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ELECTRICAL CONDUCTIVITY IN THE HUBBARD MODEL INCLUDING ELECTRON-PHONON INTERACTION

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Электропроводность в модели Хаббарда с учетом электронно-фононного взаимодействия

На основе модели Хаббарда со слабым электронно-фононным взаимодействием вычислена электропроводность σ для $U \gg t$ (U - внутриатомная кулоновская энергия, t - интеграл перекрытия между ближайшими соседями) и низких частот. Подробно исследована статическая проводимость для полузаполненной зоны и $T \gg T_D$ (T_D - температура Дебая). Эта проводимость сравнивается со статической проводимостью в модели Хаббарда без учета фононов, вычисленной в приближении $\lim_{t \to 0} \sigma / t^2$. Учет фононов отражается в конечном времени релаксации, температурная зависимость которого приводит к смещению максимума проводимости и к уменьшению проводимости для высоких температур по сравнению с T^{-2}.

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Electrical Conductivity in the Hubbard Model Including Electron-Phonon Interaction

Using the Hubbard model including weak electron-phonon coupling the electrical conductivity σ is calculated for $U \gg t$ (U, intraatomic Coulomb energy; t, nearest-neighbour hopping integral) and low frequencies. Especially the dc conductivity is investigated for the half-filled band and $T \gg T_D$ (T_D, Debye temperature). It is compared with the dc conductivity in the phononless Hubbard model calculated in the approximation $\lim_{t \to 0} \frac{\sigma}{t^2}$. The inclusion of phonons results in a finite transport relaxation time the temperature dependence of which leads to a shift of the conductivity maximum temperature to a lower value, the sharpening of the maximum, and to the decrease of the conductivity for high temperatures according to T^{-2}.

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1. INTRODUCTION

In the recent years experiments have suggested that electron-correlation models in the strong coupling region should be used to describe the properties of several real systems, such as TCNQ salts [1-3], magnetite (Fe_3O_4) [4-6], the ferrites $Me_xFe_{3-x}O_4$ (Me metal ion impurities) [7], [8], and Ti_4O_7. Therefore the calculation of the electrical conductivity σ, especially the dc conductivity, in those models is of particular interest.

Several works are concerned with the conductivity in the Hubbard model [9,10] in the strong coupling region $U \gg t$ (U, intraatomic Coulomb energy, t, nearest-neighbour hopping integral) [11-16]. In most of them a δ-function peak in the dc part of the conductivity appears [11-14]. Bari and Kaplan [14] obtained this peak in the approximation $\lim_{t \to 0} \frac{\sigma}{t^2}$. This approximation was also used in the calculation of σ in an extended Hubbard model [17,18], the Cullen-Callen model of magnetite [6,19], the Hubbard-Holstein model [20,21], and a Hubbard model modified by phonon-modulated hopping integrals [22]. In those calculations the δ-function peak which is retained even in the case of electron-phonon coupling [21,22] is assumed to be replaced in some improved approximation either by a finite value, the temperature dependence of which is assumed to be unessential [6,17] or by a temperature-independent relaxation time caused, e.g., by impurity scattering [22].

Although the assumptions concerning the δ-function peak are reasonable it is desirable to perform an improved conductivity calculation which yields a finite conductivity due to a dissipation mechanism included in the model under consideration. Considering the Hubbard model Ohata [15] has obtained a finite dc conductivity by taking into account spin disorder scattering and dynamical processes. We note that those processes do not occur in electron-correlation models for spinless fermions [4–8] which we are also interested in.

