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OPTICAL CONDUCTIVITY  
IN THE HUBBARD MODEL

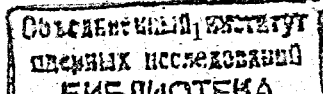
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# 1 Introduction

The discovery of high- $T_c$  superconductivity by Bednorz and Müller [1] in copper oxides has renewed interest to the Hubbard model since many unconventional properties of these materials are believed to be due to strong electron correlations [2]. Among them linear temperature dependence of resistivity and anomalous frequency dependence of optical conductivity (see, e.g., [3]). Theoretical studies of the optical conductivity for the Hubbard model [4, 5, 6] in the framework of Kubo linear response theory [7] started long time ago: it was investigated by the moment method [8], by the equation of motion method for the Green functions [9] in the Hubbard I [4] approximation [10] and in the Hubbard III [5] approximation [11, 12].

Later on most extensively the optical conductivity has been studied for the one-dimensional (1D) Hubbard model [13, 14, 15, 16, 17, 18, 19, 20, 21, 22] where results of numerical calculations for small clusters can be compared with a rigorous treatment on the basis of the Bethe ansatz exact solution [23]. For higher dimensions and in particular for the two-dimensional (2D) Hubbard model the strong coupling limit,  $U \gg t$ , has been considered mostly by numerical methods based on exact diagonalization for small clusters [24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34]. A detailed discussion of optical and photoemission sum rules for 1D and 2D Hubbard model has been given recently by Eskes et al. [35] by comparing a strong coupling perturbation theory in powers of  $t/U$  with numerical calculations. However, numerical investigations for small clusters have a poor frequency resolution to be quantitatively compared with experimental results. An analytical analysis of the frequency dependent conductivity has been given only by perturbation method [36, 37] in the limit of weak coupling,  $t \gg U$ . Therefore, an analytical investigation of one-particle and optical spectral functions in the strong coupling limit,  $t \ll U$ , is required.



To discuss physical properties of copper oxide compounds one usually starts from the multiband  $p-d$  model [38]. However, as has been recently shown [39] the two-band  $p-d$  model for copper oxide plain can be reduced to the two-band singlet-hole model which is essentially the asymmetric Hubbard model with nonequal hopping integrals  $t_{\alpha\beta}$  for the lower Hubbard band (LHB:  $\alpha = \beta = 1$ ) and the upper Hubbard band (UHB:  $\alpha = \beta = 2$ ). The LHB is occupied by one hole  $d$ -like states and the UHB is occupied by two-hole singlet states. Within the framework of this model single particle excitation spectra for the LHB and the UHB and their doping dependence have been calculated [39].

In the present paper a frequency dependent conductivity  $\sigma(\omega)$  is investigated for the asymmetric Hubbard model by applying the memory function technique [40] in terms of the Hubbard operators. A generalized Drude law with frequency and temperature dependent relaxation rates due to electron scattering on charge and spin fluctuations is obtained in the self-consistent Born approximation. It is shown that interband transitions ( $\propto t_{12}$ ) are essential for the Drude current relaxation which is proportional to  $[(t_{\alpha\alpha})^2 - (t_{12})^2]^2$  and cancels out for the symmetrical Hubbard model, ( $t_{\alpha\alpha} = t$ ). The present paper is a generalization of the optical conductivity calculations [41] for the  $p-d$  model where, however, a singlet band formation has not been taken into account and the conductivity has been considered only for the  $p$ -band.

The employment of the Hubbard operator technique has a twofold advantage. First of all by using equations of motion for the Hubbard operators we automatically take into account scattering of electrons on spin and charge fluctuations due to strong correlations as it has first been pointed out by Hubbard [5, 6]. In the Fermi liquid models (see, e.g. [42, 43, 44, 45]) one has to

introduce a phenomenological spin fluctuation scattering mechanism to obtain nonzero relaxation. To study the transport properties in the auxiliary field representation (see, e.g., [46] and the references therein) or in the gauge field technique [47, 48] one has to adopt a spin-charge separation condition which has been rigorously proved only for 1D Hubbard model. By employing the Hubbard operator representation we can also preserve rigorously restriction for no double occupancy for the LHB (or no single occupancy for the UHB) which is in the auxiliary field and the gauge field techniques has to be imposed by the local conservation law of the total number of fermions and bosons. The latter can be allowed for only approximately as, e.g., in the  $1/N$  expansion technique with  $N$  being the spin-orbital degeneracy (see, e.g., [46]). However, it is difficult to give an unambiguous physical interpretation of the obtained results for a realistic value of  $N = 2$ .

The paper is organized as follows. In the Section 2 the asymmetric Hubbard model is presented. In Section 3 a general expression for the frequency dependent conductivity in terms of the memory function is obtained. The calculation of the relaxation rate for the optical conductivity is given in Section 4. In the last Section 5 the obtained results are discussed and summarized.

## 2 Asymmetric Hubbard Model

The original one-band Hubbard model [4]

$$H = - \sum_{i \neq j \sigma} t_{ij} c_{i\sigma}^{\dagger} c_{j\sigma} + \frac{1}{2} U \sum_{i\sigma} n_{i\sigma} n_{i\bar{\sigma}} \quad (1)$$

has only two parameters: the hopping integrals  $t_{ij}$  between  $i$ -th and  $j$ -th lattice sites and the on-site Coulomb repulsion  $U$  for doubly occupied lattice sites,  $\bar{\sigma} = -\sigma$ . We introduce the Hubbard operators [6]:

$$X_i^{pq} = |i, p\rangle \langle i, q|, \quad X_i^{pq} X_i^{rs} = \delta_{qr} X_i^{ps} \quad (2)$$

for 4 possible states at a lattice site  $i$ :

$$|i, p\rangle = |i, 0\rangle, \quad |i, \sigma\rangle, \quad |i, \uparrow\downarrow\rangle \quad (3)$$

