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Микроскопическая теория ферми-жидкости для неупорядоченных узкозонных систем

Формулируется теория ферми-жидкости сильно связанных электронов в неупорядоченных системах для нахождения двухчастичных корреляционных функций L при T = 0° K. На основе неупорядоченной модели Хаббарда и использования локального лестничного приближения в канале частица-частица получена неприводимая электронно-дырочная вершинная часть, являющаяся ядром уравнения Бете-Солпитера для L. Вычислены вершинные поправки к электропроводности в рамках CPA, а также парамагнитная восприимчивость в упорядоченном случае.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Microscopic Fermi Liquid Approach to Disordered Narrow Band Systems

A Fermi liquid approach to tightly bound electrons in disordered systems is proposed to evaluate two-particle correlation functions L at T=0 K. Starting with a random Hubbard model and using a local ladder approximation in the particle-particle channel the irreducible particle-hole vertex is derived, being the kernel of the Bethe-Salpeter equation for L. CPA vertex corrections to the electrical conductivity and, for the ordered case, the correlation - enhanced paramagnetic susceptibility are calculated.

The investigation has been performed at the Laboratory of Theoretical Physics, JINR.

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1. INTRODUCTION

The microscopic calculation of correlation functions of narrow band systems in the presence of random disorder requires a tight-binding description of an inhomogeneous Fermi liquid.

The main features of such an approach are just due to lack of the translational symmetry. Consequently, an approximation scheme can be outlined as follows:

(i) The bare electron-electron interaction due to the intraatomic repulsion should be described within a random version of the Hubbard model /1/.

(ii) By means of a local ladder approximation the one-particle Green functions are dressed; for pure systems that was proposed by Babanov et al. /2/.

(iii) According to the procedure of Baym and Kadanoff /3/ one can derive selfconsistently the irreducible particle-hole vertex, being

(iv) the kernel of the Bethe-Salpeter equation for the correlation function. The corresponding integral equation for the whole vertex must be formulated in the lattice space, unlike the Landau theory of uniform Fermi liquids /4/.

(v) The configurational averaging can be performed within a coherent potential approximation (CPA). For only diagonal disorder without interactions the CPA was developed by Velický et al. /5/; the present approach rests on an extended CPA /6/.

In this paper we are working along the line (i) to (v) within a perturbative approach in terms of causal Green functions at zero temperature /7/. In Sect. 2 the functional-derivative technique is used to deduce the integral equation for the correlation function involving the irreducible particle-hole vertex. The inclusion of dynamic interactions by the local ladder approximation effects the connection between the particle-particle and particle-hole channels (Sect.3). In Sect. 4 we give the CPA result for the ac conductivity without using the Kubo formula. The spin susceptibility expression calculated in Sect. 5 for the ordered case is found to be beyond the random phase approximation (RPA).

2. CORRELATION FUNCTION AND VERTICES

Within a random lattice we consider a zero-temperature fermion system described by a tight-binding Hamiltonian H. Specifically, electron-electron correlations in disordered narrow band systems of the substitutional alloy-type A_cB_{1-c} can be treated by the Hubbard model /1/

$$H = H_\Delta + H_U , \tag{2.1}$$

where

$$H_\Delta = \sum_{i\sigma} \varepsilon_i n_{i\sigma} + \sum_{\substack{ij\sigma \\ (i\neq j)}} t_{ij} c^+_{i\sigma} c_{j\sigma} , \tag{2.2}$$

$$H_U = \frac{1}{2} \sum_{i\sigma} U_i n_{i\sigma} n_{i-\sigma} . \tag{2.3}$$

Here $c^+_{i\sigma}$ ($c_{i\sigma}$) is the creation (annihilation) operator for an electron of spin σ in the Wannier state at lattice site i, and $n_{i\sigma} = c^+_{i\sigma} c_{i\sigma}$. The spatial inhomogeneity is expressed by random atomic levels ε_i, hopping integrals t_{ij}, and strengths U_i of the local initial pair interaction. These parameters take the values ε^ν, $t^{\nu\mu}$ concerning nearest-neighbour hopping, and U^ν ($\nu,\mu = A,B$), resp., according to whether an A or B atom occupies the site i (j). In this Section we are still working within a fixed configuration $\{\nu\} = \{\nu_1, \ldots, \nu_i, \ldots, \nu_N\}$ with $\nu_i = A,B$. Then, all quantities we calculate depend on the whole configuration $\{\nu\}$.

Supposing a Schwinger source field Q which may be non-local in space and time, the one-particle causal Green function is introduced by (here the formalism is similar to [3,8,9])

$$G_{\lambda_1\lambda_1'}(t_1,t_1';Q) = -i\langle T\{c_{\lambda_1}(t_1)c^+_{\lambda_1'}(t_1')e^{-iQ}\}\rangle / \langle T e^{-iQ}\rangle, \tag{2.4}$$

where

$$Q = \sum_{\lambda_1\lambda_2}\iint_{-\infty}^{+\infty} dt_1\,dt_2\,c^+_{\lambda_1}(t_1)\,Q_{\lambda_1\lambda_2}(t_1,t_2)\,c_{\lambda_2}(t_2). \tag{2.5}$$

Here T is the time-ordering operator, $\lambda = (i,\sigma)$, the brackets denote the ground-state average corresponding to H, and the operators are written in the Heisenberg picture with respect to H. In particular, for $Q_{\lambda_1\lambda_2}(t_1,t_2) = Q_{\lambda_1\lambda_2}(t_1)\,\delta(t_1-t_2)$ the external field term $Q=\int_{-\infty}^{+\infty} H_Q(t)\,dt$ corresponds to the perturbed Hamiltonian $\widetilde{H} = H + H_Q$.

The Green function (2.4) has to fulfil the Dyson equation

$$G^{-1}(1,1';Q) = G_\Delta^{-1}(1,1') - Q(1,1') - \Sigma_U(1,1';Q), \tag{2.6}$$

where the arguments 1, 1′ include lattice site, spin, and time variables; i.e., $1 = \lambda_1 t_1 = i_1\sigma_1 t_1$ etc.. Σ_U is the self-energy related to H_U, and G_Δ is the free propagator corresponding to H_Δ from (2.2).

In the limit $Q\to 0$ the two-particle Green function defined by

$$G^{II}(1,2;1',2') = -\langle Tc(1)c(2)c^+(2')c^+(1')\rangle \tag{2.7}$$

can be expressed in terms of the total vertex part Γ as

$$\begin{aligned} G^{II}(1,2;1',2') &= G(1,1')G(2,2') - G(1,2')G(2,1') \\ &\quad + i\,G(1,\bar{3})G(2,\bar{4})\Gamma(\bar{3},\bar{4};\bar{5},\bar{6})G(\bar{5},1')G(\bar{6},2'). \end{aligned} \tag{2.8}$$

Here the bar over double repeated numbers means summation or integration over the corresponding variables; $G(1,1')$ is the Green function (2.4) in the limit $Q\to 0$.