Since in the substances mentioned above the phonons play an essential role in the electrical properties of the strongly correlated electrons, in this paper we consider the simplest model describing this situation, namely, the Hubbard model including electron-phonon interaction (see, e.g., refs. [23,24]):

$$H = \sum_{ij\sigma} t_{ij} c^{+}_{i\sigma} c_{j\sigma} + U \sum_{i} n_{i\uparrow} n_{i\downarrow} + \sum_{\vec{q}} \omega_{\vec{q}} b^{+}_{\vec{q}} b_{\vec{q}} + \sum_{\vec{q} i\sigma} A_{\vec{q}} e^{i\vec{q}\vec{R}_i} n_{i\sigma}(b_{\vec{q}} + b^{+}_{-\vec{q}}) - \mu \sum_{i\sigma} n_{i\sigma} . \tag{1}$$

The symbols have the usual meaning. The hopping integral t_{ij} is related to the band energy $\epsilon_{\vec{k}}$ by

$$t_{ij} = \frac{1}{N} \sum_{\vec{k}} \epsilon_{\vec{k}} e^{i\vec{k}(\vec{R}_i - \vec{R}_j)} . \tag{2}$$

We put $t_{ii} = 0$ without loss of generality. Furthermore, we have $A^{*}_{-\vec{q}} = A_{\vec{q}}$. For the sake of simplicity we consider only longitudinal acoustical phonons for which $|A_{\vec{q}}|^2 \propto q$ for small q. We take the U term in (1) to be much larger than the band and electron-phonon interaction terms, i.e., we consider $U \gg t$ and weak electron-phonon coupling.

Using the model (1) we calculate the conductivity and obtain a finite dc conductivity. We mainly focus our attention on the effects of phonons on the temperature dependence of the dc conductivity in the half-filled band. Furthermore, we give a justification of the approximation $\lim\limits_{t\to 0} \frac{\sigma}{t^2}$ for the half-filled band case.

2. CONDUCTIVITY CALCULATION

Considering a crystal of cubic symmetry we are concerned only with the diagonal elements of the conductivity tensor which may be expressed in terms of the Fourier transform of the retarded two-time commutator Green function [25,26]:

$$\sigma^{\nu\nu}(\omega) = -\lim_{\epsilon \to +0} \lim_{\Omega \to \infty} \frac{1}{\Omega} \langle\langle J^{\nu} ; P^{\nu} \rangle\rangle_{z=\omega+i\epsilon} . \tag{3}$$

Ω is the crystal volume and P^{ν}, J^{ν}, the ν-components of the polarization operator

$$\vec{P} = e \sum_{i\sigma} \vec{R}_i n_{i\sigma} \tag{4}$$

and the current operator

$$\vec{J} = \dot{\vec{P}} = -ie \sum_{ij\sigma} (\vec{R}_i - \vec{R}_j) t_{ij} c^{+}_{i\sigma} c_{j\sigma} , \tag{5}$$

respectively. According to (3) and (5) we write

$$\langle\langle J^{\nu}; P^{\nu} \rangle\rangle_z = -ie \sum_{ij\sigma} (R^{\nu}_i - R^{\nu}_j) t_{ij} G_{ij\sigma}(z),$$

where

$$G_{ij\sigma}(z) = \langle\langle c^{+}_{i\sigma} c_{j\sigma} ; P^{\nu} \rangle\rangle_z . \tag{6}$$

It is convenient to introduce the projection operators [12,27]

$$n^{+}_{i\sigma} = n_{i\sigma} , \qquad n^{-}_{i\sigma} = 1 - n_{i\sigma} \tag{7}$$

by means of which $G_{ij\sigma}(z)$ is resolved into four components:

$$G_{ij\sigma}(z) = \sum_{\alpha,\beta=\pm} G^{\alpha\beta}_{ij\sigma}(z),$$

where

$$G^{\alpha\beta}_{ij\sigma}(z) = \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} ; P^{\nu} \rangle\rangle_z . \qquad (8)$$

