Magnetic field dependence of conductivity and effective mass of carriers in a model of Mott-Hubbard material

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Abstract
The influence of external magnetic field $h$ on a static conductivity of Mott-Hubbard material which is described by model with correlated hopping of electrons has been investigated. By means of canonical transformation the effective Hamiltonian which takes into account strong intra-site Coulomb repulsion and correlated hopping is obtained. Using a variant of generalized Hartree-Fock approximation the single-electron Green function and quasiparticle energy spectrum of the model have been calculated. The static conductivity $\sigma$ has been calculated as a function of $h$, electron concentration $n$ and temperature $T$. The correlated hopping is shown to cause the electron-hole asymmetry of transport properties of narrow band materials.

keywords Mott-Hubbard material, conductivity, magnetic field
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The achievements of the recent years in the field of strongly correlated electron systems give us the opportunity to understand the properties of narrow-band materials, in particular those in which metal-insulator transition under the action of external influences (pressure, doping, temperature) is realized [1]. The strongly correlated electron systems demonstrate unusual transport properties [2]. For understanding of the physical mechanisms, which cause these peculiarities, the experimental and theoretical researches of the temperature dependence of conductivity are needed. The results concerning low-frequency behavior of conductivity are of the prior importance, because it gives the information about the scattering processes close to the Fermi surface. The theoretical investigation of conductivity $\sigma(\omega, T)$ are mainly concentrated in the limit $T = 0$. Behavior of the static conductivity $\sigma(T) = \sigma(\omega = 0, T)$ at $T > 0$ has not been studied sufficiently.

Theoretical investigations of the optical conductivity in the Hubbard model [3] in the frameworks of the Kubo linear response theory [4] last for many decades, we note here the investigations by analytical methods: moment method [5], in composite operators method [6], in the mean-field theory [7, 8], in the perturbative theory method [9, 10] in the limit of weak interaction ($|t| \gg U$), in method of the memory function [11, 12], in the opposite limit ($U \gg |t|$). The conductivity has been intensively studied in one-dimensional Hubbard model [13]-[15], where the numerical results can be compared with exact ones obtained by Bethe ansatz application.
For the numerical investigation of the conductivity in Hubbard model the exact diagonalization of finite clusters has been used [16] for 4 x 4 sites cluster, quantum Monte-Carlo method for 8, 10 sites [17], 3 x 3 sites [15], 8 x 8 sites [18], 12 x 12 sites [19]. The investigations by numerical methods were carried out mainly for two-dimensional lattice (this is caused by the interest to the high-temperature superconductivity phenomena [20] in systems with \( CuO \) planes), the conductivity of three-dimensional system has been studied only in narrow interval close to half-filling at weak and intermediate interactions [21].

The optical conductivity has been studied also by the dynamical mean field theory (DMFT) in the limit of infinite spatial dimension [22]. Different DMFT equations solvers were used: iterated perturbation theory IPT [23], non-crossing approximation NCA [24], second order perturbation theory 2OPT [25]. The authors have considered the symmetrical Hubbard model at half-filling close to metal-insulator transition (intra-atomic Coulomb repulsion \( U \approx 2w \), where \( 2w \) is the band width) and have obtained a good agreement with experimental data for some Mott-Hubbard systems. But for realistic models the non-local (dependent on wave vector) contributions to self-energy and transport characteristics are important. Besides, investigations in the framework of DMFT consider mainly the case of half-band filling.

In works [26]-[28] the essential importance of taking into account in the Hubbard model the correlated hopping of electrons and narrow-band model with non-equivalent Hubbard subbands has been proposed. In such a model the hopping integrals which describe translation movement of holes and doublons, differ one from the other and from the activation processes integral. Similar models have been studied intensively in recent years [29]-[31]. For the generalized model which take into account the non-equivalency of Hubbard subbands, reliable results for conductivity do not exist, so the analytical study of conductivity in the framework of the realistic models of the electronic subsystem is of importance.