The two-particle correlation function (causal response function) is defined by

$$L(1,2;1',2') = G^{II}(1,2;1',2') - G(1,1')G(2,2'). \qquad (2.9)$$

According to the Baym and Kadanoff procedure /3/ one gets, by taking the functional derivative in (2.4) directly

$$L(1,2;1',2') = -\left.\frac{\delta G(1,1';Q)}{\delta Q(2',2)}\right|_{Q=0}. \qquad (2.10)$$

From the Dyson equation (2.6) it follows via $\delta G = -G\,\delta G^{-1} G$ the relation

$$\left.\frac{\delta G(1,1';Q)}{\delta Q(2,2')}\right|_{Q=0} = G(1,2')G(2,1') + G(1,\bar{3})\left.\frac{\delta \Sigma_U(\bar{3},\bar{4};Q)}{\delta Q(2',2)}\right|_{Q=0} G(\bar{4},1'). \qquad (2.11)$$

Because Σ_U depends on Q only via G one derives from (2.11) with (2.10) the integral equation for L as

$$L(1,2;1',2') = -G(1,2')G(2,1') - iG(1,\bar{3})G(\bar{4},1')I(\bar{3},\bar{6};\bar{4},\bar{5})L(\bar{5},2;\bar{6},2'), \qquad (2.12)$$

where the irreducible particle-hole vertex I is determined by

$$\left.\frac{\delta \Sigma_U(1,1';Q)}{\delta G(2',2;Q)}\right|_{Q=0} = -iI(1,2;1',2'). \qquad (2.13)$$

Note that (2.13) is a necessary condition for approximations, too. Thus, after choosing an approximate Σ_U one has to derive I from (2.13) and to insert into (2.12) for calculating the correlation function L.

The Bethe-Salpeter equation for Γ in the particle-hole channel is found by inserting (2.8) into (2.9) and combining with (2.12) to

$$\Gamma(1,2;1',2') = I(1,2;1',2') - iI(1,\bar{3};1',\bar{4})G(\bar{4},\bar{5})G(\bar{6},\bar{3})\Gamma(\bar{5},2;\bar{6},2'). \qquad (2.14)$$

Using (2.8), (2.9), and (2.11) we get the relation

$$\left.\frac{\delta \Sigma_U(1,1';Q)}{\delta Q(2',2)}\right|_{Q=0} = -i\Gamma(1,\bar{3};1',\bar{4})G(2,\bar{3})G(\bar{4},2'), \tag{2.15}$$

which includes Ward identities.

For the Hubbard interaction term (2.3) the self-energy Σ_U can be found by making use of (2.6), (2.9) to (2.11), and the identity $\delta G = -G\,\delta G^{-1}G$, yielding (cf. /10/)

$$\begin{aligned}\Sigma_{Uij,\sigma}(t,t';Q) &= -iU_i G_{ii,-\sigma}(t,t^+;Q)\delta_{ij}\delta(t-t') \\ &\quad + iU_i \sum_{\bar{i}} \int_{-\infty}^{\infty} d\bar{t}\, G_{i\bar{i},\sigma}(t,\bar{t};Q)\, \frac{\delta \Sigma_{U\bar{i}j,\sigma}(\bar{t},t';Q)}{\delta Q_{ii,-\sigma}(t^+,t)} .\end{aligned} \tag{2.16}$$

Here Q and G have been restricted to spin diagonality, and $t^+=t+0$.

In the case Q = 0 Fourier transforms with respect to time variables are introduced as

$$G_{\lambda_1\lambda_1'}(t_1,t_1') = \int \frac{dE}{2\pi} G_{\lambda_1\lambda_1'}(E) \exp\{-iE(t_1-t_1')\} , \tag{2.17}$$

and for two-particle quantities through

$$\begin{aligned}G^{II}_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(t_1,t_2;t_1',t_2') &= \int \frac{dE_1 dE_2 dE_1' dE_2'}{(2\pi)^4} 2\pi\, \delta(E_1+E_2-E_1'-E_2') \times \\ &\quad \times G^{II}_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E_1,E_2;E_1',E_2') \exp\{-i(E_1t_1+E_2t_2-E_1't_1'-E_2't_2')\} .\end{aligned} \tag{2.18}$$

Note that the spatial Fourier transformation is not performed because of lacking the translational symmetry.

Now (2.6) can be rewritten as

$$(G^{-1}(E))_{ij,\sigma} = (G_\Delta^{-1}(E))_{ij} - \Sigma_{Uij,\sigma}(E). \tag{2.19}$$

Taking Fourier coefficients of (2.16) for $Q\to 0$ and combining with (2.15) we get

$$\Sigma_{Uij,\sigma}(E) = -iU_i\int\frac{d\bar{E}}{2\pi}G_{ii,-\sigma}(\bar{E})e^{i\varepsilon\bar{E}}\delta_{ij}$$
$$+U_i\sum_{\bar{i}_1\bar{i}_2\bar{i}_3}\int\frac{dE_1dE_2}{(2\pi)^2}G_{i\bar{i}_1,\sigma}(E_1)G_{i\bar{i}_2,-\sigma}(E_2)G_{\bar{i}_3 i,-\sigma}(E_1+E_2-E)\Gamma_{\substack{\bar{i}_1\bar{i}_2 j\bar{i}_3\\ \sigma\,-\sigma\,\sigma\,-\sigma}}(E_1,E_2;E,E_1+E_2-E). \tag{2.20}$$

For brevity, hereafter convergence factors like $e^{i\varepsilon E}$ ($\varepsilon \to +0$) are dropped (as, e.g., in the second term of (2.20)).

The four-point vertex equation (2.14) for particle-hole scattering turns into

$$\Gamma_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E_1,E_2;\omega) = I_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E_1,E_2;\omega)$$
$$-i\sum_{\mu_1\mu_2\mu_3\mu_4}\int\frac{d\bar{E}}{2\pi}I_{\lambda_1\mu_1\lambda_1'\mu_2}(E_1,\bar{E}+\omega;\omega)G_{\mu_2\mu_3}(\bar{E})G_{\mu_4\mu_1}(\bar{E}+\omega)\Gamma_{\mu_3\lambda_2\mu_4\lambda_2'}(\bar{E},E_2;\omega), \tag{2.21}$$

with the abbreviation

$$\Gamma_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E_1,E_2;E_1+\omega,E_2-\omega) \equiv \Gamma_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E_1,E_2;\omega). \tag{2.22}$$