Defining the "mixed" Green functions

$$F^{(1)\alpha\beta}_{ij\vec{q}\sigma} = \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} b_{\vec{q}} ; P^{\nu} \rangle\rangle_z , \qquad (9)$$

$$F^{(2)\alpha\beta}_{ij\vec{q}\sigma} = \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} b^{+}_{-\vec{q}} ; P^{\nu} \rangle\rangle_z$$

and using the Hamiltonian (1) we get the following equations of motion

$$\begin{aligned}
(z + U\delta_{\alpha+} - U\delta_{\beta+}) G^{\alpha\beta}_{ij\sigma}(z) &= -e(R^{\nu}_i - R^{\nu}_j)\Phi^{\alpha\beta}_{ij\sigma} + \\
&+ \sum_{\ell} t_{\ell j} \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{\ell\sigma} ; P^{\nu} \rangle\rangle_z - \\
&- \sum_{\ell} t_{i\ell} \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{\ell\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} ; P^{\nu} \rangle\rangle_z + \\
&+ \xi_{\alpha} \sum_{\ell} t_{i\ell} \langle\langle (c^{+}_{i-\sigma} c_{\ell-\sigma} - c^{+}_{\ell-\sigma} c_{i-\sigma}) c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} ; P^{\nu} \rangle\rangle_z + \\
&+ \xi_{\beta} \sum_{\ell} t_{\ell j} \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} (c^{+}_{j-\sigma} c_{\ell-\sigma} - c^{+}_{\ell-\sigma} c_{j-\sigma}) c_{j\sigma} ; P^{\nu} \rangle\rangle_z + \\
&+ \sum_{\vec{q}} A_{\vec{q}} (e^{i\vec{q}\vec{R}_j} - e^{i\vec{q}\vec{R}_i}) (F^{(1)\alpha\beta}_{ij\vec{q}\sigma}(z) + F^{(2)\alpha\beta}_{ij\vec{q}\sigma}(z)),
\end{aligned} \qquad (10)$$

$$\begin{aligned}
(z + U\delta_{\alpha+} - U\delta_{\beta+} - \omega_{\vec{q}}) F^{(1)\alpha\beta}_{ij\vec{q}\sigma}(z) &= -e(R^{\nu}_i - R^{\nu}_j)\Phi^{(1)\alpha\beta}_{ij\vec{q}\sigma} + \\
&+ \sum_{\ell} t_{\ell j} \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{\ell\sigma} b_{\vec{q}} ; P^{\nu} \rangle\rangle_z - \\
&- \sum_{\ell} t_{i\ell} \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{\ell\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} b_{\vec{q}} ; P^{\nu} \rangle\rangle_z + \\
&+ \xi_{\alpha} \sum_{\ell} t_{i\ell} \langle\langle (c^{+}_{i-\sigma} c_{\ell-\sigma} - c^{+}_{\ell-\sigma} c_{i-\sigma}) c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} b_{\vec{q}} ; P^{\nu} \rangle\rangle_z + \\
&+ \xi_{\beta} \sum_{\ell} t_{\ell j} \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} (c^{+}_{j-\sigma} c_{\ell-\sigma} - c^{+}_{\ell\sigma} c_{j-\sigma}) c_{j\sigma} b_{\vec{q}} ; P^{\nu} \rangle\rangle_z + \\
&+ \sum_{\vec{q}'} A_{\vec{q}'} (e^{i\vec{q}'\vec{R}_j} - e^{i\vec{q}'\vec{R}_i}) \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} \times \\
&\times (b_{\vec{q}'} + b^{+}_{-\vec{q}'}) b_{\vec{q}} , P^{\nu} \rangle\rangle_z + \\
&+ A_{-\vec{q}} \sum_{\ell\sigma'} e^{-i\vec{q}\vec{R}_{\ell}} \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{i-\sigma} c_{j\sigma} n_{\ell\sigma'} , P^{\nu} \rangle\rangle_z ,
\end{aligned} \qquad (11)$$

where δ is the Kronecker delta, $\xi_{\pm} = \pm 1$, and

$$\begin{aligned}
\Phi^{\alpha\beta}_{ij\sigma} &= \langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} \rangle , \\
\Phi^{(1)\alpha\beta}_{ij\vec{q}\sigma} &= \langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} b_{\vec{q}} \rangle .
\end{aligned} \qquad (12)$$

