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1. Introduction

To study the electronic transport in substitutionally disordered alloys it is important to treat simultaneously impurity and electron-phonon scattering mechanisms. Several interesting features can be expected from including off-diagonal randomness in the tight-binding model under consideration. Theoretically, this problem is connected with the appearance of vertex corrections to the conductivity arising from a random current operator.

In the phononless case, most of the work [1-8] has been devoted to transport processes in alloys with only diagonal disorder using the coherent potential approximation (CPA). Then the expression for the electrical conductivity involves no vertex corrections as has been proved in single-site CPA by Velický [1]. Various approaches [9-13] have been developed to investigate the effect of off-diagonal randomness on the conductivity. Restrictions were supposed in constructing practicable models where the transfer integrals depend additively [10,12] or multiplicatively [9,11] on the

configurations at the sites linked, and other limiting cases [13] were treated. Fukuyama et al. [10] have derived nonvanishing vertex corrections, whereas no vertex corrections occur in other extended CPA schemes [13] as in the renormalization propagator formalism of Niizeki and Endo [9]. At finite temperature, the effect of electron-phonon interaction has been investigated by Chen et al. [14]. Their CPA treatment restricted to the case of diagonal disorder yields, in analogy to [1], no vertex corrections to the conductivity.

In this paper we start with a model Hamiltonian [15] including random diagonal and off-diagonal elements caused by substitutional and thermal disorder in the binary alloy. The functional-derivative technique is used to generate the contribution of the electron-phonon interaction to the electron self-energy. The static (adiabatic) approximation is introduced to show the equivalence of statically approximated and generalized stochastic models, and the corresponding distribution functions are derived in Section 2. After specializing to additive conditions for the transfer elements, the calculation of the ac-conductivity is based on the Kubo-Greenwood formula involving the random current operator and double average (Section 3). In Section 4 we present a method for determining the vertex corrections to the conductivity which evades the renormalized cumulant perturbation series for the self-energy used in [10]. Two-particle quantities are evaluated within the modified CPA [15] using a random-phase approximation type of decoupling similarly to [1].

The vertex corrections are found by solving Bethe-Salpeter-type equations.

2. Equivalence of Statically Approximated and Stochastic Models

Consider the electron-phonon interaction in substitutionally disordered binary systems such as A_cB_{1-c}-alloys. The model Hamiltonian depending on the configuration is assumed to have the form [15]

$$H = H_e + H_{eph} + H_{ph} , \tag{2.1}$$

where

$$H_e = \sum_n \epsilon_n a_n^+ a_n + \sum_{\substack{nm \\ (n\neq m)}} h_{nm} a_n^+ a_m , \tag{2.2}$$

$$H_{eph} = \sum_{nm} \Theta_{nm} a_n^+ a_m , \text{ with } \Theta_{nm} = \sum_s (\gamma_{nm}^{(s)} b_s + (\gamma_{mn}^{(s)})^* b_s^+), \tag{2.3}$$

$$H_{ph} = \sum_s \hbar\omega_s (b_s^+ b_s + \frac{1}{2}) . \tag{2.4}$$

$a_n^+ (a_n)$ and $b_s^+ (b_s)$ are creation (annihilation) operators for an electron in the Wannier state at lattice site n and for a phonon in the state with the quantum number s, respectively. The s summation is extended over 3N normal modes of lattice vibrations, where N lattice sites are randomly occupied by atoms A or B. The atomic energies ϵ_n, the hopping integrals h_{nm} as well as the electron-phonon coupling elements $\gamma_{nn}^{(s)}$ and $\gamma_{nm}^{(s)}$ are random variables which take the values ϵ^ν, $h^{\nu\mu}$, $\gamma^{(s)\nu}$ and $\gamma^{(s)\nu\mu}$, respectively; here the superscript $\nu(\mu)$ refers to the atomic species $(\nu, \mu = A, B)$ located at site $n(m)$.

Only the nearest-neighbour (n.n.) transfer elements h_{nm} and $\gamma_{nm}^{(s)}$ are considered.

We are primarily interested in the electronic properties of the system. According to the procedure of Kadanoff and Baym /16/, the one-electron thermodynamic Green function related to $H_\lambda = H + \lambda$ is introduced by

$$G_{nm}(t,t';\lambda) = \frac{1}{i\hbar} \frac{\langle T\{S(-i\hbar\beta,0)a_n(t)\, a_m^+(t')\}\rangle}{\langle S(-i\hbar\beta,0)\rangle}, \quad (2.5)$$

where

$$S(t,t') = T\exp\{-\frac{i}{\hbar}\int_{t'}^{t}\lambda(t'')dt''\} \quad (2.6)$$

with the time-dependent auxilary field

$$\lambda(t) = \sum_{nm}\lambda_{nm}(t)\,\Theta_{nm}(t). \quad (2.7)$$

From the equation of motion for the Green function (2.5) one gets the Dyson equation

$$(i\hbar\frac{\partial}{\partial t} - \epsilon_n)G_{nm}(t,t';\lambda) - \sum_{k(\neq n)} h_{nk}G_{km}(t,t';\lambda) = \quad (2.8)$$

$$= \delta_{nm}\delta(t-t') + \sum_k \int_0^{-i\hbar\beta} dt''\Sigma_{nk}^{\{\nu\}}(t,t'';\lambda)\,G_{km}(t'',t';\lambda).$$

The electronic self-energy $\Sigma_{nk}^{\{\nu\}}(t,t'';\lambda)$ due to electron-phonon interaction in a given configuration $\{\nu\}$ is defined by

$$\sum_k \int_0^{-i\hbar\beta} dt''\Sigma_{nk}^{\{\nu\}}(t,t'';\lambda)\,G_{km}(t'',t';\lambda) = \quad (2.9)$$

$$= \frac{1}{i\hbar}\sum_k \frac{\langle T\{S(-i\hbar\beta,0)\Theta_{nk}(t)a_k(t)\,a_m^+(t')\}\rangle}{\langle S(-i\hbar\beta,0)\rangle}.$$

By exploiting the λ-dependence explicitly the relation

$$\frac{\delta G_{km}(t,t';\lambda)}{\delta\lambda_{nk}(t)} = -\frac{1}{i\hbar}\langle\Theta_{nk}(t)\rangle_{H_\lambda}G_{km}(t,t';\lambda) + \quad (2.10)$$

$$+ \frac{1}{(i\hbar)^2}\frac{\langle T\{S(-i\hbar\beta,0)\,\Theta_{nk}(t)a_k(t)a_m^+(t')\}\rangle}{\langle S(-i\hbar\beta,0)\rangle}$$

is obtained from (2.5) to (2.7) with the abbreviation

$$\langle\Theta_{nk}(t)\rangle_{H_\lambda} = \frac{\langle T\{S(-i\hbar\beta,0)\Theta_{nk}(t)\}\rangle}{\langle S(-i\hbar\beta,0)\rangle}. \quad (2.11)$$

On the other hand, via (2.8), one derives

$$\frac{\delta G_{km}(t,t';\lambda)}{\delta\lambda_{nk}(t)} = \sum_{ll}\int_0^{-i\hbar\beta}\int_0^{-i\hbar\beta} dt''d\bar{t}''G_{kl}(t,t'';\lambda)\frac{\delta\Sigma_{ll}^{\{\nu\}}(t'',\bar{t}'';\lambda)}{\delta\lambda_{nk}(t)}G_{lm}(\bar{t}'',t';\lambda). \quad (2.12)$$

Using (2.9) to (2.12) we find the functional-differential equation

$$\Sigma_{nm}^{\{\nu\}}(t,t';\lambda) = \langle\Theta_{nm}(t)\rangle_{H_\lambda}\delta(t-t') + \quad (2.13)$$

$$+ i\hbar\sum_{lk}\int_0^{-i\hbar\beta} dt''G_{lk}(t,t'';\lambda)\frac{\delta\Sigma_{km}^{\{\nu\}}(t'',t';\lambda)}{\delta\lambda_{nl}(t)}.$$

The equations (2.8), (2.12) and (2.13) determine, at least in principle in terms of mean values of phonon operators, the one-electron properties of a fictive system H_λ within a given configuration. The physically interesting quantities are obtained in the limit $\lambda \to 0$.