In this work we show that application of the variant of projection procedure for Green function allows to reproduce some peculiarities of static conductivity of narrow-band material in the limit of strong Coulomb correlation and investigate the effect of external influences like temperature change, doping, pressure and magnetic field. We apply our approach to the Hamiltonian, which, besides of intra-site Coulomb repulsion \( U \), strong in comparison with inter-site hopping \( t_{ij} \), additionally describes correlated hopping of electrons (influence of electron concentration \( n \) on the hopping processes) and show that it leads to the electron-hole asymmetry of conductivity and other characteristics.

We write the Hamiltonian of correlated electron system in representation of \( X_{ik}^{kl} \) Hubbard operators:

\[
H = H_0 + H_1 + H_1' + H_{ex},
\]

where

\[
H_0 = -\mu \sum_{is} \left( X_i^s + X_i^2 \right) + U \sum_i X_i^2 + \frac{1}{2} N V_0 \kappa u^2 + \mu_B h \sum_{is} \eta_s X_i^s,
\]

\[
H_1 = \sum_{ij} t_{ij}(n) X_i^{s0} X_j^{0s} + \sum_{ij} t_{ij}(n) X_i^{2s} X_j^{s2},
\]

(1)
\[ H' = \sum_{ij} \left( t'_{ij}(n) \eta_s X^s_0 X^2_j + h.c. \right), \]

\[ H_{ex} = -\frac{1}{2} \sum_{ij} J(ij) \left( (X^s_i + X^j_0) (X^s_j + X^2_i) + X^s_j X^2_i \right). \]

Here operator \( X_{ik} \) describes transition of site \( i \) from state \( |l⟩ \) to state \( |k⟩ \), \( \mu \) is the chemical potential, \( U \) denotes the energy of intra-site Coulomb repulsion of electrons, \( J \) stands for the direct inter-site exchange interaction, \( \kappa \) is the elastic constant, \( V_0 \) is the initial volume of the crystal, \( N \) is the number of lattice sites, \( \mu_B \) is Bohr magneton, \( h \) stands for the external magnetic field, \( \eta_s = 1 \) if \( s = \uparrow \) and \( -1 \) otherwise. Translation processes are characterized by different hopping integrals, namely \( t_{ij}(n) = (1 + \alpha \mu)(1 - \tau_1 n) t_{ij} \) and \( \tilde{t}_{ij}(n) = (1 + \alpha \mu)(1 - \tau_1 n - 2 \tau_2) t_{ij} \) are hopping parameters for holes and doublons, respectively; \( t'_{ij}(n) = (1 + \alpha \mu)(1 - \tau_1 n - \tau_2) t_{ij} \) is parameter of the hopping of an electron between doublon and hole; correlated hopping parameters \( \tau_2 \) and \( \tau_1 \) describe the influence of sites involved into the hopping process and neighbor sites, respectively; parameter \( \alpha < 0 \) takes into account the renormalization of bandwidth \( 2w = 2z|t_{ij}| \) at strain \( u [32] \), \( z \) is the number of nearest neighbor to a site.

We restrict ourselves to considering the strong correlation limit, namely \( U \gg w(n) \). In such a system at partial filling of the band the conductance is mainly due to electron hopping processes within the Hubbard subbands and interband hopping can be neglected. At these condition we apply the canonical transformation [28] to the Hamiltonian (1).

\[ H_{eff} = e^S H e^{-S}, \]

with

\[ S = \sum_{ij} \left( L(ij) \left( X^1_{ij} X^j_0 X^2_i - X^1_{ij} X^2_j \right) - h.c. \right), \]

\[ L(ij) = \frac{t'_{ij}(n)}{U}. \]

The operator \( S \) is taken to exclude the processes with pair hopping of holes and doublons in the first order in hopping parameter:

\[ H'_0 + [S; H_0] = 0. \]