The equation of motion for $F^{(2)\alpha\beta}_{ij\vec{q}\sigma}(z)$ results from (11) by the substitutions $\omega_{\vec{q}} \to -\omega_{\vec{q}}$, $b_{\vec{q}} \to b^{+}_{-\vec{q}}$, and $A_{-\vec{q}} \to -A_{-\vec{q}}$. At this step we break off the chain of equations of motion. First considering the case $i \neq j$ we employ the following decoupling procedures:

(a) The four-particle electron Green functions on the right-hand side of (10) are approximated by a decoupling also used by Kubo [12] and equivalent to that of Hubbard's first paper [9]. It is based on the following rule [10,27]: Operators for the same site are never decoupled to two parts (U>>t). Correspondingly we approximate

$$\begin{aligned}
\langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{\ell\sigma} ; P^{\nu} \rangle\rangle_z &\simeq n^{\beta}_{-\sigma} \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} c_{\ell\sigma} ; P^{\nu} \rangle\rangle_z = n^{\beta}_{-\sigma} \sum_{\gamma} G^{\alpha\gamma}_{i\ell\sigma}(z) , \\
\langle\langle n^{\alpha}_{i-\sigma} c^{+}_{\ell\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} ; P^{\nu} \rangle\rangle_z &\simeq n^{\alpha}_{-\sigma} \langle\langle c^{+}_{\ell\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} ; P^{\nu} \rangle\rangle_z = n^{\alpha}_{-\sigma} \sum_{\gamma} G^{\gamma\beta}_{\ell j\sigma}(z) ,
\end{aligned} \qquad (13)$$

$(n^{\beta}_{-\sigma} = \langle n^{\beta}_{j-\sigma}\rangle)$ and neglect the terms involving Green functions multiplied by ξ_α and ξ_β. We use this decoupling also for the mixed Green functions containing one phonon operator on the right-hand side of (11).

(b) Because we consider weak electron-phonon coupling, we approximate the mixed Green function containing two phonon operators in (11) in the lowest order in $A_{\vec q}$. Furthermore, we neglect phonon-drag effects discussed in the band limit $(U=0)$ in [28-30]. Accordingly we put

$$\langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} (b_{\vec q'} + b^{+}_{-\vec q'}) b_{\vec q}; P^{\nu}\rangle\rangle_z \simeq \delta_{\vec q',-\vec q}\, \nu_{\vec q}\, G^{\alpha\beta}_{ij\sigma}(z),$$

$$\langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} (b_{\vec q'} + b^{+}_{-\vec q'}) b^{+}_{-\vec q}; P^{\nu}\rangle\rangle_z \simeq \delta_{\vec q',-\vec q} (1+\nu_{\vec q}) G^{\alpha\beta}_{ij\sigma}(z), \tag{14}$$

where $\nu_{\vec q} = \langle b^{+}_{\vec q} b_{\vec q}\rangle = (e^{\beta\omega_{\vec q}} - 1)^{-1}$.

(c) As to the five-particle electron Green function in (11) corresponding to the indirect electron-electron interaction induced by the phonons, we first represent it exactly as $(i \neq j)$

$$\langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} n_{\ell\sigma'}; P^{\nu}\rangle\rangle_z =$$

$$= (1-\delta_{\ell i} - \delta_{\ell j}) \langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} n_{\ell\sigma'}; P^{\nu}\rangle\rangle_z +$$

$$+ (\delta_{\ell i}\, \delta_{\sigma',-\sigma}\, \delta_{\alpha +} + \delta_{\ell j} (\delta_{\sigma'\sigma} + \delta_{\sigma',-\sigma}\, \delta_{\beta +})) G^{\alpha\beta}_{ij\sigma}(z). \tag{15}$$