for an empty site, a singly occupied site by electron with spin  $\sigma = (\uparrow, \downarrow)$  and for a doubly-occupied site, respectively. For these states a completeness relation for the Hubbard operators (2) holds

$$X_i^{00} + \sum_{\sigma} X_i^{\sigma\sigma} + X_i^{22} = 1. \quad (4)$$

In terms of the Hubbard operators (2) the Hamiltonian (1) reads

$$H = E_1 \sum_{i\sigma} X_i^{\sigma\sigma} + E_2 \sum_i X_i^{22} - \sum_{i \neq j\sigma} t_{ij} \{X_i^{\sigma 0} X_j^{0\sigma} + X_i^{2\sigma} X_j^{\sigma 2} + 2\sigma (X_i^{2\bar{\sigma}} X_j^{0\sigma} + X_i^{\sigma 0} X_j^{\bar{\sigma} 2})\}. \quad (5)$$

Here  $2\sigma = \pm 1$  and we introduce energy levels  $E_1 = E_0 - \mu$  and  $E_2 = 2E_0 - 2\mu + U$  for singly and doubly occupied sites, respectively, where  $E_0$  is a reference energy and  $\mu$  is the chemical potential. The Hamiltonian (5) in the Hubbard operator representation is much easier to treat in the limit of strong correlations,  $U \gg |t_{ij}|$ , when the doubly occupied UHB is splitted from the singly occupied LHB. The algebra (2) for the Hubbard operators automatically preserves restriction of no double occupancy for the LHB (or no single occupancy for the UHB) which in the auxiliary field representation has to be imposed by local conservation law.

However, starting from the original one-band Hubbard model (1) we get a symmetrical representation (5) with equal hopping integrals  $t_{ij}$  for the LHB and UHB and their hybridization. To compare calculations with results for copper oxides in the present paper we consider a more realistic two-band  $p-d$  model reduced to a singlet-hole asymmetric Hubbard model with the LHB

occupied by one-hole Cu- $d$  like states and the UHB occupied by two-hole  $p-d$  singlet states [39]. The asymmetric Hubbard model reads:

$$H = H_0 + H_t = E_1 \sum_{i\sigma} X_i^{\sigma\sigma} + E_2 \sum_i X_i^{22} - \sum_{i \neq j\sigma} \{t_{ij}^{11} X_i^{\sigma 0} X_j^{0\sigma} + t_{ij}^{22} X_i^{2\sigma} X_j^{\sigma 2} + 2\sigma t_{ij}^{12} (X_i^{2\bar{\sigma}} X_j^{0\sigma} + X_i^{\sigma 0} X_j^{\bar{\sigma} 2})\}, \quad (6)$$

where the hopping integrals have different values for the LHB ( $t_{ij}^{11}$ ), the UHB ( $t_{ij}^{22}$ ) and the interband transitions ( $t_{ij}^{12}$ ). In the singlet-hole model the single-site repulsion energy  $U$  in (6) is given by the charge transfer energy  $\Delta = \epsilon_p - \epsilon_d$  between  $p$ - and  $d$ -levels in CuO<sub>2</sub> plane and hopping integrals for holes can be written as [39]

$$t_{ij}^{\alpha\beta} = -K_{\alpha\beta} 2t \nu_{ij} \quad (7)$$

where  $t$  is the hybridization parameter in the  $p-d$  model and the  $\nu_{ij}$  are the overlapping parameters for the Wannier oxygen states which are equal to: for the nearest neighbors  $\nu_1 = \nu_j \text{ } j \pm a_{x/y} \simeq -0.14$  and for the next nearest neighbors  $\nu_2 = \nu_j \text{ } j \pm a_x \pm a_y \simeq -0.02$  where  $a_{x/y}$  are the lattice constants. The coefficients  $K_{\alpha\beta}$  depend on the dimensionless parameter  $t/\Delta$  and for a realistic value of  $\Delta = 2t$  they are equal to [39]:

$$K_{11} \simeq -0.887, \quad K_{22} \simeq -0.477, \quad K_{12} \simeq 0.834. \quad (8)$$

These values will be used later for an estimation of relaxation rates.

In the strong coupling limit,  $U \gg |t_{ij}^{\alpha\beta}|$ , one can apply perturbation theory and further reduce the Hubbard model (5) or (6) to the one-band  $t-J$ -like model for the LHB (see, e.g., [35]). However, in this approach the dynamical effects of interband transitions are not properly taken into account which restricts the application of the  $t-J$  model only to studies of low-energy physics. A number of very important properties of the two-band model (6) as, e.g.,

weight transfer from the UHB to the LHB and changes of the spectral functions with doping (see [39]) are also lost in the  $t - J$  model. Therefore to consider optical conductivity where charge transfer between the UHB and the LHB are essential we have to consider the two band model (6). To compare our calculations with results for the conventional Hubbard model (1) (e.g., [8, 10, 11, 12]) we put all the hopping integrals to be equal:  $t_{ij}^{\alpha\beta} = t_{ij}$ .

### 3 Optical Conductivity. General Formulation

In the linear response theory of Kubo [7] the frequency dependent conductivity is defined by the current-current correlation function

$$\sigma_{xx}(\omega) = \frac{1}{V} \int_0^{\infty} dt e^{i\omega t} (J_x(t), J_x) \quad (9)$$

where  $V$  is the volume of the system,  $\Im\omega > 0$ , and

$$(A(t), B) = \int_0^{\beta} d\lambda \langle A(t - i\lambda) B \rangle \quad (10)$$

is the Kubo - Mori scalar product for the operators in the Heisenberg representation,

$$A(t) = \exp(iHt) A \exp(-iHt),$$

and  $\langle AB \rangle$  denotes equilibrium statistical averaging for a system with the Hamiltonian  $H$ ,  $\beta = 1/T$  (here  $\hbar = k_B = 1$ ).