The variable ω denotes the energy transfer. In the case of small ω which we are interested in (i.e. $\omega \ll \mu$) one can set $\omega = 0$ in I in (2.21), as has been pointed out by Landau for the uniform Fermi liquid /4/. The correlation function L defined in (2.9) on the basis of (2.8) takes the Fourier transform

$$L_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E_1,E_2;\omega) = -2\pi\delta(E_1-E_2+\omega)G_{\lambda_1\lambda_2'}(E_1)G_{\lambda_2\lambda_1'}(E_2)$$
$$+\sum_{\mu_1\mu_2\mu_3\mu_4}G_{\lambda_1\mu_1}(E_1)G_{\lambda_2\mu_2}(E_2)i\Gamma_{\mu_1\mu_2\mu_3\mu_4}(E_1,E_2;\omega)G_{\mu_3\lambda_1'}(E_1+\omega)G_{\mu_4\lambda_2'}(E_2-\omega), \tag{2.23}$$

or L in terms of I from (2.12) reads

$$L_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E_1,E_2;\omega) = -2\pi\,\delta(E_1-E_2+\omega)G_{\lambda_1\lambda_2'}(E_1)G_{\lambda_2\lambda_1'}(E_2)$$
$$-\sum_{\mu_1\mu_2\mu_3\mu_4}G_{\lambda_1\mu_1}(E_1)G_{\mu_2\lambda_1'}(E_1+\omega)\int\frac{d\bar{E}}{2\pi}\,iI_{\mu_1\mu_4\mu_2\mu_3}(E_1,\bar{E}+\omega;\omega)L_{\mu_3\lambda_2\mu_4\lambda_2'}(\bar{E},E_2;\omega). \tag{2.24}$$

In the linear response theory the effective external field Q corresponding to a weak external field Q is defined by /8/

$$G(1,\bar{3})\tilde{Q}(\bar{3},\bar{4})G(\bar{4},1') = -L(1,\bar{2};1',\bar{2}')Q(\bar{2}',\bar{2}). \qquad (2.25)$$

According to (2.10) the r.h.s. of (2.25) describes the change of the one-particle Green function $\delta G(1,1';Q)$ correctly to the first order of Q; hereby the significance of L is founded. The Fourier transform of (2.25) under the restriction $Q_{\lambda_1\lambda_1'}(t_1,t_1') = Q_{\lambda_1\lambda_1'}(t_1)\delta(t_1-t_1')$ becomes

$$\sum_{\lambda_2\lambda_2'} G_{\lambda_1\lambda_2}(E+\omega)\tilde{Q}_{\lambda_2'\lambda_2}(E+\omega,E)G_{\lambda_2\lambda_1'}(E) = -\sum_{\lambda_2\lambda_2'}\int\frac{d\bar{E}}{2\pi} L_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E+\omega,\bar{E};-\omega)Q_{\lambda_2'\lambda_2}(\omega). \qquad (2.26)$$

By inserting (2.25) into (2.12) one gets

$$\tilde{Q}(1,1') = Q(1,1') - iI(1,\bar{2};1',\bar{2}')G(\bar{2}',\bar{3})G(\bar{4},\bar{2})\tilde{Q}(\bar{3},\bar{4}). \qquad (2.27)$$

Without loss of generality, choosing $Q_{\lambda_1\lambda_1'}(t_1,t_1') = Q_{\lambda_1\lambda_1'}(t_1)\delta(t_1-t_1')$ once more, the Fourier transform of (2.27) reads

$$\begin{aligned}\tilde{Q}_{\lambda_1\lambda_1'}(E+\omega,E) &= Q_{\lambda_1\lambda_1'}(\omega)\\ &- i\sum_{\mu_1\mu_2\mu_3\mu_4}\int\frac{d\bar{E}}{2\pi} I_{\lambda_1\mu_1\lambda_1'\mu_2}(E+\omega,\bar{E};-\omega)G_{\mu_2\mu_3}(\bar{E}+\omega)G_{\mu_4\mu_1}(\bar{E})\tilde{Q}_{\mu_3\mu_4}(\bar{E}+\omega,\bar{E}).\end{aligned} \qquad (2.28)$$

Physical information of interest is contained in the expectation value of a one-particle operator $A = \sum_{\lambda_1\lambda_2} c^+_{\lambda_1} A_{\lambda_1\lambda_2} c_{\lambda_2}$ in the presence of the external field Q introduced in (2.25) and (2.27). Then, the time-dependent expectation value of A can be expressed by

$$\langle A(t)\rangle = -i\sum_{\lambda_1\lambda_2} G_{\lambda_2\lambda_1}(t,t^+;Q)A_{\lambda_1\lambda_2}(Q), \qquad (2.29)$$

where $A_{\lambda_1\lambda_2}(Q)$ refers to an explicit field dependence. In general we have to consider the first order (proportional to the applied field) change of G and of the operator A itself, too. Thus, the variation of (2.29) is written as $\delta\langle A(t)\rangle = \delta\langle A(t)\rangle^{(1)} + \delta\langle A(t)\rangle^{(2)}$.

According to (2.10) and (2.25) the correlation part of the physical response may be characterized by the change in the expectation value

$$\delta\langle A(t)\rangle^{(1)} = i\sum_{\lambda_1\lambda_2\lambda_3\lambda_4}\int dt' L_{\lambda_2\lambda_3\lambda_1\lambda_4}(t,t';t^+,t'^+)\,Q_{\lambda_4\lambda_3}(t',t')A_{\lambda_1\lambda_2}, \tag{2.30}$$

where the correlation function of coinciding time arguments occurs. Rewriting (2.30) in energy variables we get

$$\delta\langle A(\omega)\rangle^{(1)} = i\sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'}\int\frac{dE_1dE_2}{(2\pi)^2}L_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E_1,E_2;-\omega)A_{\lambda_1'\lambda_1}Q_{\lambda_2'\lambda_2}(\omega). \tag{2.31}$$

Moreover, the second contribution to the linear response arising from the change $\delta A_{\lambda_1\lambda_2}$ in (2.29) is

$$\delta\langle A(\omega)\rangle^{(2)} = -i\sum_{\lambda_1\lambda_2}G_{\lambda_2\lambda_1}(0^+)\,\delta A_{\lambda_1\lambda_2}(\omega), \tag{2.32}$$

where $G_{\lambda_2\lambda_1}(0^+) = G_{\lambda_2\lambda_1}(t,t^+)$.

3. LADDER APPROXIMATION IN TWO CHANNELS

Now we are looking for a self-consistent approximation (cf. the scheme in [9]) concerning the correlation function L. This can be realized by choosing at the beginning an approximate Σ_U, calculating then I from this Σ_U via (2.13), and inserting finally the approximate I into (2.24) to evaluate L.

