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## Optical conductivity of the Hubbard model in the strong coupling regime

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### Abstract

On the basis of a diagrammatic technique for Hubbard operators we calculate the real part of the frequency-dependent conductivity in the Hubbard model on any-dimensional cubic lattice at finite temperatures. Results in the lowest non-vanishing order of the perturbation theory are presented for various values of the parameters  $U$ ,  $t$  and band fillings. We explicitly check the sum rule within the perturbation order. The  $1/T$  behavior of the Drude weight is observed for temperatures  $t \ll kT \ll U$ .

The unusual normal state transport properties of high- $T_c$  superconductors [1] are believed to give clues to the basic mechanism responsible for superconductivity. One of the strange properties of the charge dynamics is the  $T$ -linear in-plane resistivity dependence observed over a wide temperature range within a rather narrow range of band fillings. The Hubbard model is suspected to explain at least qualitatively basic properties of high- $T_c$  superconductors [2]. One can therefore assume the Hubbard model to be the prototype for the strange metal with the linear temperature dependence of the dc resistivity.

The optical conductivity of the Hubbard model has been studied both numerically by exact diagonalization of small systems [3,4], by Monte Carlo techniques [5] and analytically by  $t$ -matrix approximation [6], by using the Gutzwiller trial wave function [7] and by performing approximate analytic mean-field calculations [8]. This paper is aimed to contribute to the current discussion on the possibility of

the non-Fermi liquid behavior of high- $T_c$  superconductors in their normal state [2,9,10].

In this paper we use the diagrammatic technique for Hubbard operators introduced by Zaitsev and developed in works of Izyumov and co-workers [11,12]. Despite its complexity it is the only systematic method for treating analytically the Hubbard model in the strong coupling limit we have at present. Let us consider a  $D$ -dimensional hypercubic lattice with  $N$  sites. The Hamiltonian of the one-band Hubbard model can be written in the form

$$H = U \sum_i n_{i+} n_{i-} + t \sum_{\langle i,j \rangle} \sum_{\sigma} a_{i\sigma}^{\dagger} a_{j\sigma} - \mu N, \quad (1)$$

where  $a_{i\sigma}$  ( $a_{i\sigma}^{\dagger}$ ) is the annihilation (creation) operator of an electron with spin  $\sigma = \pm 1$  at the site labeled by the vector  $i$ ,  $n_{i\sigma}$  is the electron-density operator at site  $i$  and  $\langle i,j \rangle$  represents summation over nearest neighbors.  $N = \sum_{i\sigma} n_{i\sigma}$  is the total particle number operator. The Hamiltonian thus describes on-site interactions of electrons with the Hubbard energy  $U$  as well as hops of electrons over lattice links with the energy  $t$ . We add the chemical potential  $\mu$  in order to fix the mean number of particles.

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To study the optical conductivity we introduce the paramagnetic current operator in the  $x$  direction as a difference in the number of right-moving and left-moving particles,

$$j_x = \frac{eA}{V\hbar} i t \sum_{i,\sigma} (a_{i\sigma}^+ a_{i+\hat{x},\sigma} - \text{h.c.}). \quad (2)$$

Here we introduced  $A$  as the lattice parameter and  $V = N A^D$  as the volume assigned to the lattice. In the following it will be useful to introduce normalized local current operators  $j_{i+}, j_{i-}$  via the formula

$$j_x = \frac{eA}{\hbar V} t \sum_{i,\sigma} j_{i\sigma}.$$

The optical conductivity as the linear response of the system to an external homogeneous and time-dependent electric field is given in the Kubo formalism by the formula (we are interested in the real part of the complex optical conductivity) [13]

$$\sigma(\omega) = -\frac{1}{\omega} \frac{V e^2 A^2}{\hbar^3} t^2 \text{Im}[P^R(\omega)], \quad (3)$$

where  $P^R(\omega)$  is the Fourier transform of the retarded current–current correlation function,

$$P^R(t-t') = -i \langle [j_x(t), j_x(t')] \rangle \theta(t-t'). \quad (4)$$

Here we assume averaging over a grand canonical ensemble and  $\theta(t-t')$  represents the step function.

