{(0,7)}$  together, we obtain:

$$\delta\sigma_{\mu\nu}^{(0,6)} + \delta\sigma_{\mu\nu}^{(0,7)} = \int d\mathbf{k} j_0^\mu(\mathbf{k}) j_0^\nu(\mathbf{k}) \frac{\partial f}{\partial \varepsilon} \left\{ \lambda^2 \tau_0(\varepsilon) \text{Re} \int \frac{d\mathbf{k}_2 W(\mathbf{k} \mathbf{k}_2)}{(\varepsilon_2 - \varepsilon + i 0)^2} - 2 \lambda^4 \tau_0^2(\varepsilon) \right. \\ \left. \times \int \frac{d\mathbf{k}_1 W(\mathbf{k}_1 \mathbf{k})}{(\varepsilon_1 - \varepsilon)_P} \int d\mathbf{k}_2 \pi \delta(\varepsilon_2 - \varepsilon) \frac{\partial W(\mathbf{k} \mathbf{k}_2)}{\partial \varepsilon_2} - 2 \lambda^4 \tau_0^2(\varepsilon) \Gamma_1(\varepsilon) \int \frac{d\mathbf{k}_1}{(\varepsilon_1 - \varepsilon)_P} \frac{\partial W(\mathbf{k}_1 \mathbf{k})}{\partial \varepsilon} \right\},$$

giving:

$$[5.9], [5.16] \quad \delta\sigma_{\mu\nu}^{(0,6)} + \delta\sigma_{\mu\nu}^{(0,7)} = \sigma_{0,6}^{\mu\nu} + \sigma_{0,7}^{\mu\nu}. \quad (6.20), (6.21)$$

The comparison shows that the only term missing is the non-Markoffian  $\delta\sigma_{\mu\nu}^{(0,10)}$  one, of [5.23]. This is due to the fact that actually only the real part [4.1] goes into the Kubo formula, and therefore  $\delta\sigma_{\mu\nu}^{(0,10)}$  has to be omitted<sup>5)</sup>.

### 8. Concluding remarks

By the present calculation we have checked the zeroth-order expression for the conductivity tensor, previously derived by VERBOVEN<sup>4</sup>). It is also possible to evaluate further higher order corrections with the same formalism. This implies, however, a non-negligible amount of calculation. In particular, we have not yet been able to obtain explicit expressions for the general  $n$ -th order contributions, because of the non-trivial integration over  $E$ , which is needed for it. Even so, we can discuss the general nature of such contributions simply by looking at (3.5), (3.23) and (6.2), respectively. What we found is in agreement with the Balescu theorem, which states that transport coefficients can always be calculated from a Markoffian Boltzmann-like equation<sup>10</sup>). In order to show this in our particular case, we follow a suggestion made to us by SWENSON<sup>11</sup>): performing the calculation on the basis of the Markoffian approximation of the general master equation, one obtains the same result as that (3.5) which is derived above without such an approximation.

We start by considering the general master equation in the following form:

$$Z_{E,t}(\alpha_0 \alpha \alpha') = \bar{h}_{E,t}(\alpha_0 \alpha \alpha') + 2\pi\lambda^2 \int_0^t dt_1 \int d\alpha_1 \bar{w}_{E,t-t_1}(\alpha_0 \alpha_1) Z_{E,t_1}(\alpha_1 \alpha \alpha') \quad (8.1)$$

where

$$\left. \begin{aligned} \bar{h}_{E,t}(\alpha_0 \alpha \alpha') &= \frac{s(t)}{2\pi^2} \int_{\gamma} dl e^{2ilt} D_{E+l}(\alpha_0) D_{E-l}(\alpha_0) \\ &\quad \times [\delta(\alpha_0 - \alpha) \delta(\alpha - \alpha') + V_{E+l, E-l}(\alpha_0 \alpha \alpha')] \end{aligned} \right\} \quad (8.2)$$