Start from a local approximation in the particle-particle channel (s-channel) by assuming a site-diagonal vertex Γ in (2.20) which depends only on the sum of energies (E_1+E_2) of the interacting electrons, i.e. $\Gamma_{\substack{iiii\\ \sigma-\sigma\sigma-\sigma}}(E_1,E_2;E,E_1+E_2-E)$ in (2.20) is replaced shortly by the scattering amplitude $T_i(E_1+E_2)$. Then it results in the local self-energy

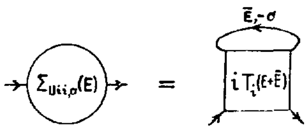
$$\Sigma_{Uii,\sigma}(E) = \int \frac{d\bar{E}}{2\pi i} G_{ii,-\sigma}(\bar{E}) T_i(E+\bar{E}), \tag{3.1a}$$

where

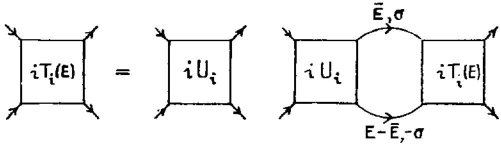
$$T_i(E) = \left[\frac{1}{U_i} + \int \frac{d\bar{E}}{2\pi i} G_{ii,\sigma}(\bar{E}) G_{ii,-\sigma}(E-\bar{E})\right]^{-1}. \tag{3.2a}$$

Here the renormalized G obeys the Dyson equation (2.19), where $\Sigma_{Uij,\sigma}(E) = \Sigma_{Uii,\sigma}(E)\,\delta_{ij}$. The convolution integral (3.2a) reflects contact interaction only between electrons having different spin directions, i.e. $T_i = T_{i,\sigma-\sigma\sigma-\sigma}$ according to the bare interaction U_i.

The diagrammatic representation of (3.1a) and (3.2a) is known as the horizontal ladder approximation (arrowed lines denote the dressed G):



(3.1b)



(3.2b)

This approximation was proposed by Babanov et al. /2/ for pure systems. A partially averaged version was given in /6/, whereas at present we consider the completely random case of the whole configuration $\{\nu\}$.

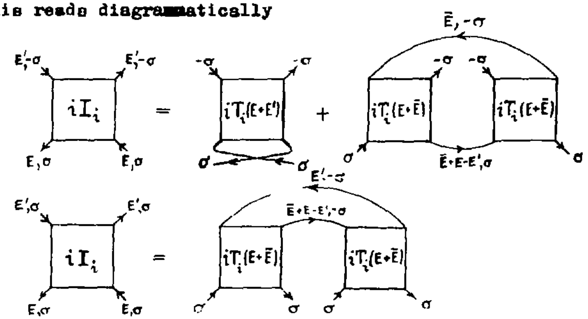
According to (2.13) the Fourier transform of the irreducible particle-hole vertex I at zero energy transfer has to satisfy the relation

$$\frac{\delta \Sigma_{ii,\sigma}(E)}{\delta G_{ii,\sigma'}(E')} = -\,i\,I_{\substack{iiii\\ \sigma\sigma'\sigma\sigma'}}(E,E';E,E') \equiv -i\,I_{i,\sigma\sigma'}(E,E'), \tag{3.3}$$

where I can be found explicitly from (3.1) and (3.2) as

$$\begin{aligned} I_{i,\sigma\sigma'}(E,E') = &-\int\frac{d\bar{E}}{2\pi i}G_{ii,-\sigma}(\bar{E})G_{ii,-\sigma}(E+\bar{E}-E')\left[T_i(E+\bar{E})\right]^2\delta_{\sigma\sigma'} \\ &+\left(T_i(E+E')-\int\frac{d\bar{E}}{2\pi i}G_{ii,-\sigma}(\bar{E})G_{ii,\sigma}(E+\bar{E}-E')\left[T_i(E+\bar{E})\right]^2\right)(1-\delta_{\sigma\sigma'}). \end{aligned} \tag{3.4a}$$

This reads diagrammatically

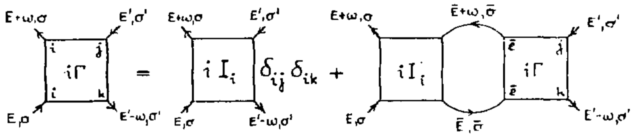


(3.4b)

From (2.21), on the basis of the locality of (3.4) one gets the equation for the total vertex in the particle-hole channel (t-channel) in the form

$$\begin{aligned} \Gamma_{\substack{ijik\\ \sigma\sigma'\sigma\sigma'}}(E,E';\omega) = &\,I_{i,\sigma\sigma'}(E,E';\omega)\delta_{ij}\delta_{ik} \\ &-i\sum_{\ell\bar{\sigma}}\int\frac{d\bar{E}}{2\pi}I_{i,\sigma\bar{\sigma}}(E,\bar{E}+\omega;\omega)G_{i\ell,\bar{\sigma}}(\bar{E})G_{\ell i,\bar{\sigma}}(\bar{E}+\omega)\Gamma_{\substack{\ell j\ell k\\ \bar{\sigma}\sigma'\bar{\sigma}\sigma'}}(\bar{E},E';\omega), \end{aligned} \tag{3.5a}$$

which can be represented graphically by



(3.5b)

It is pointed out that the ω -dependence of I can be neglected for energies near the Fermi energy (cf. (2.21)), so that I from (3.4) fits to (3.5).

4. ELECTRICAL CONDUCTIVITY

In order to evaluate the ac conductivity tensor $\sigma_{\alpha\beta}(\omega)$ defined by the relation $\langle\langle j_\alpha(\omega)\rangle\rangle_c = \sigma_{\alpha\beta}(\omega)E_\beta(\omega)$ between the configurational-averaged, induced average current $\langle\langle \vec{j}(\omega)\rangle\rangle_c$ and the spatially homogeneous external electric field $\vec{E}(\omega)$, we have to insert into (2.31), instead of $A_{\lambda_1'\lambda_1}$, the matrix elements of the α -component of the current operator j_α , and to set $Q_{\lambda_2'\lambda_2} = -\frac{1}{c}\vec{j}_{\lambda_2'\lambda_2}\cdot\vec{A}$ for coupling via the vector potential $\vec{A}$. Thus, from (2.21) and (2.22) by using $\vec{E} = -\frac{1}{c}\frac{\partial\vec{A}}{\partial t}$ one gets the real part of the conductivity tensor as ($\langle\ldots\rangle_c$ denotes configurational averaging)

$$\sigma'_{\alpha\beta}(\omega) = -\frac{1}{\omega}\,\mathrm{Re}\left\langle\sum_{\lambda_1\lambda_2\lambda_1'\lambda_2'}\int\frac{dE_1dE_2}{(2\pi)^2}L_{\lambda_1\lambda_2\lambda_1'\lambda_2'}(E_1,E_2;E_1-\omega,E_2+\omega)\,j_{\alpha,\lambda_1'\lambda_1}\,j_{\beta,\lambda_2'\lambda_2}\right\rangle_c , \qquad (4.1)$$

where the current operator given by

$$j_\alpha = -ie\sum_{ij\sigma}t_{ij}(R_{\alpha i}-R_{\alpha j})c^+_{i\sigma}c_{j\sigma} \qquad (4.2)$$

takes random matrix elements in the Wannier space if off-diagonal disorder is included. Calculating the change of the current operator via $\delta j_\alpha = \frac{ie}{c} \sum_{i\sigma\beta} R_{\alpha i} \left[n_{i\sigma}, j_\beta \right] A_\beta$ and inserting into (2.32) yields an additive conductivity term $\sigma^{(2)}_{\alpha\beta}(\omega)$ which does not contribute to the real part given in (4.1).