The following approximation scheme can be derived analogous as it has been done /17/ in treating the local electron-electron interaction in the Hubbard model. The static approximation is introduced by neglecting the time-dependence of the λ-field. Then we formally arrive at an equilibrium problem. Going over to the Fourier coefficients in (2.8), (2.12) and (2.13) within the static approximation, we get

$$(z-\epsilon_n)G_{nm}(z;\lambda) - \sum_{k(\neq n)} h_{nk}G_{km}(z;\lambda) = \tag{2.14}$$

$$= \delta_{nm} + \sum_k \Sigma^{\{\nu\}}_{nk}(z;\lambda)\, G_{km}(z;\lambda),$$

$$\frac{\partial G_{km}(z;\lambda)}{\partial \lambda_{nk}} = \sum_{l\bar{l}} G_{k\bar{l}}(z;\lambda) \frac{\partial \Sigma^{\{\nu\}}_{l\bar{l}}(z;\lambda)}{\partial \lambda_{nk}} G_{\bar{l}m}(z;\lambda), \tag{2.15}$$

$$\Sigma^{\{\nu\}}_{nm}(z;\lambda) = \langle \Theta_{nm} \rangle_{H_\lambda} - \frac{1}{\beta} \sum_{kl} G_{lk}(z;\lambda) \frac{\partial \Sigma^{\{\nu\}}_{km}(z;\lambda)}{\partial \lambda_{nl}}. \tag{2.16}$$

There are physical arguments to support this static approximation. In the sense of the Born- Oppenheimer adiabatic approximation we can suppress the ionic motion in treating the electronic problem, formally, by neglecting the time-dependence of the phonon operator Θ_{nm} or, equivalently, by neglecting the noncommutation of H_{eph} and H_{ph}. Then an electron is elastically scattered by phonons approximated as static scatterers.

Another approach to the electron-phonon interaction is based on the simulation of the interaction term by a static c-number field which acts on the electron with certain statistical fluctuations. The Hamiltonian of the stochastic model for a still fixed configuration is given by

$$\tilde{H} = H_e + \tilde{H}_{e\theta} + H_{ph}, \tag{2.17}$$

with

$$\tilde{H}_{e\theta} = \sum_{nm} \theta_{nm} a^+_n a_m, \tag{2.18}$$

where the quantities θ_{nm} fluctuate statistically according to a certain normalized distribution function $P(\{\theta\})$. . Note that θ_{nm} and $P(\{\theta\})$ are also configurational dependent.

Starting now with the Hamiltonian $\tilde{H}_\lambda = \tilde{H} + \lambda$ including the static auxiliary field

$$\lambda = \sum_{nm} \lambda_{nm} \Theta_{nm}, \tag{2.19}$$

the Fourier transform $\tilde{G}_{nm}(z;\theta)$ of the one-electron Green function obeys the equation of motion

$$(z-\epsilon_n)\tilde{G}_{nm}(z;\theta) - \sum_{k(\neq n)} h_{nk}\tilde{G}_{km}(z;\theta) = \delta_{nm} + \sum_k \theta_{nk}\tilde{G}_{km}(z;\theta). \tag{2.20}$$

The θ-averaged Green function is defined by (compare the analogous expression for the Hubbard model in [17])

$$G_{nm}(z;\lambda) = \langle \tilde{G}_{nm}(z;\theta) \frac{e^{\Lambda(\lambda,\theta)}}{\langle e^{\Lambda(\lambda,\theta)} \rangle_\theta} \rangle_\theta , \qquad (2.21)$$

where

$$\langle f(\{\theta\}) \rangle_\theta = \int P(\{\theta\}) f(\{\theta\}) \prod_{nm} d\theta_{nm} , \qquad (2.22)$$

$$\Lambda(\lambda,\theta) = -\beta \sum_{nm} \lambda_{nm} \theta_{nm} . \qquad (2.23)$$

From (2.20) and (2.21) one gets the Dyson equation

$$(z-\epsilon_n) G_{nm}(z;\lambda) - \sum_{k(\neq n)} h_{nk} G_{km}(z;\lambda) = \delta_{nm} + \sum_k \Sigma^{\{\nu\}}_{nk}(z;\lambda) G_{km}(z;\lambda) \qquad (2.24)$$

and

$$\frac{\partial G_{km}(z;\lambda)}{\partial \lambda_{nk}} = \sum_{ll} G_{kl}(z;\lambda) \frac{\partial \Sigma^{\{\nu\}}_{ll}(z;\lambda)}{\partial \lambda_{nk}} G_{lm}(z;\lambda), \qquad (2.25)$$

$$\Sigma^{\{\nu\}}_{nm}(z;\lambda) = \langle \theta_{nm} \frac{e^{\Lambda(\lambda,\theta)}}{\langle e^{\Lambda(\lambda,\theta)} \rangle_\theta} \rangle_\theta - \qquad (2.26)$$

$$- \frac{1}{\beta} \sum_{kl} G_{lk}(z;\lambda) \frac{\partial \Sigma^{\{\nu\}}_{km}(z;\lambda)}{\partial \lambda_{nl}} .$$

These equations completely coincide with the relations (2.14) to (2.16) if in determining the distribution function $P(\{\theta\})$ we make the formal identification

$$\langle \theta_{nm} \frac{e^{\Lambda(\lambda,\theta)}}{\langle e^{\Lambda(\lambda,\theta)} \rangle_\theta} \rangle_\theta = \langle \Theta_{nm} \rangle_{H_\lambda} \qquad (2.27)$$

being valid within a fixed configuration for all λ. In this way - concerning the electronic properties - the statically approximated model (2.1) is reduced to the stochastic model (2.17), i.e., to a generalized alloy model. Such a treatment of the electron-phonon interaction is not restricted to a special type of disorder.

In order to calculate the distribution function $P(\{\theta\})$, the phonon operator Θ_{nm} on the r.h.s. of (2.27) will be averaged in the spirit of the Born-Oppenheimer approximation as

$$\langle \Theta_{nm} \rangle_{H_\lambda} = \frac{\mathrm{Tr}\{e^{-\beta H}(e^{-\beta\lambda}\Theta_{nm})\}}{\mathrm{Tr}\{e^{-\beta H} e^{-\beta\lambda}\}} \approx \frac{\mathrm{Tr}\{e^{-\beta H_{ph}}(e^{-\beta\lambda}\Theta_{nm})\}}{\mathrm{Tr}\{e^{-\beta H_{ph}} e^{-\beta\lambda}\}}, \qquad (2.28)$$

where λ means the static field (2.19).