To calculate the conductivity (9) we will use the equation of motion method for the retarded two-time Green functions (GF) [9, 49] for the scalar product (10)

$$\Phi_{AB}(\omega) = ((A|B))_{\omega} = -i \int_0^{\infty} dt e^{i\omega t} (A(t), B) \quad (11)$$

and for the commutator GF

$$G_{AB}(\omega) = \langle\langle A|B \rangle\rangle_{\omega} = -i \int_0^{\infty} dt e^{i\omega t} \langle [A(t), B] \rangle \quad (12)$$

where  $\Im\omega > 0$  and the operators have zero average values:  $\langle A \rangle = \langle B \rangle = 0$ . The conventional dynamical susceptibility is given by

$$\chi_{AB}(\omega) = -\langle\langle A|B \rangle\rangle_{\omega}. \quad (13)$$

The GF (11), (12) are coupled by the equation

$$\omega \langle\langle A|B \rangle\rangle_{\omega} = \langle\langle A|B \rangle\rangle_{\omega} - \langle\langle A|B \rangle\rangle_{\omega=0}. \quad (14)$$

We have also the following useful relations:

$$\langle\langle i\dot{A}|B \rangle\rangle_{\omega} = \langle\langle A| -i\dot{B} \rangle\rangle_{\omega} = \langle\langle A|B \rangle\rangle_{\omega} \quad (15)$$

$$(i\dot{A}, B) = (A, -i\dot{B}) = \langle [A, B] \rangle \quad (16)$$

where  $i\dot{A} = i dA/dt = [A, H]$ . The static isolated, or Kubo, susceptibility (13)  $\chi_{AB}(\omega = 0)$  and isothermal susceptibility  $\chi_{AB}^0 = (A, B)$ , obtained by differentiating the free energy with respect to an external field, in general case are nonequal:

$$\chi_{AB}(0) = \chi_{AB}^0 - \beta \langle A^0 B^0 \rangle. \quad (17)$$

Only for ergodic systems where correlations decay with time the invariant part of correlation functions with respect to the evolution with the Hamiltonian  $H$  is absent

$$\langle A^0 B^0 \rangle = \lim_{t \rightarrow \infty} \langle A(t) B \rangle = 0$$

and both the susceptibilities are equal.

By using the above given definitions and writing the current operator as the time derivative of the polarization operator of the system,  $J_x = \dot{P}_x$ , we obtain the following equivalent representation for the optical conductivity (9)

$$\sigma(\omega) = \frac{i}{V} \langle\langle J|J \rangle\rangle_{\omega} = \frac{1}{V} \langle\langle P|J \rangle\rangle_{\omega} = \frac{i}{V\omega} [\chi_{JJ}(0) - \chi_{JJ}(\omega)] \quad (18)$$

where we have omitted the indexes for the operators  $J_x, P_x$ . By employing the standard dispersion relation [9] for the GF (12) or susceptibility (13) we readily get the sum rule for the real, or absorptive part of the conductivity (18):

$$\int_0^\infty d\omega \Re \sigma_{xx}(\omega) = \frac{1}{V} \int_0^\infty d\omega \frac{\Im \chi_{JJ}(\omega)}{\omega} = \frac{\pi}{2V} \Re \chi_{JJ}(0) = \frac{i\pi}{2V} \langle [J_x, P_x] \rangle. \quad (19)$$

The sum rules (19) has been extensively used by many authors to discuss the metal-insulator transitions in the Hubbard model (see, e.g., [13, 14, 15, 16, 17, 18, 19, 26, 28, 30, 33, 35]) since the right hand side of (19) can be calculated from the static correlation functions.

The formula for the conductivity (9) has been obtained by Kubo [7] by considering a linear response to an external electric field. Starting from the linear response theory in respect to the vector potential  $A(\mathbf{r}, t)$  a formula for the frequency dependent conductivity for the Hubbard model (1) with nearest neighbors hopping can be written in the form (see, e. g., [33]):

$$\sigma(\omega) = \frac{i}{V\omega} [-e^2 a_x^2 \langle H_t \rangle - \chi_{JJ}(\omega)]. \quad (20)$$

where  $\langle H_t \rangle$  is the average kinetic (hopping) energy in the model (1). It results in the formula for the absorptive part of conductivity:

$$\Re \sigma(\omega) = \bar{D} \delta(\omega) + \frac{1}{V\omega} \Im \chi_{JJ}(\omega) \quad (21)$$

where the Drude spectral weight can be written as

$$\bar{D} = \frac{\pi}{V} [\chi_{JJ}^0 - \Re \chi_{JJ}(\omega = 0)]. \quad (22)$$

if one uses the formula for the static susceptibility  $\chi_{JJ}^0$  in terms of the kinetic energy for the Hubbard model with nearest neighbors hopping (see (58)). As it was mentioned above, for the ergodic system (at least, nonsuperconducting) the isothermal,  $\chi_{JJ}^0$ , and the static isolated,  $\chi_{JJ}(\omega = 0)$ , susceptibilities are

equal and  $\bar{D} \equiv 0$  in (22). However, in the numerical calculations for finite clusters one can observe nonzero Drude weight (22) which is caused by transitions between lowest energy levels of the finite system and essentially is a finite size effect (see [18]). In the thermodynamic limit,  $N \rightarrow \infty$ , for a real system it should tends to zero.

To calculate the effective Drude spectral weight in the Hubbard model one can use a partial sum rule:

$$Z(\omega) = \int_0^\omega dz \Re \sigma_{xx}(z) \quad (23)$$

by defining the Drude weight as  $(1/2)D = Z(\omega_0)$  with the cut-off frequency  $\omega_0$  below the interband transition energy of order  $U$ . Then at the metal-insulator transition the Drude weight tends to zero in the insulating phase at half-filled band. The latter approach has been used in a number of numerical calculations (see, e.g. [18, 28]).