Comparison with (2.26) shows that it is convenient to introduce the external field vertex Λ_α into (4.1) by

$$\sigma'_{\alpha\beta}(\omega) = \frac{1}{\omega} \mathrm{Re} \Big\langle \sum_{\lambda_1\lambda_2\lambda'_1\lambda'_2} j_{\alpha,\lambda'_1\lambda_1} \int \frac{dE_1}{2\pi} G_{\lambda_1\lambda'_2}(E_1+\omega) \Lambda_{\beta,\lambda'_2\lambda_2}(E_1+\omega,E_1) G_{\lambda_2\lambda'_1}(E_1) \Big\rangle_c . \tag{4.3a}$$

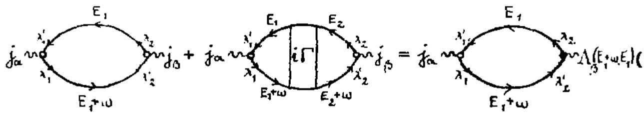
According to $Q_{\lambda'_2\lambda_2}(\omega) = -\frac{1}{c} \vec{j}_{\alpha,\lambda_2\lambda'_2} \cdot \vec{A}_\alpha(\omega)$ we separate the current vertex Λ_α from the effective external field $\tilde{Q}$ by $\tilde{Q}_{\lambda'_2\lambda_2}(E+\omega,E) = -\frac{1}{c} \sum_\alpha \Lambda_{\alpha,\lambda'_2\lambda_2} A_\alpha(\omega)$. Thus, the integral equation (2.28) can be rewritten as

$$\Lambda_{\alpha,\lambda_1\lambda'_1}(E+\omega,E) = j_{\alpha,\lambda_1\lambda'_1} - i \sum_{\mu_1\mu_2\mu_3\mu_4} \int \frac{d\bar{E}}{2\pi} I_{\lambda_1\mu_1\lambda'_1\mu_2}(E+\omega,\bar{E};\omega) G_{\mu_2\mu_3}(\bar{E}+\omega) G_{\mu_4\mu_1}(\bar{E}) \Lambda_{\alpha,\mu_3\mu_4}(\bar{E}+\omega,\bar{E}) . \tag{4.4a}$$

On the other hand, (4.4a) can be verified by combining (4.1) and (4.3) with (2.24). To express Λ_α directly in terms of the total vertex Γ from (2.23), (4.1), and (4.3), we write

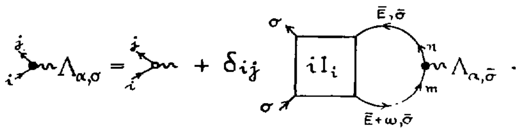
$$\Lambda_{\alpha,\lambda_1\lambda'_1}(E+\omega,E) = j_{\alpha,\lambda_1\lambda'_1} - i \sum_{\mu_1\mu_2\mu_3\mu_4} \int \frac{d\bar{E}}{2\pi} \Gamma_{\lambda_1\mu_1\lambda'_1\mu_2}(E+\omega,\bar{E};-\omega) G_{\mu_2\mu_3}(\bar{E}+\omega) G_{\mu_4\mu_1}(\bar{E}) j_{\alpha,\mu_3\mu_4} . \tag{4.5}$$

The connection between (4.3a) and (4.5) can be illustrated by electron-hole bubbles:



(4.3b)

Further, the diagrams of (4.4a) with the local kernel I of (3.4) are



(4.4b)

Note that (4.4) involving three I terms has an analogous form to the vertex equation for the ordered case in /11/. Writing out Λ_α in detail with (4.4) we have two terms

$$\sigma'_{\alpha\beta}(\omega) = \frac{1}{\omega}\,\mathrm{Re}\int\frac{dE}{2\pi}\left\langle \mathrm{tr}\left\{ j_\alpha G(E+\omega)\, j_\beta G(E)\right\}\right\rangle_c + \tilde\sigma'_{\alpha\beta}(\omega), \tag{4.6}$$

where

$$\tilde\sigma'_{\alpha\beta}(\omega) = \frac{1}{\omega}\,\mathrm{Re}\int\frac{dE_1}{2\pi}\left\langle \sum_{i\sigma} K_{\alpha,ii,\sigma}(E_1,E_1+\omega)\Lambda_{\beta,ii,\sigma}(E_1+\omega,E_1)\right\rangle_c , \tag{4.7}$$

$$K_{\alpha,ii,\sigma}(E_1,E_2) = \sum_{j\bar j} G_{ij,\sigma}(E_1)\, j_{\alpha,j\bar j}\, G_{\bar j i,\sigma}(E_2). \tag{4.8}$$

The trace in the first term of (4.6) is to be taken over one-electron λ states with spin included.

The problem of configurational averaging in (4.7) is beyond the CPA. To proceed, we employ a chain factorization by setting $\langle K_\alpha\Lambda_\beta\rangle_c = \langle K_\alpha\rangle_c\langle\Lambda_\beta\rangle_c$. Thus, working in k-space one gets with (4.2) the off-diagonal CPA result /12/

$$\begin{aligned} K^R_{\alpha,\sigma}(z_1,z_2) &= \langle G_\sigma(z_1)\, j_\alpha G_\sigma(z_2)\rangle_{c,ii} \\ &= \frac{e}{N}\sum_{\vec k} \mathcal{G}_{\vec k\sigma}(z_1)\mathcal{G}_{\vec k\sigma}(z_2)\frac{\partial}{\partial k_\alpha}\left\{t^{BB}s(\vec k)+\frac{1}{2}\left(\Sigma_\sigma(\vec k,z_1)+\Sigma_\sigma(\vec k,z_2)\right)\right\}. \end{aligned} \tag{4.9}$$

The superscript "R" refers to the resolvent obtained by analytical continuation to retarded and (or) advanced Green functions (cf. also (4.11) to (4.13)); the subscript "c,ii" means taking the site-diagonal element after averaging. The coherent quantities on the r.h.s. of (4.9) are defined below (see (4.16) to (4.18)).

Using the time reversal symmetry relation (f being an arbitrary function)

$$\sum_{\vec{k}} f(s(\vec{k}))\,\frac{\partial s(\vec{k})}{\partial k_\alpha} = 0\,, \tag{4.10}$$

one can prove that $K^R_{\alpha\sigma}$ given by (4.9) vanishes identically, i.e. $\tilde{\sigma}'_{\alpha\beta}(\omega) = 0$. This conclusion seems to be more general because products (4.8) with inner factors j_α should vanish. A similar proof for the ordered case yields immediately $\tilde{\sigma}'_{\alpha\beta}(\omega) = 0$ within the local approximation.