Finally, we obtain the effective Hamiltonian:

\[ H_{eff} = H_0 + H_1 + H_{ex} + \tilde{H}_{ex}, \]

where

\[ \tilde{H}_{ex} = -\frac{1}{2} \sum_{ij} \tilde{J}(ij) \left( X^s_i X^s_j - X^s_i X^s_j \right) \]

with the indirect exchange interaction parameter \( \tilde{J}(ij) = \frac{(t'_{ij}(n))^2}{U}. \)
Using the projection procedure \cite{33} for the case of \( n < 1 \) we obtain for the single particle energy spectrum:

\[
E_s(k) = -\mu - zJn_\sigma - z\tilde{J}n_\bar{\sigma} + \alpha_s t_k(n) + \beta_s,
\]

where the correlated narrowing of the band and spin-dependent shift of subband center are

\[
\alpha_s = \frac{2 - n + \eta_m}{2} + \frac{n^2 - m^2}{2(2 - n + \eta_m)},
\]

\[
\beta_s = -\frac{2}{(2 - n + \eta_m)} \sum_k t_k(n) \langle X_i^{s0} X_j^{0s} \rangle_k,
\]

respectively, and \( z \) is the number of nearest neighbors to a site. The respective results for \( n > 1 \):

\[
\tilde{E}_s(k) = -\mu + U - zJn_\sigma - z\tilde{J}n_\bar{\sigma} + \tilde{\alpha}_s \tilde{t}_k(n) + \tilde{\beta}_s,
\]

\[
\tilde{\alpha}_s = \frac{n + \eta_m}{2} + \frac{n^2 - m^2}{2(n + \eta_m)},
\]

\[
\tilde{\beta}_s = -\frac{2}{(n + \eta_m)} \sum_k \tilde{t}_k(n) \langle X_i^{s2} X_j^{s2} \rangle_k,
\]

describe upper Hubbard subband of halfbandwidth \( \tilde{w}(n) = z|\tilde{t}_{ij}(n)| \).

With use of the method of works \cite{34, 35}, we calculate the \( xx \)-component of static electronic conductivity \( \sigma_{xx} = \sigma + \tilde{\sigma} \), where

\[
\sigma = -\frac{e^2 \tau z}{2Na} \sum_{ij} \langle X_i^{s0} X_j^{0s} \rangle t_{ij}(n),
\]

is the conductivity of lower \((0 - s)\)-subband,

\[
\tilde{\sigma} = -\frac{e^2 \tau z}{2Na} \sum_{ij} \langle X_i^{s2} X_j^{s2} \rangle \tilde{t}_{ij}(n),
\]

is the conductivity of upper \((\uparrow \downarrow - \bar{s})\)-subband.

The magnetization can be calculated from the equation

\[
\exp \left( \frac{2h + \beta_\uparrow - \beta_\downarrow + zJ_{eff}m}{\Theta} \right) = \frac{\sinh \left( \frac{w(n)\alpha_\uparrow}{\Theta} \frac{1-n}{1-n_\uparrow} \right) \sinh \left( \frac{w(n)\alpha_\downarrow}{\Theta} \frac{n}{1-n_\downarrow} \right)}{\sinh \left( \frac{w(n)\alpha_\uparrow}{\Theta} \frac{1-n}{1-n_\uparrow} \right) \sinh \left( \frac{w(n)\alpha_\downarrow}{\Theta} \frac{n}{1-n_\downarrow} \right)}
\]

for \( n < 1 \) and corresponding equation in which the substitutions \( n \rightarrow 2 - n, w(n) \rightarrow \tilde{w}(n), \alpha_s \rightarrow \tilde{\alpha}_s, \beta_s \rightarrow \tilde{\beta}_s \) are made. Here \( J_{eff} = J - \tilde{J} \). Using these expressions we have
numerically calculated the static conductivity $\sigma_{xx}$ as a function of electron concentration (Figs. 1, 2), temperature (Fig. 4), and magnetic field (Fig. 3).