As is usual in the perturbation theory we first calculate the Matsubara correlation function

$$P(\tau-\tau') = -\langle T_\tau(j_x(\tau)j_x(\tau')) \rangle \quad (5)$$

and at the end we perform an analytical continuation  $P^R(\omega) = P(i\nu_n)|_{i\nu_n=\omega+i0}$ . We introduced the “imaginary time” ordering  $T_\tau$ .

Our aim in this paper is to calculate the correlation function  $\mathcal{P}(i\nu_n)$  as the Fourier transform of (5) in the framework of the perturbation theory developed for Hubbard operators. For this purpose we have to express the current operators  $j_{i,\sigma}$  in terms of the Hubbard  $X$  operators,

$$j_{i,+} = i \sum_{\hat{x}, \hat{x}'} (\psi_{i,\hat{x}}^+ \hat{\tau}_{\hat{x}\hat{x}'} \psi_{i+\hat{x},\hat{x}'} - \text{h.c.}),$$

$$j_{i,-} = i \sum_{\eta, \eta'} (\psi_{i,\eta}^+ \hat{\tau}_{\eta\eta'} \psi_{i+\hat{x},\eta'} - \text{h.c.}). \quad (6)$$

At the step we adopt the notation from Ref. [11],

$$\psi_+ = \begin{pmatrix} X^{0+} \\ X^{-2} \end{pmatrix}, \quad \psi_- = \begin{pmatrix} X^{0-} \\ -X^{+2} \end{pmatrix},$$

and  $\tau_{\hat{x}\hat{x}'}$  ( $\tau_{\eta\eta'}$ ) is a  $2 \times 2$  matrix with unity elements. The Hubbard operators are defined via the division of the standard Fermi operators:  $a_\sigma = X^{0\sigma} + \sigma X^{-\sigma^2}$ . When substituting Eq. (6) into Eq. (5) one is able, in general, to construct diagrams for the current–current correlation function  $\mathcal{P}$ . Such diagrams exhibit rather complex and complicated structure (in the order of  $t^3$  one gets about 250 diagrams which may serve as a base for further approximations), and generalized, schematic picture of these diagrams within a chosen hierarchy system is also too lengthy and complicated. In this paper we restrict ourselves to calculations in the lowest non-vanishing order and discussion of further approximations will be given elsewhere. In fact we are going to calculate the correlation function in the second order of perturbation theory. In this order we have to calculate

$$\mathcal{P}^{(2)}(\tau-\tau') = -\langle T_\tau(j_x(\tau)j_x(\tau')) \rangle_0, \quad (7)$$

where averaging is over the distribution generated by the Hamiltonian

$$H_0 = \sum_i n_{i+} n_{i-} - \mu N.$$

In order to get  $\mathcal{P}^{(2)}(i\nu_n)$ , one must calculate the Fourier transform of the quantity

$$\mathcal{P}_{++}^{(2)}(\mathbf{i}-\mathbf{j}, \tau-\tau') = -\langle T_\tau(j_{i+}(\tau)j_{j+}(\tau')) \rangle_0. \quad (8)$$

We note that  $\mathcal{P}_{--}^{(2)} = \mathcal{P}_{++}^{(2)}$  and  $\mathcal{P}_{+-}^{(2)} = \mathcal{P}_{-+}^{(2)} = 0$  in the order under consideration and for the symmetry between up- and down-spin currents. Thus we get the following scheme for calculating  $\sigma(\omega)$ . First we derive  $\mathcal{P}_{++}^{(2)}(\mathbf{0}, i\nu_n)$  as the Fourier picture of (8), next we have  $\mathcal{P}^{(2)}(i\nu_n) = (2N/V^2) \mathcal{P}_{++}^{(2)}(\mathbf{0}, i\nu_n)$  and by analytical continuation we come to  $\sigma(\omega) \sim \text{Im}[P^R(\omega)]$ .