Next we go over from causal Green functions in (4.6) to advanced ("a") and retarded ("r") ones. Using the abbreviations

$$D(\omega) = \int \frac{dE}{2\pi}\,\Pi(E+\omega,E) \tag{4.11}$$

and

$$\Pi(E+\omega,E) = G_{\lambda_1\lambda_2'}(E+\omega)\,G_{\lambda_2\lambda_1'}(E) \tag{4.12}$$

one can perform analytical continuation by spectral theorems to write

$$D(\omega) = \int_{-\infty}^{\infty} \frac{dE}{2\pi}\Big[f(E+\omega)\,\Pi^{aa}(E+\omega,E) - f(E)\,\Pi^{rr}(E+\omega,E) + \big(f(E)-f(E+\omega)\big)\,\Pi^{ra}(E+\omega,E)\Big],\quad \omega>0. \tag{4.13}$$

Here Π^{aa} means replacing both Green functions in (4.12) by advanced ones, etc.; at zero temperature we have the Fermi function $f(E) = \Theta(E-\mu)$ with μ being the chemical potential. An analogous expression to (4.13) can be derived for $\omega < 0$.

Using (4.11) to (4.13) and combining with the relations $G^r_{\lambda\lambda'} = (G^a_{\lambda'\lambda})^*$, $j_{\alpha,\lambda\lambda'} = (j_{\alpha,\lambda'\lambda})^*$, and $\sigma_{\alpha\beta} = \sigma_{\beta\alpha}$ (fulfilled in cubic lattices), from (4.6) we obtain

$$\sigma^{r'}_{\alpha\beta}(\omega) = \frac{1}{4\pi}\int_{-\infty}^{\infty} dE \left(\frac{f(E)-f(E+\omega)}{\omega}\right)\Big\langle tr\Big\{ j_\alpha G^r(E+\omega) j_\beta G^a(E) + j_\alpha G^a(E+\omega) j_\beta G^r(E) - j_\alpha G^r(E+\omega) j_\beta G^r(E) - j_\alpha G^a(E+\omega) j_\beta G^a(E)\Big\}\Big\rangle_c . \tag{4.14}$$

This is the Kubo-Greenwood formula, but with Green functions renormalized by electron correlations within the ladder approximation (3.1) and (3.2). Note that $\sigma^{r'}_{\alpha\beta}(\omega)$ reflects the retarded response valid for all ω ; in getting (4.14) we have used the Bose-type relation $\sigma'_{\alpha\beta}(\omega) = \mathrm{sign}\,\omega\ \sigma^{r'}_{\alpha\beta}(\omega)$.

To average configurationally in the presence of off-diagonal randomness, we restrict ourselves to nearest-neighbour hopping integrals in the additive limit $t^{AB} = \frac{1}{2}(t^{AA}+t^{BB})$. The CPA result including current vertex corrections due to the off-diagonal disorder is /12/

$$\langle tr\{ j_\alpha G(z_1) j_\alpha G(z_2)\}\rangle_c = e^2 \sum_{\vec{k}\sigma} \mathcal{G}_{\vec{k}\sigma}(z_1)\mathcal{G}_{\vec{k}\sigma}(z_2)\Big[\frac{\partial}{\partial k_\alpha}\Big\{ t^{BB} s(\vec{k}) + \frac{1}{2}(\Sigma_\sigma(\vec{k},z_1)+\Sigma_\sigma(\vec{k},z_2))\Big\}\Big]^2 + e^2\sum_{\vec{k}\sigma}\big[\sigma_{2\sigma}(z_1)\mathcal{G}_{\vec{k}\sigma}(z_2) + \sigma_{2\sigma}(z_2)\mathcal{G}_{\vec{k}\sigma}(z_1)\big]\Big[\frac{\partial s(\vec{k})}{\partial k_\alpha}\Big]^2, \tag{4.15}$$

where

$$\mathcal{G}_{\vec{k}\sigma}(z) = \langle G_\sigma(z)\rangle_{c,\vec{k}} = (z - \varepsilon^B - t^{BB} s(\vec{k}) - \Sigma_\sigma(\vec{k},z))^{-1}, \tag{4.16}$$

$$\Sigma_\sigma(\vec{k},z) = \sigma_{0\sigma}(z) + 2\sigma_{1\sigma}(z) s(\vec{k}) + \sigma_{2\sigma}(z) s^2(\vec{k}), \tag{4.17}$$

$$s(\vec{k}) = \sum_{j(\neq i)}{}' e^{i\vec{k}(\vec{R}_j - \vec{R}_i)}. \tag{4.18}$$

Here $\mathcal{G}_{\vec{k}\sigma}(z)$ is the coherent Green function, $\Sigma_\sigma(k,z)$ is the coherent potential, and $s(k)$ denotes the nearest-neighbour structure factor (cf. (4.9)). The self-energy parts $\sigma_{0\sigma}$, $\sigma_{1\sigma}$, $\sigma_{2\sigma}$

including $\Sigma_{U ii,\sigma}$ from (3.1) and (3.2) can be determined within the coherent ladder approximation scheme given in /6/. It should be mentioned that (4.15) is consistent with the Ward identity reflecting the gauge invariance of the configurationally averaged system.

In the case of only diagonal disorder we have no vertex corrections. Then, the dissipative part of the scalar dc conductivity becomes

$$\sigma'(\omega \to 0) = \frac{1}{\pi} \sum_{k,\sigma} j_{\alpha,k}^{2} \left[\operatorname{Im} \mathcal{G}_{k\sigma}^{+}(\mu) \right]^{2}. \tag{4.19}$$

Note that (4.19) involves the undamped conductivity result for the ordered case, too.

5. MAGNETIC SUSCEPTIBILITY (ORDERED CASE)

As a first step for treating the magnetic analog to the situation described in Section 4, we calculate in the following the magnetic susceptibility for pure systems. The longitudinal spin susceptibility at T=0 is given by

$$\chi_{ij}(\omega) = -\mu_B^2 \sum_{\sigma\sigma'} \int \frac{dE_1 dE_2}{(2\pi)^2}\, i L_{\substack{ij\,ij \\ \sigma\sigma'\sigma\sigma'}}(E_1, E_2; E_1 - \omega, E_2 + \omega)\,\sigma\sigma', \tag{5.1}$$

where μ_B is the Bohr magneton. This expression reflects the linear response to a weak external magnetic field $h_i(t) = h_0 e^{i(\vec{k}\vec{R}_i - \omega t)}$ applied parallel to the z-axis. By inserting $A = m_i = \mu_B \sum_\sigma \sigma\, n_{i\sigma}$, i.e. $A_{\lambda_1\lambda_2} = A_{mn} = \mu_B \sigma \delta_{\sigma\sigma'} \delta_{ni} \delta_{mi}$, and $Q_{\lambda_1\lambda_2}(t) = Q_{mn}(t) = -\mu_B h_m(t) \cdot \sigma^{\sigma\sigma'} \delta_{\sigma\sigma'} \delta_{mn}$, one gets (5.1) via the relation $\delta\langle m_i(\omega)\rangle = \sum_j \chi_{ij}(\omega) h_j(\omega)$. Here $\delta\langle m_i(\omega)\rangle$ is the change of the magnetic moment on site $\vec{R}_i$ arising from the expectation value of the operator m_i. It is pointed out that the contribution to χ coming from (2.32) tends to zero (in the paramagnetic phase).