From Fig. 1 one can see that in the considered model with correlated hopping of electrons the conductivity provided by carriers in upper subband is lower than the conductivity, provided by carriers from upper subband. This effect was discussed in work [35], it is a manifestation of the electron-hole asymmetry, inherent to real transition metal compounds. Other important feature is the change of current carrier type from metallic to semiconducting type in the vicinity of $n = 2/3, 4/3$ and from semiconducting type to metallic one at $n = 1$. Increasing the correlated hopping we shift maxima of the conductivity closer to the half-filling. External magnetic field changes the concentration dependence of $\sigma$ qualitatively (see Fig. 2). The higher is the electron concentration, the less pronounced is the effect of applied magnetic field. At small concentration of electrons the band is fully polarized, in such a ferromagnetic system the conductivity is considerably lower than in paramagnetic state. If electron concentration increase, the decrease of magnetization leads to the increase of conductivity, $\sigma$ approaches its value in paramagnetic state. At the same time, due to the changes in the correlation band narrowing and the shift of subband center, the position of conductivity maximum changes from $n = 2/3$ in saturated ferromagnetic state (Fig 2, 2) to $n = 0.5$ in ferromagnetic state (Fig 2, 3). The change of conductivity with increase of the applied field can be very sharp at low temperature, (Fig 3, solid curve). The increase of temperature leads to the decrease of $\sigma$ and its changes become more smooth. Plateau of $\sigma(h)$ dependence signifies, that at
low temperatures the fully polarized state is reached in very low field. Much higher field is needed to polarize spins at higher temperatures (Fig 7, long-dashed and short dashed curves). Sharp increases of $\sigma$ with increase of temperature is related to the transition from the polarized ferromagnetic state to paramagnetic one, in each state the conductivity decreases with rise of temperature. Very small changes of electron concentration can greatly affect the temperature dependence of conductivity (see Fig. 4).

In the framework of the considered model one can naturally introduce the notions of "wide" (lower) and "narrow" (upper) energy bands and, correspondingly, "light" and "heavy" current carriers with the effective masses

$$m^*_s = \left(\frac{\partial^2 E_s(k)}{\partial k^2}\right)^{-1}, \quad \bar{m}^*_s = \left(\frac{\partial^2 \bar{E}_s(k)}{\partial k^2}\right)^{-1},$$

(16)

where $E_s(k)$ is the energy spectrum of current carriers in lower ($s - 0$) band, $\bar{E}_s(k)$ is the energy spectrum of current carriers in upper ($\bar{s} - \uparrow\downarrow$) subband.

We have obtained that effective mass of heavy carriers can increase substantially with the increase of electron concentration. Because of the correlated hopping the heavy carriers can be realized in lower ($s - 0$) subband as well. It is worthwhile to note that the notion "effective mass of current carrier" has conditional sense, different from the standard one, used in band theory. The definitions (16) are related to the expressions for band spectrum which describe the transitions between $|s\rangle$- and
$|0\rangle$-states as well as $|\uparrow\downarrow\rangle$- and $|\bar{s}\rangle$-states. Then $m^*$ and $\tilde{m}^*$ are effective masses of respective transitions; for the cases when subbands are almost empty or almost full, $m^*$ and $\tilde{m}^*$ can be interpreted as effective masses of electronic and hole states. In the paramagnetic state for the case $n \ll 1$ the value $m_1^* = \frac{\hbar}{2a^2|t(n)|} \simeq \frac{\hbar}{2a^2|t|}$ can be identified as an effective mass of $|s\rangle$-states, i.e. electrons, for the case $n = 1 - \varepsilon$ ($\varepsilon \ll 1$) the value $m_2^* = \frac{\hbar}{2a^2|t(n)|}|_{n=1}$ is an effective mass of a hole. If $n > 1$, then for $n = 1 + \varepsilon$ we have translational motion of doublons ("extra electrons") with masses $\tilde{m}_1^* = \frac{\hbar}{2a^2|\tilde{t}(n)|}|_{n=1}$, and for $n = 2 - \varepsilon$ we have the effective mass of holes $\tilde{m}_2^* = \frac{\hbar}{2a^2|\tilde{t}(n)|}|_{n=2}$. From these results one can see that the effective mass of carrier in upper band can differ substantially from the effective masses in the case when the conductivity is due to $s-0$-transitions. It is important to note that passing from the regime of conductivity provided by the carriers in lower band to the regime when it is provided by $\bar{s}-\uparrow\downarrow$-transitions, the effective mass increase stepwise at the point $n = 1$ (the behavior of the effective mass dependence on the electron concentration is shown in Fig. 5).