For practical calculations the reduced distribution function

$$P_{nm}(\theta_{nm}) = \int P(\{\theta\}) \prod'_{ij(\neq nm)} d\theta_{ij} \qquad (2.29)$$

is needed. Writing the phonon average of any function $f(\Theta_{nm})$ in the form (compare [14])

$$\langle f(\Theta_{nm})\rangle_{ph} = \frac{Tr\{e^{-\beta H_{ph}} f(\Theta_{nm})\}}{Tr\{e^{-\beta H_{ph}}\}} = \int P_{nm}(\theta_{nm}) f(\theta_{nm}) d\theta_{nm}, \quad (2.30)$$

by means of Bloch's theorem one finds the normalized distribution function

$$P_{nm}(\theta_{nm}) = \frac{1}{\sqrt{2\pi a_{nm}}} \exp\{-\frac{\theta_{nm}^2}{2a_{nm}}\}, \quad (2.31)$$

$$\text{with} \quad a_{nm} = \sum_s |\gamma_{nm}^{(s)}|^2 \coth\frac{\beta\hbar\omega_s}{2}.$$

Obviously, the Gaussian (2.31) identified with (2.29) fulfils the condition (2.27) within the approximation (2.28) by setting $\lambda_{ij} = \lambda_{nm}\ \delta_{ij,nm}$. In an analogous manner, the reduced two-dimensional distribution function $P_{nm,kl}(\theta_{nm}, \theta_{kl})$ defined by

$$P_{nm,kl}(\theta_{nm}, \theta_{kl}) = \int P(\{\theta\}) \prod''_{ij(\neq nm, \neq kl)} d\theta_{ij}, \quad (nm \neq kl) \quad (2.32)$$

is obtained after extensive calculations as

$$P_{nm,kl}(\theta_{nm}, \theta_{kl}) = \quad (2.33)$$

$$= \frac{1}{2\pi\sqrt{\tilde{a}_{nm,kl}}} \exp\{-(\frac{\theta_{nm}^2}{2\tilde{a}_{nm}} + \frac{\theta_{kl}^2}{2\tilde{a}_{kl}} - \frac{a_{nm,kl}}{2\tilde{a}_{nm,kl}}\theta_{nm}\theta_{kl})\},$$

where (under the subsidiary condition $\tilde{a}_{nm,kl} > 0$)

$$\tilde{a}_{nm} = a_{nm} - \frac{1}{4}\frac{a_{nm,kl}^2}{a_{kl}}, \quad \tilde{a}_{kl} = a_{kl} - \frac{1}{4}\frac{a_{nm,kl}^2}{a_{nm}}, \quad (2.34)$$

$$\tilde{a}_{nm,kl} = a_{nm}a_{kl} - \frac{1}{4}a_{nm,kl}^2,$$

with

$$a_{nm,kl} = \sum_s ((\gamma_{nm}^{(s)})^* \gamma_{kl}^{(s)} + \gamma_{nm}^{(s)} (\gamma_{kl}^{(s)})^*) \coth\frac{\beta\hbar\omega_s}{2}. \quad (2.35)$$

Note that the interference term (proportional to $a_{nm,kl}$)) reflects phonon-assisted correlations between different lattice sites.

3. Symmetric Model and Conductivity Formula

The description of the electron-phonon interaction in alloy analogy allows one to apply a modified CPA for calculating electronic properties as the conductivity. Therefore, we specialize the off-diagonal randomness by assuming the additive and symmetric conditions /15/

$$h^{AB} = \frac{1}{2}(h^{AA} + h^{BB}), \quad (3.1)$$

$$\gamma^{(s)AB} = \frac{1}{2}(\gamma^{(s)AA} + \gamma^{(s)BB}). \qquad (3.2)$$

Then the general Hamiltonian (2.1) can be rewritten as

$$H = H_e^B + \sum_n V_n + H_{ph}, \qquad (3.3)$$

with

$$V_n = (E_n+\Theta_n)a_n^+a_n + \sum_{m(\neq n)}{}' (h_n+\bar{\Theta}_n)(a_n^+a_m + a_m^+a_n), \qquad (3.4)$$

where the prime indicates that only nearest neighbours are included in the summation. H_e^B is the one-electron Hamiltonian (2.2) for a perfect B-crystal. The random quantities $[E_n, h_n; \Theta_n, \bar{\Theta}_n]$ are equal to $[\epsilon^A - \epsilon^B, \frac{1}{2}(h^{AA}-h^{BB}); \Theta^A, \bar{\Theta}^A]$ or $[0, 0; \Theta^B, \bar{\Theta}^B]$ according to whether an A or B atom occupies the n-th site, respectively, where

$$\Theta^\nu = \sum_s (\gamma^{(s)\nu} b_s + (\gamma^{(s)\nu})^* b_s^+), \qquad (3.5)$$

$$\bar{\Theta}^\nu = \frac{1}{2}\sum (\gamma^{(s)\nu\nu} b_s + (\gamma^{(s)\nu\nu})^* b_s^+), (\nu = A,B). \qquad (3.6)$$

In alloy analogy (2.17), the stochastic model corresponding to the symmetric model (3.3) takes now the form

$$\tilde{H} = H_e^B + \sum_n \tilde{V}_n + H_{ph} = \tilde{H}_e + H_{ph}, \qquad (3.7)$$

where

$$\tilde{V}_n = (E_n + \theta_n) a_n^+ a_n + \sum_{m(\neq n)}{}' (h_n + \bar{\theta}_n)(a_n^+ a_m + a_m^+ a_n) \qquad (3.8)$$

$\tilde{H}_e$ denotes the electronic part of the generalized alloy Hamiltonian (3.7). The equation of motion for the Fourier transform $\tilde{G}_{nm}(z;\theta)$ of the one-electron Green function is obtained as

$$(z-\epsilon^B-E_n)\tilde{G}_{nm}(z;\theta) - \sum_{k(\neq n)}{}' (h^{BB}+h_n+h_k)\tilde{G}_{km}(z;\theta) = \qquad (3.9)$$
$$= \delta_{nm} + \theta_n \tilde{G}_{nm}(z;\theta) + \sum_{k(\neq n)}{}' (\bar{\theta}_n + \bar{\theta}_k)\tilde{G}_{km}(z;\theta).$$

Adopting the formalism developed in Section 2, one immediately recognizes the special case of the symmetric model as

$$\Theta_{nn} = \Theta_n, \quad \Theta_{nm} = \bar{\Theta}_n + \bar{\Theta}_m \qquad (3.10)$$

and

$$\theta_{nm} = \theta_n, \quad \theta_{nm} = \bar{\theta}_n + \bar{\theta}_m, \ (n,m:n.n.). \qquad (3.11)$$

Especially, one recovers with (3.10) and (3.11) the equation (2.27) for determining the distribution function $P(\{\theta\})$.

Adapting the CPA formalism we introduce from (3.7) and (3.9) the totally averaged one-electron Green function (or the propagator) in the physical limit $\lambda \to 0$ as

$$\mathcal{G}(z) = \langle\langle \tilde{G}(z;\theta)\rangle_\theta\rangle_c = \langle\langle (z-\tilde{H}_e)^{-1}\rangle_\theta\rangle_c = (z - H_e^B - \Sigma(z))^{-1}, \qquad (3.12)$$

where $\langle\ldots\rangle_c$ implies the configuration averaging and Σ is the electronic self-energy operator.