According to (2.26) one can introduce the spin vertex Λ by

$$\begin{aligned} \chi(\vec{k},\omega) &= \frac{1}{N}\sum_{ij}\chi_{ij}(\omega)e^{-i\vec{k}(\vec{R}_i-\vec{R}_j)} \\ &= \frac{\mu_B^2}{N}\sum_{ij\sigma}\sigma\int\frac{dE_1}{2\pi}G_{ij,\sigma}(E_1+\omega)\,i\Lambda_{j\sigma}(E_1+\omega,E_1)G_{ji,\sigma}(E_1)e^{-i\vec{k}\vec{R}_i}, \end{aligned} \tag{5.2a}$$

where Λ has been separated from the external field $\tilde{Q}$ through $\tilde{Q}_{\lambda_1\lambda_2}(E+\omega,E) = -\mu_B h_o e^{i\omega t}\Lambda_{\lambda_1}(E+\omega,E)\,\delta_{\lambda_1\lambda_2}$. Note that the spin-flip situation is excluded.

From (2.28) we get

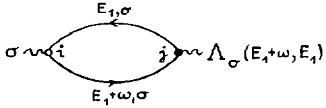
$$\Lambda_{i\sigma}(E+\omega,E) = \sigma e^{i\vec{k}\vec{R}_i} - \sum_{j\sigma'}\int\frac{d\bar{E}}{2\pi}\,i\,I_{i,\sigma\sigma'}(E+\omega,\bar{E};-\omega)G_{ij,\sigma'}(\bar{E}+\omega)G_{ji,\sigma'}(\bar{E})\Lambda_{j\sigma'}(\bar{E}+\omega,\bar{E}), \tag{5.3}$$

and, more explicitly, by using I at $\omega = 0$ from (3.4) it follows

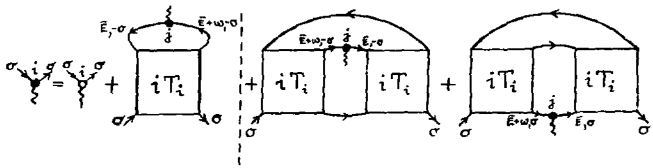
$$\begin{aligned} \Lambda_{i\sigma}(E+\omega,E) &= \sigma e^{ik\vec{R}_i} - \sum_{j}\int\frac{d\bar{E}}{2\pi}\,iT_i(E+\bar{E})G_{ij,-\sigma}(\bar{E}+\omega)G_{ji,-\sigma}(\bar{E})\Lambda_{j-\sigma}(\bar{E}+\omega,\bar{E}) \\ &+ \sum_{j}\int\frac{d\bar{E}\,d\bar{\bar{E}}}{(2\pi)^2}G_{ii,-\sigma}(\bar{\bar{E}})G_{ii,\sigma}(E+\bar{\bar{E}}-\bar{E})\left[T_i(E+\bar{\bar{E}})\right]^2G_{ij,-\sigma}(\bar{E}+\omega)G_{ji,-\sigma}(\bar{E})\Lambda_{j-\sigma}(\bar{E}+\omega,\bar{E}) \\ &+ \sum_{j}\int\frac{d\bar{E}\,d\bar{\bar{E}}}{(2\pi)^2}G_{ii,-\sigma}(\bar{\bar{E}})G_{ii,-\sigma}(E+\bar{\bar{E}}-\bar{E})\left[T_i(E+\bar{\bar{E}})\right]^2G_{ij,\sigma}(\bar{E}+\omega)G_{ji,\sigma}(\bar{E})\Lambda_{j\sigma}(\bar{E}+\omega,\bar{E}). \end{aligned} \tag{5.4a}$$

To generalize later the calculations to the disordered case, we retain the dummy index i for the quantities I_i, T_i and G_{ii}. Note that the off-diagonal elements of Λ in spin and lattice spaces vanish identically, provided a local vertex I is only taken into account. The equation (5.3) can be verified on the basis of (2.24), too.

Diagrams representing (5.2a) and (5.4a) take the form



(5.2b)



(5.4b)

Further, the unperturbed system is assumed to be paramagnetic, i.e. $\Sigma_{Uii,\sigma} = \Sigma_{Uii,-\sigma} = \Sigma_{Uii}$, implying $G_{ii,\sigma} = G_{ii,-\sigma} = G_{ii}$. Then, by making the ansatz $\Lambda_{i\sigma}(E+\omega,E) = \sigma\Lambda_i(E+\omega,E)$ eq. (5.4) simplifies to

$$\Lambda_i(E+\omega,E) = e^{i\vec{k}\vec{R}_i} + \sum_j \int \frac{d\bar{E}}{2\pi} iT_i(E+\bar{E})G_{ij}(\bar{E}+\omega)G_{ji}(\bar{E})\Lambda_j(\bar{E}+\omega,\bar{E}), \qquad (5.5)$$

which can be performed by putting $\Lambda_i(E+\omega,E) = \Lambda_{\vec{k}}(E+\omega,E)e^{i\vec{k}\vec{R}_i}$ to

$$\Lambda_{\vec{k}}(E+\omega,E) = 1 + \int \frac{d\bar{E}}{2\pi} iT_i(E+\bar{E}) \frac{1}{N}\sum_{\vec{k}'} G_{\vec{k}'+\vec{k}}(\bar{E}+\omega)G_{\vec{k}'}(\bar{E})\Lambda_{\vec{k}}(\bar{E}+\omega,\bar{E}). \qquad (5.6)$$

Now from (5.2) one obtains the dynamic paramagnetic susceptibility

$$\chi(\vec{k},\omega) = \frac{2\mu_B^2}{N}\sum_{\vec{k}'}\int \frac{d\bar{E}}{2\pi} G_{\vec{k}'+\vec{k}}(\bar{E}+\omega)G_{\vec{k}'}(\bar{E}) i\Lambda_{\vec{k}}(\bar{E}+\omega,\bar{E}). \qquad (5.7)$$

For practical calculations the system of eqs. (5.6) and (5.7) is not convenient. Following /13/, by approximating the energy dependence of the scattering amplitude in (5.6) (compare (3.1)) as

$$T_i(E+\bar{E}) \longrightarrow \bar{T}_i(E) = \frac{\Sigma_{Uii}(E)}{n_i} \qquad (5.8)$$

we get the result

$$\chi(\vec{k},\omega) = \frac{\frac{2\mu_B^2}{N} i \sum_{\vec{k}'} \int \frac{d\bar{E}}{2\pi} G_{\vec{k}'+\vec{k}}(\bar{E}+\omega) G_{\vec{k}'}(\bar{E})}{1 - \frac{i}{n_i} \frac{1}{N} \sum_{\vec{k}'} \int \frac{d\bar{E}}{2\pi} G_{\vec{k}'+\vec{k}}(\bar{E}+\omega) G_{\vec{k}'}(\bar{E}) \Sigma_{Uii}(\bar{E})} \quad . \tag{5.9}$$

Here Σ_{Uii} must be determined by solving strictly (3.1) and (3.2) together with (2.19), n_i being the average electron number per site per spin, where the index i in Σ_{Uii} and n_i is again fictitious.