To calculate the current-current correlation function for conductivity (18) it is convenient to employ the memory function approach of Mori [50] in the form slightly different then that one used by Götze et al. [40]. We define the memory function  $M_{JJ}(\omega) \equiv M(\omega)$  by the equation

$$\Phi_{JJ}(\omega) = ((J|J))_\omega = \frac{\chi_0}{\omega + M(\omega)} \quad (24)$$

where  $\chi_0 = \chi_{JJ}^0$  and

$$M(\omega \pm i\delta) = M'(\omega) \pm iM''(\omega).$$

Here  $M'(\omega) = \Re M(\omega)$  and  $M''(\omega) = \Im M(\omega)$  are real functions.

We calculate the memory function by using equation of motion for the GF

$$\Phi_{JJ}(t-t') = ((J(t); J(t'))).$$

By differentiating it in respect to time  $t$  and  $t'$  we readily get an equation for its Fourier transform (11):

$$\Phi(\omega) = \Phi_0(\omega) + \Phi_0(\omega)M_0(\omega)\Phi_0(\omega) \quad (25)$$

where

$$\Phi_0(\omega) = \frac{\chi_0}{\omega} \quad (26)$$

and the "scattering matrix"

$$M_0(\omega) = -(1/\chi_0)((F_x|F_x))_\omega(1/\chi_0) \quad (27)$$

is given by the correlation function for forces

$$F_x = i\dot{J}_x = [J_x, H]. \quad (28)$$

We have also used the relation of orthogonality for current and force:

$$(F_x, J_x) = (i\dot{J}_x, J_x) = \langle [J_x, J_x] \rangle = 0.$$

From eqs. (24), (25) we obtain the following relation for the memory function  $M(\omega)$  and  $M_0(\omega)$  (27):

$$M_0(\omega) = -[M(\omega)/\chi_0] - [M(\omega)/\chi_0]\Phi_0(\omega)M_0(\omega). \quad (29)$$

A formal solution of this equation by iteration shows that the memory function is just the irreducible part of the scattering matrix (27) which has no parts connected by single zero order GF  $\Phi_0(\omega)$ :

$$M(\omega) = ((F_x|F_x))_\omega^{(irred)}(1/\chi_0). \quad (30)$$

In solving eq. (29) by perturbation expansion one should be cautious since the solution is a non-analytical function in  $(\omega, \text{coupling constant})$  [51]. The exact meaning of the irreducibility is really given by Mori in his definition of the memory function in terms of the operators with the projected time evolution.

Recently a rigorous solution in the closed form to the Mori formula (24) has been obtained in terms of the correlation functions with unprojected time evolution by applying perturbation expansion for the projected operator [52]. In this way the equivalence between the Mori formula, eq. (24), and the Kubo formula, eq. (18), has been established [53].

A more general than Mori, frequency dependent projection technique has been proposed by Tserkovnikov[49]. By applying his method we obtain an exact representation for the memory function, or the self-energy operator for the GF (24), in the form

$$\begin{aligned} -\chi_0 M(\omega) &= ((i\dot{J}_x| - i\dot{J}_x))_\omega^{(irred)} = \\ &= ((i\dot{J}_x| - i\dot{J}_x))_\omega - ((i\dot{J}_x|J_x))_\omega((J_x|J_x))_\omega^{-1}((J_x| - i\dot{J}_x))_\omega. \end{aligned} \quad (31)$$

In this representation all the operators in correlation functions have the time evolution with the full, unprojected Liouville operator. By using eq.(15) we readily regain from the Mori representation (24) the Kubo formula in terms of current-current susceptibility, eq.(18). However, a practical calculation within the exact representation (31) is not straightforward. So in the next Section we will use the representation (30) and calculate the force-force correlation function in the leading order of  $|t_{\alpha\beta}|/U$  for the Hubbard model (6). As we will see the irreducibility condition defined above will be preserved in the adopted approximation.

Now we can write the frequency dependent conductivity (18) by using the representation for the GF (24) in the form of the generalized Drude law:

$$\sigma(\omega) = \frac{\chi_0}{V} \frac{m}{\tilde{m}(\omega)} \frac{1}{\tilde{\Gamma}(\omega) - i\omega} \quad (32)$$

where the effective optical mass and the relaxation rate are given by

$$\frac{\tilde{m}(\omega)}{m} = 1 + \lambda(\omega), \quad \tilde{\Gamma}(\omega) = \frac{\Gamma(\omega)}{1 + \lambda(\omega)} \quad (33)$$

where the Bose-like operators have been introduced:

$$\begin{aligned}
B_{j\sigma\sigma'}^{11} &= (X_j^{00} + X_j^{\sigma\sigma})\delta_{\sigma'\sigma} + X_j^{\bar{\sigma}\sigma}\delta_{\sigma'\bar{\sigma}}, \\
B_{j\sigma\sigma'}^{12} &= (X_j^{00} + X_j^{\sigma\sigma})\delta_{\sigma'\bar{\sigma}} - X_j^{\bar{\sigma}\sigma}\delta_{\sigma'\sigma}, \\
B_{j\sigma\sigma'}^{22} &= (X_j^{22} + X_j^{\sigma\sigma})\delta_{\sigma'\sigma} + X_j^{\bar{\sigma}\sigma}\delta_{\sigma'\bar{\sigma}}, \\
B_{j\sigma\sigma'}^{21} &= (X_j^{22} + X_j^{\sigma\sigma})\delta_{\sigma'\bar{\sigma}} - X_j^{\bar{\sigma}\sigma}\delta_{\sigma'\sigma}.
\end{aligned} \tag{45}$$