The real part of the conductivity tensor at finite frequency ω is given by the Kubo-Greenwood formula

$$\sigma'_{\alpha\beta}(\omega) = \frac{2\pi}{V}\int_{-\infty}^{\infty} d\eta \left(\frac{f(\eta)-f(\eta+\omega)}{\omega}\right) \langle\langle \mathrm{tr}\{\delta(\eta-\tilde{H}_e) j_\alpha \delta(\eta+\omega-\tilde{H}_e) j_\beta\}\rangle\rangle_c , \tag{3.13}$$

where

$$f(\eta) = (1 + \exp\{(\eta-\mu)/k_B T\})^{-1} \tag{3.14}$$

is the Fermi distribution function, V is the volume of the system, μ is the chemical potential and j_α is the α-component of the one-electron current operator. The trace is to be taken over one-eletron states, and the two possible spin orientations are already taken into account by an extra factor of 2. Equivalently, the conductivity can be expressed in terms of $\tilde{G}(z;\theta)$ as

$$\sigma'_{\alpha\beta}(\omega) = \frac{1}{2\pi V}\int_{-\infty}^{\infty} d\eta \left(\frac{f(\eta)-f(\eta+\omega)}{\omega}\right) \langle\langle \mathrm{tr}\{\tilde{G}(\eta^+) j_\alpha \tilde{G}(\eta^-+\omega) j_\beta +$$

$$+ \tilde{G}(\eta^-) j_\alpha \tilde{G}(\eta^+ + \omega) j_\beta - \tilde{G}(\eta^+) j_\alpha \tilde{G}(\eta^+ + \omega) j_\beta - \tag{3.15}$$

$$- \tilde{G}(\eta^-) j_\alpha \tilde{G}(\eta^- + \omega) j_\beta\}\rangle\rangle ,$$

where $\eta^{\pm} = \eta \pm i0$ and the notation has been simplified by dropping θ-arguments and the indices from the double average.

The current operator in tight-binding representation takes the form

$$j_\alpha = -ie\sum_n R_{\alpha n}[a_n^+ a_n, \tilde{H}] = j_\alpha^{(0)} + j_\alpha^{(1)} , \tag{3.16}$$

with

$$j_\alpha^{(0)} = -ieh^{BB}\sum_n \sum'_{m(\neq n)} (R_{\alpha n} - R_{\alpha m}) a_n^+ a_m , \tag{3.17}$$

$$j_\alpha^{(1)} = \sum j_{\alpha n}^{(1)} = -ie\sum_n \sum'_{m(\neq n)} (h_n + \bar{\theta}_n)(R_{\alpha n} - R_{\alpha m})(a_n^+ a_m - a_m^+ a_n), \tag{3.18}$$

where $\vec{R}_n$ denotes the position vector of site n in the static lattice. Here $j_\alpha^{(0)}$ refers to the unperturbed current related to H_e^B. The part $j_\alpha^{(1)}$ including both electronic and phononic contributions is configurational dependent. Additionally, the phonon-assisted current (proportional to θ_n) is subjected to statistical fluctuations.

4. Vertex Corrections within a Modified CPA

Substituting (3.16) into (3.15) the diagonal part of σ which we are primarily interested in can be written in terms of expressions

$$\langle\langle \mathrm{tr}\{\tilde{G}(z_1) j_\alpha \tilde{G}(z_2) j_\alpha\}\rangle\rangle = \langle\langle \mathrm{tr}\{\tilde{G}(z_1) j_\alpha^{(0)} \tilde{G}(z_2) j_\alpha^{(0)}\}\rangle\rangle +$$

$$+ \langle\langle \mathrm{tr}\{\tilde{G}(z_1) j_\alpha^{(1)} \tilde{G}(z_2) j_\alpha^{(0)}\}\rangle\rangle + \langle\langle \mathrm{tr}\{\tilde{G}(z_1) j_\alpha^{(0)} \tilde{G}(z_2) j_\alpha^{(1)}\}\rangle\rangle + \tag{4.1}$$

$$+ \langle\langle \mathrm{tr}\{\tilde{G}(z_1) j_\alpha^{(1)} \tilde{G}(z_2) j_\alpha^{(1)}\}\rangle\rangle .$$

We must therefore consider averages of the following types:

$$K^{(0)} = \langle\langle \tilde{G}(z_1) j_a^{(0)} \tilde{G}(z_2) \rangle\rangle = \tag{4.2}$$

$$= \mathcal{G}(z_1)[j_a^{(0)} + \langle\langle T(z_1)\, \mathcal{G}(z_1) j_a^{(0)} \mathcal{G}(z_2) T(z_2) \rangle\rangle]\, \mathcal{G}(z_2),$$

$$K^{(1)} = \langle\langle \tilde{G}(z_1) j_a^{(1)} \tilde{G}(z_2) \rangle\rangle = \mathcal{G}(z_1)[\langle\langle j_a^{(1)} \rangle\rangle + \langle\langle T(z_1)\, \mathcal{G}(z_1) j_a^{(1)} \rangle\rangle +$$

$$+ \langle\langle j_a^{(1)} \mathcal{G}(z_2) T(z_2) \rangle\rangle + \langle\langle T(z_1)\, \mathcal{G}(z_1) j_a^{(1)} \mathcal{G}(z_2) T(z_2) \rangle\rangle] \mathcal{G}(z_2), \tag{4.3}$$

$$L = \langle\langle \tilde{G}(z_1) j_a^{(1)} \tilde{G}(z_2) j_a^{(1)} \rangle\rangle = \mathcal{G}(z_1)[\langle\langle j_a^{(1)} \mathcal{G}(z_2) j_a^{(1)} \rangle\rangle +$$

$$+ \langle\langle j_a^{(1)} \mathcal{G}(z_2) T(z_2)\, \mathcal{G}(z_2) j_a^{(1)} \rangle\rangle +$$

$$+ \langle\langle T(z_1)\, \mathcal{G}(z_1) j_a^{(1)} \mathcal{G}(z_2) j_a^{(1)} \rangle\rangle + \tag{4.4}$$

$$+ \langle\langle T(z_1) \mathcal{G}(z_1) j_a^{(1)} \mathcal{G}(z_2) T(z_2)\, \mathcal{G}(z_2) j_a^{(1)} \rangle\rangle],$$

where the scattering operator T corresponding to the perturbation $(\sum_n \tilde{V}_n - \Sigma)$ is defined by

$$\tilde{G} = \mathcal{G} + \mathcal{G} T \mathcal{G} \tag{4.5}$$

with the self-consistency requirement $\langle\langle T \rangle\rangle = 0$.