This representation guarantees that the electron correlations on the same site are taken into account exactly. We decouple the Green function on the right-hand side of (15) following the rule used in (a):

$$\langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} n_{\ell\sigma'}; P^{\nu}\rangle\rangle_z \simeq n_{\sigma'} G^{\alpha\beta}_{ij\sigma}(z) +$$

$$+ \Phi^{\alpha\beta}_{ij\sigma} \langle\langle n_{\ell\sigma'}; P^{\nu}\rangle\rangle_z . \tag{16}$$

Since $t \ll U$ we take into account only terms in the lowest order in t and correspondingly neglect the second term in (16). Thus we get

$$\langle\langle n^{\alpha}_{i-\sigma} c^{+}_{i\sigma} n^{\beta}_{j-\sigma} c_{j\sigma} n_{\ell\sigma'}; P^{\nu}\rangle\rangle_z \simeq (n_{\sigma'} + \delta_{\ell i} (\delta_{\sigma',-\sigma}\, \delta_{\alpha +} - n_{\sigma'}) +$$

$$+ \delta_{\ell j} (\delta_{\sigma'\sigma} + \delta_{\sigma',-\sigma}\, \delta_{\beta +} - n_{\sigma'})) G^{\alpha\beta}_{ij\sigma}(z). \tag{17}$$

Considering the case $i = j$ the equation of motion (10) reduces to that of the pure Hubbard model for which Kubo [12] has shown that the Fourier transform $G^{\alpha\beta}_{\vec k\sigma}$ (equation (18)) is an odd function of $\vec k$ and therefore $G^{\alpha\beta}_{ii\sigma} = 0$.

Inserting the approximations (13), (14), (17) into (10), (11) and introducing the Fourier transforms

$$G^{\alpha\beta}_{\vec k\sigma} = \frac{1}{N} \sum_{i,j} G^{\alpha\beta}_{ij\sigma}\, e^{-i\vec k(\vec R_i - \vec R_j)}$$

$$\Phi^{\alpha\beta}_{\vec k\sigma} = \frac{1}{N} \sum_{i,j} \Phi^{\alpha\beta}_{ij\sigma}\, e^{-i\vec k(\vec R_i - \vec R_j)} \tag{18}$$

$$F^{(1)\alpha\beta}_{\vec k\vec q\sigma} = \frac{1}{N} \sum_{i,j} F^{(1)\alpha\beta}_{ij\vec q\sigma}\, e^{-i\vec k\vec R_i}\, e^{i(\vec k+\vec q)\vec R_j} =$$

$$= \frac{1}{N^2} \sum_{\vec k_1,\vec k_2} \langle\langle \rho^{\alpha}_{\vec k_1 -\sigma}\, \rho^{\beta}_{\vec k_2 -\sigma}\, c^{+}_{-\vec k_1 - \vec k\sigma}\, c_{\vec k_2 - \vec k - \vec q\sigma}\, b_{\vec q}; P^{\nu}\rangle\rangle_z \tag{19}$$

$$\Phi^{(1)\alpha\beta}_{\vec k\vec q\sigma} = \frac{1}{N} \sum_{i,j} \Phi^{(1)\alpha\beta}_{ij\vec q\sigma}\, e^{-i\vec k\vec R_i}\, e^{i(\vec k+\vec q)\vec R_j}, \tag{20}$$

where $\rho^{\alpha}_{\vec k-\sigma} = \sum_i e^{i\vec k\vec R_i} n^{\alpha}_{i-\sigma}$, and analogous expressions for $F^{(2)\alpha\beta}_{\vec k\vec q\sigma}$ and $\Phi^{(2)\alpha\beta}_{\vec k\vec q\sigma}$ we obtain