According to this scheme let us calculate the value of  $\mathcal{P}_{++}^{(2)}(\mathbf{0}, i\nu_n)$ . When substituting  $j_{i+}$  from Eq. (6) into Eq. (8) and applying the Wick theorem we obtain the diagrams shown in Fig. 1. We remind that we adopt the notation from Ref. [11]. Here we note that we choose connected diagrams only (the sites  $i, i+\hat{x}$  are connected with the sites  $j, j+\hat{x}$ ) because discon-

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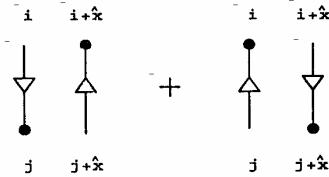


Fig. 1. Relevant diagrams for deriving the Matsubara current-current correlation function (see Eq. (8)).

nected parts represent the term  $\langle j_{i+} \rangle \langle j_{j+} \rangle$  which is zero when averaging over an equilibrium distribution.

By standard rules we can find the following analytical expression of the above graphs,

$$\mathcal{P}_{++}^{(2)}(\mathbf{q}, i\nu_l) = \frac{2}{\beta\hbar} \sum_n g_+^{(0)}(i\omega_n) g_+^{(0)}(i\omega_n - i\nu_l), \quad (9)$$

where  $\omega_n$  ( $\nu_n$ ) stands for the Fermi (Bose) Matsubara frequencies and

$$g_+^{(0)}(i\omega_n) = \frac{1 - n_-}{i\omega_n - \epsilon_1} + \frac{n_-}{i\omega_n - \epsilon_2}$$

is the spin-up free propagator with energies  $\epsilon_1 = -\mu$  and  $\epsilon_2 = U - \mu$  (see Ref. [11]). Here we introduced the mean number of spin-up and spin-down electrons as  $n_+$  and  $n_-$ , respectively.

After summing up Eq. (9) and proceeding through our scheme we finally obtain the real part of the complex optical conductivity in the form (we assume  $\omega \geq 0$ )

$$\sigma^{(2)}(\omega) = D\delta(\omega) + R\delta(\omega - U/\hbar), \quad (10)$$

with the Drude part

$$D = 2\sigma_0 \frac{t^2}{\hbar} \frac{1}{kT} (1-x)x$$

and with the high-frequency weight

$$R = \sigma_0 \frac{t^2}{\hbar} \frac{1}{U} (1-x)^2,$$

where we introduced  $\sigma_0 = \pi e^2 / \hbar \Delta$  and  $x \geq 0$  represents the doping of holes for a half-filled band.

In deriving Eq. (10) we assumed  $t \ll kT \ll U$  and we eliminated the chemical potential by considering the mean number of particles at a site as fixed,



Fig. 2. First order diagram for the Matsubara Green's function (Eq. (13)).

$$n_e = \frac{2}{N} \sum_{k,\sigma} \frac{1}{\beta} \times \sum_m \exp(i\omega_m \eta) \eta g_+^{(0)}(i\omega_m, \mathbf{k}) = 1 - x,$$

where  $\omega_m = (\pi/\beta\hbar)(2m + 1)$  and  $\eta$  goes to zero at the end of the calculation. Before discussing this result let us turn to check explicitly the  $f$ -sum rule for the Hubbard model in the thermodynamical limit [5]. For this purpose we calculate the average of the kinetic energy term

$$\langle T \rangle^{(2)} = \frac{2}{\beta} \sum_m \exp(i\omega_m \eta) \sum_k t(\mathbf{k}) g_+^{(1)}(\mathbf{k}, \omega_m). \quad (12)$$