The additive random operator $\sum_n \tilde{V}_n$ suggests to decompose the self-energy in the form $\Sigma = \sum_n \Sigma_n$ and to introduce the single-site scattering operator T_n as

$$T_n = (\tilde{V}_n - \Sigma_n)[1 - \mathcal{G}(\tilde{V}_n - \Sigma_n)]^{-1}. \tag{4.6}$$

It is pointed out that $\tilde{V}_n, \Sigma_n, T_n$ and, recalling (3.18), $j_{an}^{(1)}$ are finite ranged quantities in the Wannier space. The total scattering operator can be expressed in terms of T_n as multiple scattering series /1,14/

$$T = \sum_n T_n + \sum_{\substack{nm \\ (n \neq m)}} T_n \mathcal{G} T_m + \sum_{\substack{nml \\ (n \neq m,\ m \neq l)}} T_n \mathcal{G} T_m \mathcal{G} T_l + \dots . \tag{4.7}$$

To calculate the averages (4.2) to (4.4) we are working within a modified single-site CPA /15/ based on the self-consistency condition

$$\langle\langle T_n \rangle\rangle = 0. \tag{4.8}$$

Moreover, in view of the statistical correlations, a random-phase approximation type of decoupling similarly to /1/ is used which can be characterized, for instance, by

$$\langle\langle T_n \mathcal{G} T_m \rangle\rangle = \langle\langle T_n \mathcal{G} T_n \rangle\rangle \delta_{nm}, \langle\langle T_n \mathcal{G} j_{am}^{(1)} \rangle\rangle =$$

$$= \langle\langle T_n \mathcal{G} j_{an}^{(1)} \rangle\rangle \delta_{nm}, \langle\langle j_{an}^{(1)} \mathcal{G} j_{am}^{(1)} \rangle\rangle = \begin{cases} \ll j_{an}^{(1)} \mathcal{G} j_{an}^{(1)} \gg \text{ if } n = m, \\ \ll j_{an}^{(1)} \gg \mathcal{G} \ll j_{am}^{(1)} \gg \text{ if } n \neq m, \end{cases} \tag{4.9}$$

etc. The higher products of random quantities are averaged analogously.

Beginning with the expression $K^{(1)}$ (4.3) and defining the vertex operator $\Gamma^{(1)}$ as

$$\Gamma^{(1)}(z_1, j_\alpha^{(1)}, z_2) = \ll T(z_1)\mathcal{G}(z_1) j_\alpha^{(1)} \mathcal{G}(z_2) T(z_2) \gg , \quad (4.10)$$

we obtain the Bethe-Salpeter-type equations (arguments $z_1 (z_2)$ to the left (right) of $j_\alpha^{(1)}$)

$$K^{(1)} = \mathcal{G}[\ll j_\alpha^{(1)} \gg + \ll T\, \mathcal{G} j_\alpha^{(1)} \gg + \ll j_\alpha^{(1)} \mathcal{G} T \gg + \sum_n \Gamma_n^{(1)}]\, \mathcal{G}, \quad (4.11)$$

with

$$\Gamma_n^{(1)} = \ll T_n K^{(1)} T_n \gg + \quad (4.12)$$

$$+ \ll T_n \mathcal{G} j_{\alpha n}^{(1)} - \ll j_{\alpha n}^{(1)} \gg - \ll T_n \mathcal{G}\, j_{\alpha n}^{(1)} \gg - \ll j_{\alpha n}^{(1)} \mathcal{G} T_n \gg - \Gamma_n^{(1)}] \mathcal{G} T_n \gg .$$

Iteration of this closed system yields the formal solution for $\Gamma^{(1)}$ as

$$\Gamma^{(1)} = \sum_n \ll T_n \mathcal{G}[\ll j_\alpha^{(1)} \gg + \ll T\, \mathcal{G} j_\alpha^{(1)} \gg + \ll j_\alpha^{(1)} \mathcal{G} T \gg +$$

$$+ j_{\alpha n}^{(1)} - \ll j_{\alpha n}^{(1)} \gg - \ll T_n \mathcal{G}\, j_{\alpha n}^{(1)} \gg - \ll j_{\alpha n}^{(1)} \mathcal{G}\, T_n \gg] \mathcal{G}\, T_n \gg + \quad (4.13)$$

$$+ \sum_{\substack{nm \\ (n \neq m)}} \ll T_n \mathcal{G} \ll T_m \mathcal{G}[\ll j_\alpha^{(1)} \gg + \ll T\, \mathcal{G}\, j_\alpha^{(1)} \gg + \ll j_\alpha^{(1)} \mathcal{G}\, T \gg +$$

$$+ j_{\alpha m}^{(1)} - \ll j_{\alpha m}^{(1)} \gg - \ll T_m \mathcal{G}\, j_{\alpha m}^{(1)} \gg - \ll j_{\alpha m}^{(1)} \mathcal{G}\, T_m \gg] \mathcal{G}\, T_m \gg \mathcal{G} T_n \gg +$$

$$+ \ldots \ .$$

The corresponding equations for $K^{(0)}$ (4.2) and the vertex operator

$$\Gamma^{(0)}(z_1, j_\alpha^{(0)}, z_2) = \ll T(z_1) \mathcal{G}(z_1) j_\alpha^{(0)} \mathcal{G}(z_2) T(z_2) \gg \quad (4.14)$$

are a special case of (4.11) to (4.13) if $j_\alpha^{(1)}$ is replaced by the non-random current $j_\alpha^{(0)}$.

The contributions to (4.4) which are retained by the single-site CPA can be classified in the form (with dropping the z-arguments)

$$L_1 = \ll j_\alpha^{(1)} \mathcal{G}(z_2) j_\alpha^{(1)} \gg = \sum_n \{\ll j_{\alpha n}^{(1)} \mathcal{G}\, j_{\alpha n}^{(1)} \gg + \quad (4.15)$$

$$+ \sum_{m(\neq n)} \ll j_{\alpha n}^{(1)} \gg \mathcal{G} \ll j_{\alpha m}^{(1)} \gg \},$$

$$L_2 = \ll j_\alpha^{(1)} \mathcal{G}(z_2) T(z_2) \mathcal{G}(z_2) j_\alpha^{(1)} \gg = \quad (4.16)$$

$$= \sum_n \{\ll j_{\alpha n}^{(1)} \mathcal{G}\, T_n \mathcal{G} j_{\alpha n}^{(1)} \gg + \ll j_{\alpha n}^{(1)} \mathcal{G} T_n \gg \mathcal{G} \sum_{m(\neq n)} \ll j_{\alpha m}^{(1)} \gg +$$

$$+ \sum_{m(\neq n)} \ll j_{\alpha m}^{(1)} \gg \mathcal{G} \ll T_n \mathcal{G}\, j_{\alpha n}^{(1)} \gg + \ll j_{\alpha n}^{(1)} \mathcal{G}\, T_n \gg \mathcal{G} \sum_{m(\neq n)} \ll T_m \mathcal{G} j_{\alpha m}^{(1)} \gg \},$$

$$L_3 = \ll T(z_1) \mathcal{G}(z_1) j_\alpha^{(1)} \mathcal{G}(z_2) j_\alpha^{(1)} \gg =$$

$$= \sum_n \{\ll T_n \mathcal{G} j_{\alpha n}^{(1)} \mathcal{G} j_{\alpha n}^{(1)} \gg + \ll T_n \mathcal{G}\, j_{\alpha n}^{(1)} \gg \mathcal{G} \sum_{m \neq n} \ll j_{\alpha m}^{(1)} \gg +$$

$$+ \ll T_n \mathcal{G} \sum_{m(\neq n)} \ll j_{\alpha m}^{(1)} \gg \mathcal{G}\, j_{\alpha n}^{(1)} \gg + \quad (4.17)$$

$$+ \ll T_n \mathcal{G} \sum_{m(\neq n)} \ll T_m \mathcal{G} j_{\alpha m}^{(1)} \gg \mathcal{G}\, j_{\alpha n}^{(1)} \gg \},$$

and with (4.12)

$$L_4 = \langle\langle T(z_1)\mathcal{G}(z_1)j^{(1)}_{\alpha}\ \mathcal{G}(z_2)T(z_2)\ \mathcal{G}(z_2)j^{(1)}_{\alpha}\rangle\rangle =$$