$$\bar{w}_{E,t}(\alpha_0 \alpha) = \frac{1}{2\pi^2} \int_{\gamma} dl e^{2ilt} D_{E+l}(\alpha_0) D_{E-l}(\alpha_0) W_{E+l, E-l}(\alpha_0 \alpha), \quad (8.3)$$

$$Z_{E,t}(\alpha_0 \alpha \alpha') = \frac{s(t)}{2\pi^2} \int_{\gamma} dl e^{2ilt} Z_{E+l, E-l}(\alpha_0 \alpha \alpha') \quad \left. \right\} \quad (8.4)$$

and

$$Z_t(\alpha_0 \alpha \alpha') = \int_{-\infty}^{+\infty} dE Z_{E,t}(\alpha_0 \alpha \alpha') \quad \left. \right\} \quad (8.4)$$

One obtains (8.1) for  $t \neq 0$ , directly from (2.8) by standard calculation<sup>2</sup>)<sup>3</sup>).

The Markoffian approximation of the non-Markoffian master equation (8.1) is given by:

$$\left. \begin{aligned} Z_{E,t}^M(\alpha_0 \alpha \alpha') &= \bar{h}_{E,t}(\alpha_0 \alpha \alpha') + 2\pi\lambda^2 \int d\alpha_1 \left[ \int_0^{\infty} dt_1 \bar{w}_{E,t_1}(\alpha_0 \alpha_1) \right] Z_{E,t}^M(\alpha_1 \alpha \alpha') \\ &= \bar{h}_{E,t}(\alpha_0 \alpha \alpha') + \lambda^2 D_{E+i0}(\alpha_0) D_{E-i0}(\alpha_0) \\ &\quad \times \int d\alpha_1 W_{E \mp i0, E \pm i0}(\alpha_0 \alpha_1) Z_{E,t}^M(\alpha_1 \alpha \alpha') \end{aligned} \right\} \quad (8.5)$$

In (8.5) the upper signs stand for  $t > 0$ , the lower ones for  $t < 0$ . The evaluation of (3.1) in the Markoffian approximation gives\*):

$$\left. \begin{aligned} \tilde{A}_{\pm}^M &= \lim_{T \rightarrow \pm \infty} \int d\alpha_0 A(\alpha_0) \int_{-\infty}^{+\infty} dE \int_0^T dt Z_{E,t}^M(\alpha_0 \alpha \alpha') = \lim_{T \rightarrow \pm \infty} \frac{1}{2\pi} \int d\alpha_0 A(\alpha_0) \\ &\times \int_{-\infty}^{+\infty} dE D_{E+i0}(\alpha_0) D_{E-i0}(\alpha_0) \left. \begin{aligned} &\left| \pm \delta(\alpha_0 - \alpha) \delta(\alpha - \alpha') \pm V_{E \mp i0, E \pm i0}(\alpha_0 \alpha \alpha') \right. \right. \\ &+ 2\pi \lambda^2 \int d\alpha_1 W_{E \mp i0, E \pm i0}(\alpha_0 \alpha_1) \int_0^T dt Z_{E,t}^M(\alpha_1 \alpha \alpha') \left. \right. \end{aligned} \right\} \end{aligned} \right\} \quad (8.6)$$

Looking at (2.8) one easily recognizes that for large  $T$ , ( $\leq 0$ ), and after integration over  $\alpha_0$ ,  $2\pi \int_0^T dt Z_{E,t}^M(\alpha_0 \alpha \alpha')$  obeys the same equation as  $\pm Z_{E \mp i\eta, E \pm i\eta}(\alpha_0 \alpha \alpha')$  for small  $\eta$ . Therefore, considering (3.5) we obtain:

$$\tilde{A}_{\pm}^M = \tilde{A}_{\pm} \quad (8.7)$$

which represents the desired result.

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\* We are allowed to evaluate (3.1) using (8.1) (which is valid only for  $t \neq 0$ ), instead of (2.7) (which is also valid for  $t = 0$ ), because in both cases the lower limit of the time integral of (3.1) gives a vanishing contribution.