The transition to the static paramagnetic susceptibility is performed in the so-called k-limit /4/ (see also the k-limit discussion in /14/) yielding the correlation-enhanced expression

$$\chi(\vec{k}\to 0, \omega=0) = \frac{2\mu_B^2 i \int \frac{d\bar{E}}{2\pi} (G^2(\bar{E}))_{ii}}{1 - \frac{i}{n_i} \int \frac{d\bar{E}}{2\pi} (G^2(\bar{E}))_{ii} \Sigma_{Uii}(\bar{E})} \quad . \tag{5.10}$$

The form of (5.10) refers to instabilities of the paramagnetic phase towards ferromagnetic ordering, arising from the condition $\chi^{-1}(\vec{k}\to 0, \omega=0) = 0$. In the Hartree-Fock approximation $\Sigma_{Uii} = Un_i$, from (5.10) one gets immediately the well-known RPA result (according to the vertex $\Gamma = -U/(1-U\varrho(\mu))$, cf. (3.5))

$$\chi^{HF} = \frac{2\mu_B^2 \varrho(\mu)}{1 - U\varrho(\mu)} \quad , \tag{5.11}$$

which gives for noninteracting electrons the Pauli susceptibility $\chi_0 = 2\mu_B^2 \varrho_0(\mu)$. $\varrho(\mu)$ is the single-particle density of states (per site per spin) at the Fermi level.

Next, we discuss the Ward identity related to the susceptibility calculation (cf., e.g., /15/). Starting with the Fourier transform of (2.15) we can express the first order variation of the self-energy Σ_U with respect to the external field δQ by

$$\delta\Sigma_{U\lambda_1\lambda_1'}(E+\omega, E; Q) = -\sum_{\lambda_2\lambda_2'\lambda_3\lambda_4} \int \frac{d\bar{E}}{2\pi} i\Gamma_{\lambda_1\lambda_3\lambda_1'\lambda_4}(E+\omega, \bar{E}; -\omega) G_{\lambda_2\lambda_3}(\bar{E}) G_{\lambda_4\lambda_2'}(\bar{E}+\omega) \delta Q_{\lambda_2'\lambda_2}(\omega) . \tag{5.12}$$

By inserting into (5.12) the inhomogeneous magnetic field $h_i = he^{i(\vec{k}\vec{R}_i-\omega t)}$ via δQ (compare the context of (5.1)) we get by performing $\lim_{\vec{k}\to 0}\lim_{\omega\to 0}$ the Ward identity

$$\left(\frac{\partial \Sigma_{Uii,\sigma}(E;h)}{\partial h}\right)_{h=0} = \mu_B \sum_{jk\sigma'} \int \frac{d\bar{E}}{2\pi} i\Gamma_{\substack{ijik\\ \sigma\sigma'\sigma\sigma'}}(E,\bar{E})\left(G_{\sigma'}(\bar{E})\sigma' G_{\sigma'}(\bar{E})\right)_{jk}, \qquad (5.13)$$

where the vertex $\Gamma_{ijik}(E,\bar{E}) = \Gamma_{ijik}(E,\bar{E};E,\bar{E})$ denotes zero energy transfer. Substituting (3.5) at $\omega=0$ into (5.13) one finds

$$\left(\frac{\partial \Sigma_{Uii,\sigma}(E;h)}{\partial h}\right)_{h=0} = \mu_B \sum_{\sigma'} \int \frac{d\bar{E}}{2\pi} i I_{ii,\sigma\sigma'}(E,\bar{E})\left(G_{\sigma'}(\bar{E})\sigma' G_{\sigma'}(\bar{E})\right)_{ii}$$
$$- \sum_{j\sigma'} \int \frac{d\bar{E}}{2\pi} i I_{ii,\sigma\sigma'}(E,\bar{E}) G_{ij,\sigma'}(\bar{E}) G_{ji,\sigma'}(\bar{E}) \left(\frac{\partial \Sigma_{Ujj,\sigma'}(\bar{E};h)}{\partial h}\right)_{h=0}. \qquad (5.14)$$

Comparison of (5.14) with the k-limit of (5.3) leads to

$$\left(\frac{\partial \Sigma_{Uii,\sigma}(E;h)}{\partial h}\right)_{h=0} = \mu_B\left(\sigma - \Lambda_{i\sigma}(E,E)\right), \qquad (5.15)$$

where the index i is retundant.

By inserting $\Lambda_{i\sigma}$ from (5.15) into the $\vec{k}$-limit of (5.2) one verifies the static susceptibility $\chi \equiv \chi(\vec{k}\to 0,\omega=0)$ to be

$$\chi = \mu_B i \sum_\sigma \sigma \int \frac{dE}{2\pi}\left(G_\sigma^2(E)\right)_{ii}\left(\mu_B\sigma - \left(\frac{\partial \Sigma_{Uii\sigma}(E;h)}{\partial h}\right)_{h=0}\right) = -\mu_B i \sum_\sigma \sigma \int \frac{dE}{2\pi}\left(\frac{\partial G_{ii,\sigma}(E;h)}{\partial h}\right)_{h=0}, \qquad (5.16)$$

which is equivalent to $\chi = \sum_\sigma \sigma \left(\frac{\partial n_{i\sigma}(h)}{\partial h}\right)_{h=0}$.

Moreover, within the approximation (5.8), from (5.5), (5.2), and (5.15) in the paramagnetic phase one can deduce the relation

$$\left(\frac{\partial \Sigma_{Uii,\sigma}(E;h)}{\partial h}\right)_{h=0} = -\sigma \frac{\Sigma_{Uii}(E)}{2\mu_B n_i}\chi. \qquad (5.17)$$

6. CONCLUSION

In order to calculate correlation functions in substitutionally disordered systems with narrow energy bands, we have proposed a microscopic Fermi liquid approach in terms of Wannier functions. When the kernel, appearing in the vertex and (or) correlation function equations, is of short range (say local), we have derived explicit expressions for the electrical conductivity and magnetic susceptibility. The latter was found in the ordered case.

The equations (5.16) and (5.17) can be used as a starting point to calculate the static spin susceptibility with disorder included. Then, we have to replace, for instance, Σ_{Uii}, G_{ii}, and n_i by the corresponding configuration-dependent quantities, yielding a site-dependent susceptibility χ_i.

Approximations were constructed as to make them useful for a numerical analysis. Numerical results based on the present approximation will be reported in a subsequent paper.

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