$$= \sum_n \{\langle\langle T_n\ \mathcal{G}j^{(1)}_{\alpha n}\ \mathcal{G}T_n\mathcal{G}\,j^{(1)}_{\alpha n}\rangle\rangle + \langle\langle T_n\mathcal{G}\sum_{m(\neq n)}\langle\langle j^{(1)}_{\alpha m}\rangle\rangle\mathcal{G}T_n\mathcal{G}\,j^{(1)}_{\alpha n}\rangle\rangle +$$

$$+ \langle\langle T_n\mathcal{G}\sum_{m(\neq n)}\langle\langle T_m\,\mathcal{G}j^{(1)}_{\alpha m}\rangle\rangle\mathcal{G}T_n\ \mathcal{G}\,j^{(1)}_{\alpha n}\rangle\rangle +$$

$$+ \langle\langle T_n\mathcal{G}\sum_{m(\neq n)}\langle\langle j^{(1)}_{\alpha m}\mathcal{G}T_m\rangle\rangle\mathcal{G}T_n\mathcal{G}j^{(1)}_{\alpha n}\rangle\rangle + \qquad (4.18)$$

$$+ \langle\langle T_n\,\mathcal{G}j^{(1)}_{\alpha m}\rangle\rangle\,\mathcal{G}\sum_{m(\neq n)}\langle\langle T_m\,\mathcal{G}j^{(1)}_{\alpha m}\rangle\rangle +$$

$$+ \langle\langle T_n\mathcal{G}\sum_{m(\neq n)}\langle\langle j^{(1)}_{\alpha m}\mathcal{G}T_m\rangle\rangle\mathcal{G}\,j^{(1)}_{\alpha n}\rangle\rangle +$$

$$+ \Gamma^{(1)}_n\mathcal{G}[\sum_{m(\neq n)}(\langle\langle j^{(1)}_{\alpha m}\rangle\rangle + \langle\langle T_m\,\mathcal{G}j^{(1)}_{\alpha m}\rangle\rangle)] + \langle\langle T_n\mathcal{G}\sum_{m(\neq n)}\Gamma^{(1)}_m\mathcal{G}\,j^{(1)}_{\alpha n}\rangle\rangle +$$

$$+ \langle\langle T_n\mathcal{G}\sum_{m(\neq n)}\Gamma^{(1)}_m\mathcal{G}\,T_n\mathcal{G}\,j^{(1)}_{\alpha n}\rangle\rangle\}.$$

Further calculations are performed in the momentum representation. Using the translational symmetry, the propagator (3.12) takes the $\vec{k}$ -transform

$$\mathcal{G}_{\vec{k}}(z) = [z - \epsilon^B - h^{BB}s(\vec{k}) - \Sigma(\vec{k},z)]^{-1}, \qquad (4.19)$$

where the nearest-neighbour structure factor

$$s(\vec{k}) = \sum'_{m(\neq n)} e^{i\vec{k}(\vec{R}_m - \vec{R}_n)} \qquad (4.20)$$

is associated with the static lattice. The self-energy

$$\Sigma(\vec{k},z) = \sigma_0(z) + 2\sigma_1(z)s(\vec{k}) + \sigma_2(z)\,s^2(\vec{k}) \qquad (4.21)$$

is expressed in terms of $\sigma_0, \sigma_1, \sigma_2$ which obey the CPA conditions $\langle\langle t_{ln}\rangle\rangle = 0$ $(l = 0,1,2)$ /15/ arising from the T_n operator in the $\vec{k}$ -transformed version

$$\langle\vec{k}|T_n|\vec{k}'\rangle = \frac{1}{N}e^{-i(\vec{k}-\vec{k}')\vec{R}_n}[t_{0n} + t_{1n}(s(\vec{k}) + s(\vec{k}')) + t_{2n}\,s(\vec{k})s(\vec{k}')]. \qquad (4.22)$$

Combining (4.6) with (4.8) to $\Sigma_n = \langle\langle \tilde{V}_n\rangle\rangle + \langle\langle \tilde{V}_n\ \mathcal{G}\ T_n\rangle\rangle$, we can derive with (3.8) the useful equations (by averaging the index n disappears)

$$\sigma_0 = c\Lambda_0 + \langle\langle(E_n + \theta_n)t_{0n}\rangle\rangle F_0 + \langle\langle(h_n + \bar{\theta}_n)t_{0n}\rangle\rangle F_1 + \qquad (4.23)$$

$$+ \langle\langle(E_n + \theta_n)t_{1n}\rangle\rangle F_1 + \langle\langle(h_n + \bar{\theta}_n)t_{1n}\rangle\rangle F_2,$$

$$\sigma_1 = c\frac{\Lambda_1}{12} + \langle\langle(h_n + \theta_n)t_{0n}\rangle\rangle F_0 + \langle\langle(h_n + \bar{\theta}_n)t_{1n}\rangle\rangle F_1, \qquad (4.24)$$

$$\sigma_2 = \langle\langle(h_n + \bar{\theta}_n)t_{1n}\rangle\rangle F_0 + \langle\langle(h_n + \bar{\theta}_n)t_{2n}\rangle\rangle F_1, \qquad (4.25)$$

where

$$F_\ell(z) = \frac{1}{N}\sum_{\vec{k}}\mathcal{G}_{\vec{k}}(z)[s(\vec{k})]^\ell, \quad (\ell = 0,1,2). \qquad (4.26)$$

Here we have made use of the Gaussian (2.31) and the definitions $\Delta_0 = \epsilon^A - \epsilon^B, \Delta_1 = 6(h^{AA} - h^{BB})$ (e.g., for a simple cubic lattice); c being the concentration of the A component. By transforming (3.17) and (3.18) we arrive at the diagonal current

$$j^{(0)}_{\alpha k} = e h^{BB} \frac{\partial s(\vec{k})}{\partial \vec{k}_\alpha} \tag{4.27}$$

and the matrix elements

$$\langle \vec{k} | j^{(1)}_{\alpha n} | \vec{k}' \rangle = \frac{e}{N} e^{-i(\vec{k}-\vec{k}')\vec{R}_n} (h_n + \bar{\theta}_n) \left[\frac{\partial s(\vec{k})}{\partial \vec{k}_\alpha} + \frac{\partial s(\vec{k}')}{\partial \vec{k}'_\alpha} \right], \tag{4.28}$$

which lead, by using $\ll h_n + \bar{\theta}_n \gg = c \frac{\Delta_1}{12}$, , to the average

$$\ll j^{(1)}_\alpha \gg_{\vec{k}} = ec \frac{\Delta_1}{6} \frac{\partial s(\vec{k})}{\partial \vec{k}_\alpha}. \tag{4.29}$$

Having introduced the momentum representation, the quantity $K^{(1)}$ we are looking for can be obtained in the following way. To begin with, we get, via (4.22) and (4.28), the expressions

$$\ll\langle \vec{k} | j^{(1)}_{\alpha n} \mathcal{G} T_n | \vec{k}' \rangle\gg =$$

$$= \frac{e}{N} e^{-i(\vec{k}-\vec{k}')\vec{R}_n} [\tau_0 F_0 + \tau_1 (F_0 s(\vec{k}') + F_1) + \tau_2 F_1 s(\vec{k}')] \frac{\partial s(\vec{k})}{\partial \vec{k}_\alpha}, \tag{4.30}$$

$$\lll \vec{k} | T_n \mathcal{G} j^{(1)}_{\alpha n} | \vec{k}' \ggg = \tag{4.31}$$

$$= \frac{e}{N} e^{-i(\vec{k}-\vec{k}')\vec{R}_n} [\tau_0 F_0 + \tau_1 (F_0 s(\vec{k}) + F_1) + \tau_2 F_1 s(\vec{k})] \frac{\partial s(\vec{k}')}{\partial \vec{k}'_\alpha}$$

implying the relation

$$\ll j^{(1)}_\alpha \mathcal{G} T \gg_{\vec{k}} = \ll T \mathcal{G} j^{(1)}_\alpha \gg_{\vec{k}} = \tag{4.32}$$

$$= e[\tau_0 F_0 + \tau_1 (F_0 s(\vec{k}) + F_1) + \tau_2 F_1 s(\vec{k})] \frac{\partial s(\vec{k})}{\partial \vec{k}_\alpha},$$

where

$$\tau_\ell = \ll (h_n + \bar{\theta}_n) t_{ln} \gg, \quad (\ell = 0,1,2). \tag{4.33}$$