There are only two independent operators in eq. (45) since the Hubbard operators obey the completeness relation, eq. (4). They describe electron scattering on spin and charge fluctuations resulted from nonfermionic commutation relations (kinematical interaction) for the Fermi-like Hubbard operators in the current operator (39). It can be demonstrated explicitly by using the following representation

$$\begin{aligned}
(X_j^{22} + X_j^{\sigma\sigma}) + X_j^{\bar{\sigma}\sigma} &= \frac{1}{2}(\sum_{\sigma} X_j^{\sigma\sigma} + 2X_j^{22}) + \frac{1}{2}(X_j^{\sigma\sigma} - X_j^{\bar{\sigma}\bar{\sigma}}) + X_j^{\bar{\sigma}\sigma} = \\
&= \frac{1}{2}N_j + 2\sigma S_j^z + S_j^{\sigma}
\end{aligned} \tag{46}$$

where  $S_j^z = \pm 1/2$  and  $S_j^{\sigma} = S_j^{\pm}$  for  $2\sigma = \pm 1$ . From eq. (46) it follows that the operators (45) can be written in terms of the number  $N_j$  and spin  $S_j^{\sigma}$  operators.

In the following we neglect higher order corrections to the interband force (43) which are given by the products of operators from the different bands in eq. (44), as, e.g.,  $X_i^{\sigma 0} X_l^{\sigma' 2}$ . We neglect also high-energy contributions in eq. (44) from creations of electron pairs given by the products of the type  $X_j^{02} X_l^{2\sigma}$ . However, we keep three site scattering terms in the force (44) with  $i \neq j \neq l, i \neq l$  which give an important contribution to conductivity (see, e.g., [35]). By omitting these high-energy contributions, irrelevant for the Drude

relaxation, we write the force (44) in  $\mathbf{q}$ -representation as

$$\begin{aligned}
F_x^{int} &= -\frac{e}{\sqrt{N}} \sum_{k,q} \sum_{\sigma\sigma'} v_x(k) \gamma(k-q) (t_{11}^2 X_k^{\sigma 0} X_{k-q}^{0\sigma'} B_{q\sigma\sigma'}^{11} + t_{12}^2 X_k^{\bar{\sigma} 0} X_{k-q}^{0\sigma'} B_{q\sigma\sigma'}^{21} \\
&\quad + t_{22}^2 X_k^{2\sigma} X_{k-q}^{\sigma' 2} B_{q\sigma\sigma'}^{22} + t_{21}^2 X_k^{2\bar{\sigma}} X_{k-q}^{\sigma' 2} B_{q\sigma\sigma'}^{12}) - \text{H. c.}
\end{aligned} \tag{47}$$

where the following functions in  $\mathbf{q}$  representation were introduced

$$\begin{aligned}
B_{q\sigma\sigma'}^{\alpha\beta} &= \frac{1}{\sqrt{N}} \sum_i B_{i\sigma\sigma'}^{\alpha\beta} e^{-i\mathbf{q}\mathbf{R}_i}, \\
t^{\alpha\beta}(\mathbf{q}) &= t_{\alpha\beta} \gamma(\mathbf{q}), \quad v_x(q) = -\partial \gamma(\mathbf{q}) / \partial q_x.
\end{aligned} \tag{48}$$

Now we can calculate the relaxation rates (36) both for the interband transitions given by the force (43) and for the intraband scattering, the Drude part, given by the force (47). By applying the self-consistent Born approximation for the electron-hole time-dependent correlation functions

$$\langle X_q^{2\bar{\sigma}} X_q^{0\sigma} X_q^{\sigma' 0}(t) X_q^{\bar{\sigma}' 2}(t) \rangle \simeq \delta_{q,q'} \delta_{\sigma,\sigma'} \langle X_q^{2\bar{\sigma}} X_q^{\bar{\sigma} 2}(t) \rangle \langle X_q^{0\sigma} X_q^{\sigma 0}(t) \rangle \tag{49}$$

we obtain the following equation for the interband relaxation rate

$$\begin{aligned}
\Gamma_0(\omega) &= \frac{1 - \exp(\beta\omega)}{2\chi_0\omega} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle F_x^0 F_x^0(t) \rangle = \frac{2\pi e^2 U^2 t_{12}^2}{\chi_0\omega} \int_{-\infty}^{\infty} dz \sum_q (v_x(q))^2 \\
&\quad \{ [n(z-\omega) - n(z)] A_1(q, z-\omega) A_2(q, z) - [n(z+\omega) - n(z)] A_1(q, z+\omega) A_2(q, z) \}.
\end{aligned} \tag{50}$$

Here the spectral functions

$$\begin{aligned}
A_1(q, \omega) &= -\frac{1}{\pi} \Im \langle \langle X_q^{0\sigma} | X_q^{\sigma 0} \rangle \rangle_{\omega+i\delta}, \\
A_2(q, \omega) &= -\frac{1}{\pi} \Im \langle \langle X_q^{\sigma 2} | X_q^{2\sigma} \rangle \rangle_{\omega+i\delta},
\end{aligned} \tag{51}$$

define the spectra of electronic excitations by the full one-electron GF for the LHB and the UHB, respectively, and  $n(\omega) = (\exp \beta\omega + 1)^{-1}$ . In the decoupling (49) we have neglected nondiagonal correlation functions, as, e.g.,



with

$$\lambda(\omega) = \frac{M'(\omega)}{\omega}, \quad \Gamma(\omega) = M''(\omega). \quad (34)$$

The real and imaginary parts of the memory function are coupled by the dispersion relation

$$M'(\omega) = \frac{1}{\pi} \int_{-\infty}^{\infty} dz \frac{M''(z)}{z - \omega}. \quad (35)$$

It is also convenient, by using the spectral representation for the GF, to write the relaxation rate given by eq.(34) in terms of the conventional time-dependent force-force correlation function:

$$\Gamma(\omega) = \frac{1 - \exp(\beta\omega)}{2\chi_0\omega} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle F_x F_x(t) \rangle \quad (36)$$

where

$$\chi_0 = (J_x, J_x) = i \langle [J_x, P_x] \rangle \quad (37)$$

is the static susceptibility.