Here we denoted

$$t(\mathbf{k}) = 2t \sum_A \cos(\mathbf{k} \cdot \mathbf{A}),$$

with a nearest-neighbor vector  $\mathbf{A}$  and  $g_+^{(1)}$  is the Matsubara Green's function given in the first order by the diagram in Fig. 2 with the analytical expression

$$g_+^{(1)}(\mathbf{k}, i\omega_m) = t(\mathbf{k}) g_+^{(0)}(i\omega_m) g_+^{(0)}(i\omega_m). \quad (13)$$

After summing up Eq. (12) we obtain in the limit  $t \ll kT \ll U$

$$\langle T \rangle^{(2)} = -zt^2 N \left( \frac{1}{kT} (1-x)x + \frac{1}{U} (1-x)^2 \right). \quad (14)$$

Here  $z$  is the number of nearest neighbors.

Thus we checked the  $f$ -sum rule (as well as our calculations) which relates the just obtained average of the kinetic energy with the optical spectral weight,

$$N_{\text{total}} = \int_0^\infty \sigma(\omega) d\omega = -\sigma_0 \frac{\langle T \rangle}{\hbar} \frac{1}{zN}. \quad (15)$$

Our results clearly indicate the existence of the Drude weight at  $\omega = 0$  which is inversely proportional to temperature (what is indicated in experiments for a narrow range of band fillings). One sees that this term

does not depend (at  $t \ll kT \ll U$ ) on the Hubbard repulsive energy  $U$ . This is due to the fact that this part is connected with the electron motion to empty sites available when  $x \neq 0, 1$ . In his classical paper [14] Kohn showed that  $D$  can serve as a parameter for the Mott metal–insulator transition. In our case for large  $U$  this weight is zero for a half-filled band ( $x = 0$ ) and naturally for an empty lattice ( $x = 1$ ). For small doping the Drude conductivity depends linearly on the hole-doping concentration  $x$ . The second term in Eq. (10) manifests explicitly transitions across the Hubbard gap resulting in a double occupancy. In our crude approximation its weight does not depend on temperature and decreases rapidly as  $1/U$  for large  $U$ . We do not know about experimental observations of such transitions [4]. We emphasize that doping shifts the spectral weight from high-frequency excitation to low-frequency one as found in experiments [15]. The present calculation, however, cannot explain the width of the observed peaks since we do not introduce any responsible dissipative mechanism and we are dealing with temperatures  $kT \gg t$ .

Summarizing, we have studied analytically the real part of the frequency- and temperature-dependent conductivity for the Hubbard model in the framework of the Kubo formalism. We found that in a non-half-filled case the system exhibits a large  $\delta$ -type peak at low frequencies which can be associated with a Drude peak. The height of the peak is inversely proportional to temperature indicating a connection with experimental results. In our crude approximation we observe another peak at large frequencies whose weight is temperature-independent and decreases linearly with increasing  $U$ . We connected this peak with transitions across the Hubbard gap.

Our results reproduce qualitatively and generalize numerical calculations performed for small systems in the strong-coupling limit. However a quantitative comparison is not possible since the calculations are carried at zero temperature. We believe that calculations based on chosen diagrams as a basis for Dyson's or Larkin's equations will enrich our results which are valid in the strong-coupling regime only and can say nothing about the very interesting region of  $kT \ll t$  and  $U \sim t$ . We expect on the basis of the spectral properties of the Hubbard Hamiltonian derived in more sophisticated approximations (as the Hubbard I, II or GRPA) that the high-frequency peak observed in

our calculations will be accompanied with a family of peaks with their weight corresponding to the perturbation order used. We add that our result is independent of the dimensionality of a model lattice. This is due to the fact that within our approximation there are possible only electronic hops between nearest neighbors so we expect a significant role of the dimensionality for higher-order calculations in which elementary plaquettes can serve as a trajectory for the electronic hopping.

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