The examination of the equation (4.13) for $\Gamma^{(1)}$ shows that each term in the series expansion in $\vec{k}$-representation contains the factor $\lll \vec{k} | T_n \mathcal{G} A \mathcal{G} T_n | \vec{k}' \ggg$, where A decomposes, in view of (4.28) to (4.32), into summands of the type $f(s(\vec{k}_1))[a \frac{\partial s(\vec{k}_1)}{\partial \vec{k}_{1\alpha}} + b \frac{\partial s(\vec{k}_2)}{\partial \vec{k}_{2\alpha}}]$ ($\vec{k}_1, \vec{k}_2$ are summed over finally). Using the symmetry relation (f being an arbitrary function)

$$\sum_{\vec{k}} f(s(\vec{k})) \frac{\partial s(\vec{k})}{\partial \vec{k}_\alpha} = 0, \tag{4.34}$$

one can prove that the vertex part $\Gamma^{(1)}$ vanishes. Moreover, the same conclusion is drawn for the vertex part $\Gamma^{(0)}$ defined in (4.14). From (4.2) and (4.27) one immediately obtains

$$K^{(0)}_{\vec{k}} = eh^{BB}\ \frac{\partial s(\vec{k})}{\partial \vec{k}_a} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2). \qquad (4.35)$$

The next step consists in differentiating the self-energy (4.21) expressed in terms of (4.23) to (4.25) and in comparing the result with (4.29), (4.32) and (4.33):

$$\frac{\partial \Sigma}{\partial \vec{k}_a} = 2[c\frac{\Lambda_1}{12} + r_0F_0 + r_1(F_0 s(\vec{k}) + F_1) + r_2F_1 s(\vec{k})]\frac{\partial s(\vec{k})}{\partial \vec{k}_a} =$$

$$= \frac{1}{e}[\ll j^{(1)}_a \gg_{\vec{k}} + \ll T\,\mathcal{G}\, j^{(1)}_a \gg_{\vec{k}} + \ll j^{(1)}_a\, \mathcal{G}T \gg_{\vec{k}}]. \qquad (4.36)$$

Recalling the z-arguments from (4.3), with (4.36) and vanishing $\Gamma^{(1)}$ in (4.11) we get the final expression

$$K^{(1)}_{\vec{k}} = \frac{e}{2}[\frac{\partial \Sigma(\vec{k}, z_1)}{\partial \vec{k}_a} + \frac{\partial \Sigma(\vec{k}, z_2)}{\partial \vec{k}_a}]\mathcal{G}_{\vec{k}}(z_1)\,\mathcal{G}_{\vec{k}}(z_2), \qquad (4.37)$$

which includes vertex corrections arising from the terms $\ll T(z_1)\,\mathcal{G}(z_1) j^{(1)}_a \gg$ and $\ll j^{(1)}_a\,\mathcal{G}(z_2)T(z_2) \gg$. The relation (4.37)

plays the role of a generalized Ward's identity [18].

Let us outline the procedure for calculating the quantity L defined in (4.4). Substituting (4.22), (4.28) to (4.33) into (4.15) and (4.16) we find, with (4.24), (4.25) and (4.36), the k-transformed contributions

$$L_{1\vec{k}} = e^2[\ll(h_n+\bar{\theta}_n)^2 \gg - (c\frac{\Delta_1}{12})^2][F_0(\frac{\partial s(\vec{k})}{\partial \vec{k}_a})^2 + \frac{1}{N}\hat{F}] +$$

$$+ (\ll j^{(1)}_a \gg_{\vec{k}})^2 \mathcal{G}_{\vec{k}}, \qquad (4.38)$$

$$L_{2\vec{k}} = e^2[\ll(h_n+\bar{\theta}_n)^2 t_{0n} \gg F_0^2 + 2\ll(h_n+\bar{\theta}_n)^2 t_{1n} \gg F_0F_1 +$$

$$+ \ll(h_n+\bar{\theta}_n)^2 t_{2n} \gg F_1^2 - (\sigma_1 + c\frac{\Delta_1}{12})(r_0F_0^2 + 2r_1F_0F_1 + r_2F_1^2) -$$

$$-\sigma_2(r_0F_0F_1 + r_1(F_1^2 + F_0F_2) + r_2F_1F_2)](\frac{\partial s(\vec{k})}{\partial \vec{k}_a})^2 + \qquad (4.39)$$

$$+ (e\frac{\partial \Sigma}{\partial \vec{k}_a} - \ll j^{(1)}_a \gg_{\vec{k}} \ll j^{(1)}_a \gg_{\vec{k}} \mathcal{G}_{\vec{k}} + \frac{1}{4}(e\frac{\partial \Sigma}{\partial \vec{k}_a} - \ll j^{(1)}_a \gg_{\vec{k}})^2 \mathcal{G}_{\vec{k}},$$

where

$$\hat{F}(z) = \sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z)[\frac{\partial s(\vec{k})}{\partial \vec{k}_a}]^2. \qquad (4.40)$$

The quantity $L_{2\vec{k}}$ can be simplified by using the identity

$$\ll j^{(1)}_{\alpha n}\,\mathcal{G}T_n\mathcal{G}\tilde{V}_n \gg = \ll j^{(1)}_{\alpha n}\mathcal{G}\,T_n \gg (1+\mathcal{G}\,\Sigma_n) + \qquad (4.41)$$

$$+ \ll j^{(1)}_{\alpha n} \gg \mathcal{G}\Sigma_n - \ll j^{(1)}_{\alpha n}\,\mathcal{G}\,\tilde{V}_n \gg,$$

which yields the relation

$$\begin{aligned}
&\langle\langle (h_n+\bar{\theta}_n)^2 t_{0n}\rangle\rangle F_0^2 + 2\langle\langle (h_n+\bar{\theta}_n)^2 t_{1n}\rangle\rangle F_0 F_1 + \\
&+ \langle\langle (h_n+\bar{\theta}_n)^2 t_{2n}\rangle\rangle F_1^2 = \sigma_2 + \\
&+ \sigma_1 (r_0 F_0^2 + 2 r_1 F_0 F_1 + r_2 F_1^2) + \\
&+ \sigma_2 (r_0 F_0 F_1 + r_1 (F_1^2 + F_0 F_2) + r_2 F_1 F_2) + \\
&+ c\frac{\Delta_1}{12}(\sigma_1 F_0 + \sigma_2 F_1) - \langle\langle (h_n+\bar{\theta})^2\rangle\rangle F_0 .
\end{aligned} \tag{4.42}$$