In the next Section we calculate the force-force correlation function and relaxation rate (36) for the asymmetric Hubbard model (6).

## 4 Relaxation Rates

We start with a definition of the polarization operator for the Hubbard model (6):

$$P = e \sum_i \mathbf{R}_i N_i = e \sum_i \mathbf{R}_i \left( \sum_{\sigma} X_i^{\sigma\sigma} + 2X_i^{22} \right) \quad (38)$$

where  $\mathbf{R}_i$  are coordinates of electrons with charge  $e$  on a 2D square lattice. From this definition the following expression for the current operator results

$$\begin{aligned} J_x &= -i[P_x, H] = \\ &= ie \sum_{i \neq j\sigma} (R_i^x - R_j^x) \{ t_{ij}^{11} X_i^{\sigma 0} X_j^{0\sigma} + t_{ij}^{22} X_i^{2\sigma} X_j^{\sigma 2} + 2\sigma t_{ij}^{12} (X_i^{2\bar{\sigma}} X_j^{0\sigma} + X_i^{\sigma 0} X_j^{\bar{\sigma} 2}) \}. \end{aligned} \quad (39)$$

By introducing the  $\mathbf{q}$ -representation for the Hubbard operators and the hopping integrals

$$\begin{aligned} X_{\mathbf{q}}^{\alpha\beta} &= \frac{1}{\sqrt{N}} \sum_i X_i^{\alpha\beta} e^{-i\mathbf{q}\mathbf{R}_i}, \\ t^{\alpha\beta}(\mathbf{q}) &= \sum_{i \neq 0} t_{oi}^{\alpha\beta} e^{-i\mathbf{q}\mathbf{R}_i}, \end{aligned} \quad (40)$$

the current operator (39) can be written as

$$J_x = e \sum_{q\sigma} \{ v_x^{11}(q) X_q^{\sigma 0} X_q^{0\sigma} + v_x^{22}(q) X_q^{2\sigma} X_q^{\sigma 2} + 2\sigma v_x^{12}(q) (X_q^{2\bar{\sigma}} X_q^{0\sigma} + X_q^{\sigma 0} X_q^{\bar{\sigma} 2}) \} \quad (41)$$

where  $v_x^{\alpha\beta}(q) = -\partial t^{\alpha\beta}(\mathbf{q}) / \partial q_x$  are electron velocities.

Now we calculate the force (28) for the current (41) which can be written as a sum of two terms:

$$F_x = F_x^0 + F_x^{int} = [J_x, H_0] + [J_x, H_t]. \quad (42)$$

The first term has a contribution only from interband transitions:

$$F_x^0 = -eU \sum_{q\sigma} 2\sigma v_x^{12}(q) (X_q^{2\bar{\sigma}} X_q^{0\sigma} - X_q^{\sigma 0} X_q^{\bar{\sigma} 2}). \quad (43)$$

The second term, being proportional to the square of the hopping integrals, has contributions both from electron hopping in one band and from interband transitions. In the coordinate space it reads

$$\begin{aligned} F_x^{int} &= -ie \sum_{i \neq j \neq l} \sum_{\sigma\sigma'} (R_i^x - R_j^x) (t_{ij}^{11} X_i^{\sigma 0} + 2\sigma t_{ij}^{12} X_i^{2\bar{\sigma}}) \\ &\quad \{ (t_{jl}^{11} X_l^{0\sigma'} B_{j\sigma\sigma'}^{11} + 2\sigma t_{il}^{12} X_l^{\sigma' 2} B_{j\sigma\sigma'}^{12}) - X_j^{02} (t_{jl}^{22} X_l^{2\sigma} - 2\sigma t_{jl}^{12} X_l^{\bar{\sigma} 0}) \} \\ &\quad -ie \sum_{i \neq j \neq l} \sum_{\sigma\sigma'} (R_i^x - R_j^x) (t_{ij}^{22} X_i^{2\sigma} - 2\sigma t_{ij}^{12} X_i^{\bar{\sigma} 0}) \\ &\quad \{ (t_{jl}^{22} X_l^{\sigma' 2} B_{j\sigma\sigma'}^{22} - 2\sigma t_{il}^{12} X_l^{0\sigma'} B_{j\sigma\sigma'}^{21}) - X_j^{02} (t_{jl}^{11} X_l^{\sigma 0} + 2\sigma t_{jl}^{12} X_l^{2\bar{\sigma}}) \} \\ &\quad - \text{H. c.} \end{aligned} \quad (44)$$

$\langle X_q^{2\bar{\sigma}} X_q^{\sigma 0}(t) \rangle$ , since they give higher order corrections in  $t_{12}/U$  which have been already omitted in the force (47). Since the difference between the UHB and the LHB energy is of order  $U$  the interband relaxation rate is nonzero only for this region of high energy around  $|\omega| \simeq U$ . To analyze its temperature and doping dependence we need self-consistent solutions for the one-electron GF in eq. (51).