The effective mass dependence on the magnetization and external magnetic field is shown in Figs. 6 and 7, respectively. Rise of magnetization leads to the rise of difference in effective masses of spin-up and spin-down current carriers (Fig. 6). The slope of the dependencies $m_{\text{eff}}(m)$ changes with the rise of $m$, too. This leads to the decrease of overall transport in ferromagnetic state, though effective masses of carrier with majority becomes lower. The results shown in Fig. 6 qualitatively agree with the corresponding plot of work [36], where Gutzwiller approximation has been used to calculate effective masses of current carriers. The correlated hopping, favoring localization, shift effective masses up. Different possible scenarios of $m_{\text{eff}}(\hbar)$ dependence are shown in Fig. 7. At high temperature $m_{\text{eff}}$ changes monotonically (Fig. 7, dotted curve) while at low temperature system in unstable towards the transition to polarized state (Fig. 7, solid curve). Direct exchange interaction can stabilize ferromagnetically polarized state in the less then half-filled band even in weak magnetic field (Fig. 7, dash-dotted curve). In this paper we have used a model with correlated hopping of electrons to study the influence of external magnetic field, temperature and doping on a static conductivity of Mott-Hubbard material. In the regime of strong Coulomb interaction hybridization of the Hubbard subbands do not contribute essentially to the transport properties so we have excluded it from the effective Hamiltonian by means of canonical transformation. The single-electron Green
Figure 6: The dependence of current carriers effective mass $m_{\text{eff}}/m_0$ on the magnetization at $n = 0.2$, $\Theta/w = 0.02$, $zJ_{\text{eff}}/w = 0$: solid curves correspond to $\tau_1 = \tau_2 = 0$; dashed curves – to $\tau_1 = \tau_2 = 0.1$.

Figure 7: The dependence of current carriers effective mass $m_{\text{eff}}/m_0$ on the applied magnetic field: solid curves correspond to $zJ_{\text{eff}}/w = 0$, $\Theta/w = 0.02$; dotted curves – to $zJ_{\text{eff}}/w = 0$, $\Theta/w = 0.05$; dash-dotted curves – to $zJ_{\text{eff}}/w = 0.05$, $\Theta/w = 0.02$.

The function and quasiparticle energy spectrum of the model have been calculated using a variant of generalized Hartree-Fock approximation. This procedure has allowed us to obtain analytical expression for the band narrowing factor and relatively simple and transparent equations for calculation of spin-dependent shift of the band center, magnetization, static conductivity and effective mass of the current carrier. The results of our study generalize the results of works [6, 16], where the static conductivity of the Hubbard model has been calculated as a function of electron concentration $n$, for a wider class of systems, for which the correlated hopping should be taken into account. In the limiting case of the absence of correlated hopping our results agree with the concentrational dependencies obtained in the composite operator method [6], exact diagonalization [16] and Monte-Carlo simulations [18] results. The temperature dependence of conductivity in paramagnetic state, calculated in this work, agrees with the corresponding results of DMFT [24, 37]. In the magnetic field static conductivity reflects the changes of single electron energy spectrum through correlation narrowing of the band and shift of subband center. The temperature and concentration dependencies of $\sigma$ are governed by changes of system magnetization in external magnetic field. We have found that in the ground state the saturated ferromagnetic state is stable while at non-zero temperature magnetization has the concentration dependence which agrees with work [38]. Such behavior of magnetization leads to $\sigma(n)$ dependence with maxima at quarter and three-quarter fillings in distinction from paramagnetic ones, obtained in work [35]. At non-zero temperatures the sharp changes of $\sigma(n)$ dependence are possible. It is due to complicated character of temperature dependence of band narrowing factor. Effective mass of quasi-particles appear to be spin-dependent and
substantially varies with magnetic field. These results are in agreement with the analysis of work [36] and experimental data of work [39] for heavy-fermion compounds. Taking into account the correlated hopping which is inherent to real narrow band materials allows us to describe electron-hole asymmetry of these processes which is observed in real materials.

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