Then we get

$$\begin{aligned}
L_{1\vec{k}} + L_{2\vec{k}} &= e\left[\langle\langle (h_n+\bar{\theta}_n)^2\rangle\rangle - (c\frac{\Delta_1}{12})^2\right]\frac{1}{N}\hat{F} + \\
&+ e^2\sigma_2 \left(\frac{\partial s(\vec{k})}{\partial \vec{k}_\alpha}\right)^2 + \frac{1}{4}\left(e\frac{\partial \Sigma}{\partial \vec{k}_\alpha} + \langle\langle j_\alpha^{(1)}\rangle\rangle_{\vec{k}}\right)^2 \mathcal{G}_{\vec{k}} .
\end{aligned} \tag{4.43}$$

By inserting the expressions (4.22), (4.28) to (4.33), (4.36) and (4.42) into (4.17) and (4.18) we obtain the remaining contributions to L in the form

$$\begin{aligned}
\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1) L_{3\vec{k}} &= e^2\{[\sigma_2(z_1) - (\langle\langle (h_n+\bar{\theta}_n)^2\rangle\rangle - \\
&- (c\frac{\Delta_1}{12})^2) F_0(z_1)]\hat{F}(z_2) + [\sigma_1(z_1) + c\frac{\Delta_1}{12}] B_1 + \sigma_2(z_1) B_2\} + \\
&+ \frac{1}{2}\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2)[e\frac{\partial \Sigma(z_1)}{\partial \vec{k}_\alpha} - \langle\langle j_\alpha^{(1)}\rangle\rangle_{\vec{k}}]\langle\langle j_\alpha^{(1)}\rangle\rangle_{\vec{k}} ,
\end{aligned} \tag{4.44}$$

$$\begin{aligned}
\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1) L_{4\vec{k}} &= e^2\left[(\sigma_1(z_2) - c\frac{\Delta_1}{12})B_1 + \sigma_2(z_2) B_2\right] + \\
&+ \frac{1}{4}\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2)[e\frac{\partial \Sigma(z_1)}{\partial \vec{k}_\alpha} - \langle\langle j_\alpha^{(1)}\rangle\rangle_{\vec{k}}] \times \\
&\times [e\frac{\partial \Sigma(z_2)}{\partial \vec{k}_\alpha} - \langle\langle j_\alpha^{(1)}\rangle\rangle_{\vec{k}}] ,
\end{aligned} \tag{4.45}$$

with the abbreviations

$$B_1 = r_0 F_0 H_0 + r_1 (F_1 H_0 + F_0 H_1) + r_2 F_1 H_1 , \tag{4.46}$$

$$B_2 = r_0 F_0 H_1 + r_1 (F_1 H_1 + F_0 H_2) + r_2 F_1 H_2 , \tag{4.47}$$

being valid for $r_\ell = r_\ell(z_1)$, $F_\ell = F_\ell(z_1)$ and

$$H_\ell(z_1, z_2) = \sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2)\left[\frac{\partial s(\vec{k})}{\partial \vec{k}_\alpha}\right]^2 [s(\vec{k})]^\ell , \tag{4.48}$$

$(\ell = 0,1,2)$.

Here we have used (4.34) in getting the equation (4.45).

Now one can prove, by means of (4.24) and (4.25), the relations

$$\sigma_1(z_1)B_1 + \sigma_2(z_1)B_2 =$$

$$= \frac{1}{4}\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2)[(\frac{\partial\Sigma(z_1)}{\partial\vec{k}_\alpha})^2 - \frac{1}{e}\frac{\partial\Sigma(z_1)}{\partial\vec{k}_\alpha}\ll j_\alpha^{(1)}\gg_{\vec{k}}], \quad (4.49)$$

$$\sigma_1(z_2)B_1 + \sigma_2(z_2)B_2 =$$

$$= \frac{1}{4}\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2)[\frac{\partial\Sigma(z_1)}{\partial\vec{k}_\alpha}\frac{\partial\Sigma(z_2)}{\partial\vec{k}_\alpha} - \quad (4.50)$$

$$- \frac{1}{e}\frac{\partial\Sigma(z_2)}{\partial\vec{k}_\alpha}\ll j_\alpha^{(1)}\gg_{\vec{k}}].$$

Combining (4.44) and (4.45) with the last two equations we find

$$\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)(L_{3\vec{k}} + L_{4\vec{k}}) =$$

$$= e^2[\sigma_2(z_1) - (\ll(h_n + \bar{\theta}_n)^2\gg - (c\frac{\Delta_1}{12})^2)F_0(z_1)]\hat{F}(z_2) +$$

$$+ \frac{1}{4}\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2)[e^2(\frac{\partial\Sigma(z_1)}{\partial k_\alpha})^2 + \quad (4.51)$$

$$+ 2e^2\frac{\partial\Sigma(z_1)}{\partial k_\alpha}\frac{\partial\Sigma(z_2)}{\partial k_\alpha} - 2e\frac{\partial\Sigma(z_2)}{\partial k_\alpha}\ll j_\alpha^{(1)}\gg_{\vec{k}} - (\ll j_\alpha^{(1)}\gg_{\vec{k}})^2].$$

After recalling the z-arguments in (4.43), all contributions to the quantity tr{L} can be now summarized as

$$\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)[L_{1\vec{k}} + L_{2\vec{k}} + L_{3\vec{k}} + L_{4\vec{k}}] =$$

$$= \frac{e^2}{4}\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2)[\frac{\partial\Sigma(z_1)}{\partial k_\alpha} + \frac{\partial\Sigma(z_2)}{\partial k_\alpha}]^2 + \quad (4.52)$$

$$+ e^2[\sigma_2(z_1)\hat{F}(z_2) + \sigma_2(z_2)\hat{F}(z_1)].$$

Returning with (4.27), (4.35), (4.37) and (4.52) to the starting point (4.1), one obtains the final result

$$\ll \mathrm{tr}\{\tilde{G}(z_1)j_\alpha\tilde{G}(z_2)j_\alpha\}\gg =$$

$$= e^2\sum_{\vec{k}} \mathcal{G}_{\vec{k}}(z_1)\mathcal{G}_{\vec{k}}(z_2)[\frac{\partial}{\partial k_\alpha}\{h^{BB}\vec{s}(\vec{k}) + \frac{1}{2}(\Sigma(\vec{k},z_1) + \Sigma(\vec{k},z_2))\}]^2 + \quad (4.53)$$

$$+ e^2\sum_{\vec{k}}[\sigma_2(z_1)\mathcal{G}_{\vec{k}}(z_2) + \sigma_2(z_2)\mathcal{G}_{\vec{k}}(z_1)][\frac{\partial\vec{s}(k)}{\partial k_\alpha}]^2.$$

This equation represents, in view of (3.15), the formal CPA solution of the ac-conductivity problem expressed in terms of the totally averaged one-electron Green function and the electron self-energy. The nonvanishing vertex corrections resulting from the random current operator are proportional to σ_1 and σ_2, i.e., assotiated with the off-diagonal disorder. The simultaneous action of impurity and electron-phonon scattering mechanisms is taken into account. In the phononless case, the formula (4.53) corresponds exactly to the solution of the static-conductivity problem obtained by Fukuyama et al. /10/ . Note that the corresponding result /10/ was found via a diagram analysis on the basis of Yonezawa's perturbation series for the self-energy.

The numerical evaluation of the expression (4.53) is connected with the solution of the CPA self-consistency problem[15]. Numerical results showing the effect of the vertex corrections on the temperature - dependent conductivity will be reported in a subsequent paper.

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