The intraband relaxation rate is given by the following equation

$$\Gamma_{int}(\omega) = \frac{1 - \exp(\beta\omega)}{2\chi_0\omega} \int_{-\infty}^{\infty} dt e^{i\omega t} \langle F_x^{int} F_x^{int}(t) \rangle. \quad (52)$$

To calculate the many-particle time-dependent correlation functions in the right-hand side of eq. (52) we apply the mode-coupling approximation in terms of an independent propagation of electron-hole and charge-spin fluctuations. This approximation is essentially equivalent to the self-consistent Born approximation in which vertex corrections are neglected. The proposed approximation is defined by the following decoupling of the time-dependent correlation function:

$$\begin{aligned} & \langle X_k^{\sigma 0} X_{k-q}^{0\sigma'} B_{q\sigma\sigma'}^{11} | X_{k-q}^{s'0}(t) X_{k'}^{0s}(t) (B_{q's's'}^{11}(t))^\dagger \rangle \\ & \simeq \delta_{k,k'} \delta_{q,q'} \delta_{s,\sigma} \delta_{s',\sigma'} \langle X_k^{\sigma 0} X_k^{0\sigma}(t) \rangle \langle X_{k-q}^{0\sigma'} X_{k-q}^{s'0}(t) \rangle \langle B_{q\sigma\sigma'}^{11} (B_{q\sigma\sigma'}^{11}(t))^\dagger \rangle \end{aligned} \quad (53)$$

There are 16 correlation functions of the type given by eq.(53) for the LHB and for the UHB. However, by using the symmetry relations for the correlations functions in terms of the Bose-like operators (45) we can write the final result for the intraband relaxation rate in a compact form:

$$\begin{aligned} \Gamma_{int}(\omega) &= \frac{\exp(\beta\omega) - 1}{\chi_0\omega} \int_{-\infty}^{\infty} d\omega_1 \int_{-\infty}^{\infty} d\omega_2 n(\omega_1) [1 - n(\omega_2)] N(\omega - \omega_1 + \omega_2) \\ & \times \frac{2e^2}{N} \sum_{k,q} g_x^2(k, k-q) \chi_{cs}''(q, \omega - \omega_1 + \omega_2) \end{aligned}$$

$$\times \{ (t_{11}^2 - t_{12}^2)^2 A_1(k, \omega_1) A_1(k-q, \omega_2) + (t_{22}^2 - t_{12}^2)^2 A_2(k, \omega_1) A_2(k-q, \omega_2) \}, \quad (54)$$

where the momentum dependent vertex is given by

$$g_x(k, k-q) = v_x(k) \gamma(k-q) - v_x(k-q) \gamma(k) \quad (55)$$

and the charge-spin susceptibility  $\chi_{cs}(q, \omega)$  is defined by the equation:

$$\begin{aligned} \langle \rho_{cs}(q) | \rho_{cs}(-q, t) \rangle &= \frac{1}{4} \langle N_q | N_{-q}(t) \rangle + \sum_{\alpha} \langle S_q^{\alpha} | S_{-q}^{\alpha}(t) \rangle \\ &= \frac{1}{\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega t} N(\omega) \chi_{cs}''(q, \omega). \end{aligned} \quad (56)$$

Here  $N(\omega) = (\exp \beta\omega - 1)^{-1}$  and  $\chi_{cs}''(q, \omega) = \Im \chi_{cs}(q, \omega + i\delta)$ . The formula (54) generalize the result obtained for the relaxation rate for  $p$ -band electrons in the  $p-d$  model in Ref. [41].

To conclude this Section we calculate the static current-current susceptibility (37) in the denominators of eqs.(50), (54) which is also define the sum rule for the conductivity, eq.(19). By performing the commutation between the polarization operator (38) and the current (41) we readily get

$$\begin{aligned} \chi_0 &= (J_x, J_x) = i \langle [J_x, P_x] \rangle \\ &= \sum_{i \neq j, \sigma} (R_i^x - R_j^x)^2 \{ t_{ij}^{11} \langle X_i^{\sigma 0} X_j^{0\sigma} \rangle + t_{ij}^{22} \langle X_i^{2\sigma} X_j^{\sigma 2} \rangle + 2\sigma t_{ij}^{12} \langle (X_i^{2\bar{\sigma}} X_j^{0\sigma} + X_i^{\sigma 0} X_j^{\bar{\sigma} 2}) \rangle \}. \end{aligned} \quad (57)$$

For the Hubbard model with only the nearest neighbors hopping,  $(R_i^x - R_j^x)^2 = a_x^2$ , the static susceptibility (57) is equal to the average kinetic energy, the hopping term  $H_t$  in eq.(6), multiplied by a constant:

$$\chi_0 = -e^2 a_x^2 (1/2) \langle H_t \rangle. \quad (58)$$

The latter equation for the conventional Hubbard model (5) has been used by many authors to study the conductivity sum rule (19) (see, e.g. [13, 14,

15, 16, 18, 19, 20, 21, 26, 28, 30, 31, 35]). In the  $q$ -representation the static susceptibility (57) reads:

$$\chi_0 = -e^2 \sum_{q,\sigma} \left\{ \frac{\partial^2 t^{11}(q)}{\partial q_x^2} \langle X_q^{\sigma 0} X_q^{0\sigma} \rangle + \frac{\partial^2 t^{22}(q)}{\partial q_x^2} \langle X_q^{2\sigma} X_q^{\sigma 2} \rangle + 2\sigma \frac{\partial^2 t^{12}(q)}{\partial q_x^2} \langle (X_i^{2\sigma} X_j^{0\sigma} + X_i^{\sigma 0} X_j^{\bar{\sigma} 2}) \rangle \right\}. \quad (59)$$

By introducing the band masses:  $1/m_x^{\alpha\beta} = -\partial^2 t_q^{\alpha\beta} / \partial q_x^2$  one can write the susceptibility as  $\chi_0/V = ne^2/m_{eff}$  in terms of the doping and temperature dependent effective mass  $m_{eff}$ ,  $n = N/V$ . The latter can be calculated by using the solution for the one-electron GF including the nondiagonal ones (see, e.g. [39]).

## 5 Results and Discussion

In the present paper we have derived a closed set of formulas for the frequency dependent conductivity for the asymmetric Hubbard model (6) in the form of the generalized Drude law (32) with the relaxation rates for the interband transitions (50) and the intraband scattering (54). The former gives a contribution for the optical conductivity in the high frequency range around  $\omega \simeq U$ . The latter describes the Drude relaxation due to electron scattering on spin and charge fluctuations both in the LHB and UHB. The static current-current susceptibility (59) defines the sum rule (19) and enter as a normalization factor in the definition of the relaxation rates (50), (54).

For an estimation of the relaxation rates we can use a Hubbard I type approximation for the one-electron GF (51) (see, e.g. [39]):

$$A_1(q, \omega) = \chi_1 \delta(\omega - \Omega_{1q}), \quad A_2(q, \omega) = \chi_2 \delta(\omega - \Omega_{2q}) \quad (60)$$

where

$$\chi_1 = \langle X_i^{00} + X_i^{\sigma\sigma} \rangle, \quad \chi_2 = \langle X_i^{\sigma\sigma} + X_i^{22} \rangle$$

and  $\chi_1 = 1 - \chi_2 = 1 - n/2$ . The functions  $\Omega_{1q}$  and  $\Omega_{2q}$  are the one-electron spectra for the LHB and the UHB, respectively. They have been calculated for the asymmetric Hubbard model (6) allowing for the interband hybridization by projection technique for the GF in Ref.[39]. By using eqs.(60) we get the following expressions for the relaxation rates

$$\Gamma_0(\omega) = \frac{2\pi e^2 U^2 t_{12}^2}{\chi_0 \omega} \chi_1 \chi_2 \sum_q (v_x(q))^2 [n(\Omega_{1q}) - n(\Omega_{2q})][\delta(\Omega_{2q} - \Omega_{1q} - \omega) - \delta(\Omega_{2q} - \Omega_{1q} + \omega)] \quad (61)$$

$$\Gamma_{int}(\omega) = \frac{\exp(\beta\omega) - 1}{\chi_0 \omega} \frac{2e^2}{N} \sum_{k,q} g_x^2(k, k-q)$$

$$\{ (t_{11}^2 - t_{12}^2)^2 \chi_1^2 n(\Omega_{1k}) [1 - n(\Omega_{1k-q})] N(\omega - \Omega_{1k} + \Omega_{1k-q}) \chi_{cs}''(q, \omega - \Omega_{1k} + \Omega_{1k-q}) + (t_{22}^2 - t_{12}^2)^2 \chi_2^2 n(\Omega_{2k}) [1 - n(\Omega_{2k-q})] N(\omega - \Omega_{2k} + \Omega_{2k-q}) \chi_{cs}''(q, \omega - \Omega_{2k} + \Omega_{2k-q}) \} \quad (62)$$

These are conventional formulas for the optical (61) and the Drude (62) relaxation rates calculated in the Born approximation for a two-band model. However, the relaxation rates and the conductivity (32) have quite a complicated temperature and doping dependence due to very specific dependence of the one-electron spectra  $\Omega_{1q}$  and  $\Omega_{2q}$  on that parameters (see [39]). It can be studied only by numerical solution of a self-consistent system of equations for the GF which will be considered elsewhere. Here we only point out that the Drude relaxation rate (54) disappears for the symmetric Hubbard model (5) with  $t_{\alpha\beta} = t$  independently of the approximations for the one-electron GF due to a cancellation of the intraband ( $\propto t_{\alpha\alpha}$ ) and interband  $\propto t_{12}$  contributions. If one neglects the latter a final relaxation rate results (see, e.g. [11]).

To estimate the Drude relaxation rates for copper-oxides we can use the hopping parameters given by eqs.(7), (8). The calculations show that for

electronically doped copper oxides (the chemical potential in the LHB) the relaxation rate (54) being proportional to  $(K_{11}^2 - K_{12}^2)^2 \simeq 0.01$  should be much smaller than for hole doped ones (the chemical potential in the UHB) where it is proportional to  $(K_{22}^2 - K_{12}^2)^2 \simeq 0.22$ . The latter one has been calculated in Ref.[41] for a simplified model of  $p$ -band by the formula close to (62) but neglecting  $t_{12}$  term which has resulted in a higher value for the spin-fluctuation resistivity and frequency dependent relaxation rate.

For discussion of a very important in the Hubbard model (1) or (6) problem of the Mott-Hubbard metal-insulator transition around half-filling ( $n = 1$ ) we have to calculate more accurately the one-electron GF given by eq.(60) including the non-diagonal GF  $\langle X_q^{\sigma 0} X_q^{\bar{\sigma} 2} \rangle$  which define the static susceptibility (59). An estimation in the leading order of  $t_{12}/U$  for a model with nearest neighbors hopping results in the formula

$$\chi_0 = e^2 a^2 \sum_q \{ \gamma(q) [t_{11} \chi_1 n(\Omega_{1q}) + t_{22} \chi_2 n(\Omega_{2q})] + 2(t_{12} \gamma(q))^2 \chi_1 \chi_2 \frac{n(\Omega_{1q}) - n(\Omega_{2q})}{\Omega_{2q} - \Omega_{1q}} \}. \quad (63)$$

For a half-filled band, ( $n = 1$ ), at low temperature  $n(\Omega_{1q}) = 1$ ,  $n(\Omega_{2q}) = 0$  and there is only the interband contribution of the order  $\chi_0/N \simeq e^2 a^2 (t_{12}^2/2U)$ . This small value of  $\chi_0$  greatly enhances the interband relaxation rate  $\Gamma_0(\omega \simeq U) \simeq U$ . However, at a final concentration of charge carriers  $\delta = 1 - n$  a contribution from the LHB (or the UHB) in (63) of the order  $\chi_0/N \simeq e^2 a^2 t_{\alpha\alpha} \delta$  appears and at some concentration  $\delta \simeq (t_{12}^2/t_{\alpha\alpha} U)$  a crossover from interband to intraband scattering takes place.

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