$$(z + U\delta_{\alpha+} - U\delta_{\beta+}) G^{\alpha\beta}_{\vec k\sigma} = -ie \frac{\partial}{\partial k^\nu}\Phi^{\alpha\beta}_{\vec k\sigma} + n^{\beta}_{-\sigma}\epsilon_{\vec k}\sum_\gamma G^{\alpha\gamma}_{\vec k\sigma} - n^{\alpha}_{-\sigma}\epsilon_{\vec k}\sum_\gamma G^{\gamma\beta}_{\vec k\sigma} + \sum_{\vec q} A_{\vec q}\big(F^{(1)\alpha\beta}_{\vec k\vec q\sigma} + F^{(2)\alpha\beta}_{\vec k\vec q\sigma} - F^{(1)\alpha\beta}_{\vec k-\vec q,\vec q\sigma} - F^{(2)\alpha\beta}_{\vec k-\vec q,\vec q\sigma}\big), \qquad (21)$$

$$(z+U\delta_{\alpha+} - U\delta_{\beta+} - \omega_{\vec q}) F^{(1)\alpha\beta}_{\vec k\vec q\sigma} = -ie\frac{\partial}{\partial k^\nu}\Phi^{\alpha\beta}_{\vec k\vec q\sigma} + n^\beta_{-\sigma}\epsilon_{\vec k+\vec q}\sum_\gamma F^{(1)\alpha\gamma}_{\vec k\vec q\sigma} - n^\alpha_{-\sigma}\epsilon_{\vec k}\sum_\gamma F^{(1)\gamma\beta}_{\vec k\vec q\sigma} + A_{-\vec q}\{(1+\delta_{\beta+} - n + \nu_{\vec q})G^{\alpha\beta}_{\vec k\sigma} - (n-\delta_{\alpha+}+\nu_{\vec q})G^{\alpha\beta}_{\vec k+\vec q\sigma}\}, \qquad (22)$$

$$(z+U\delta_{\alpha+} - U\delta_{\beta+}+\omega_{\vec q})F^{(2)\alpha\beta}_{\vec k\vec q\sigma} = -ie\frac{\partial}{\partial k^\nu}\Phi^{(2)\alpha\beta}_{\vec k\vec q\sigma} + n^\beta_{-\sigma}\epsilon_{\vec k+\vec q}\sum_\gamma F^{(2)\alpha\gamma}_{\vec k\vec q\sigma} - n^\alpha_{-\sigma}\epsilon_{\vec k}\sum_\gamma F^{(2)\gamma\beta}_{\vec k\vec q\sigma} + A_{-\vec q}\{(n-\delta_{\beta+}+\nu_{\vec q})G^{\alpha\beta}_{\vec k\sigma} - (1+\delta_{\alpha+} - n+\nu_{\vec q})G^{\alpha\beta}_{\vec k+\vec q\sigma}\}. \qquad (23)$$

$n = n_\sigma + n_{-\sigma}$ is the given electron concentration. We note that the first term in (17) gives no contribution because of $\delta_{\vec q,0} A_{\vec q} = 0$. As we are interested in the low-frequency region, especially in the dc conductivity, we consider the case $\omega \ll U$. Because additionally $t \ll U$

discard the off-diagonal terms in (21) to (23), i.e., we put $G^{\alpha\gamma(\neq\beta)}_{\vec k\sigma} = 0$, $G^{\gamma(\neq\alpha)\beta}_{\vec k\sigma}=0$, $F^{(1)\alpha\gamma(\neq\beta)}_{\vec k\vec q\sigma}=0$ etc., since the inclusion of those terms would give rise to correlations of order $O(t^2/U^2)$ in the Green functions [12,15]. Furthermore, because of $\omega \ll U$ we neglect the Green functions $G^{\alpha\neq\beta}_{\vec k\sigma}$ (which vanish for $\omega\ll U$ and $A_{\vec q}=0$ [15]) and therefore consider only intraband transitions. For brevity we replace the superscripts "$\alpha\alpha$" by "α" hereafter.

Calculating the mean value $\Phi^\alpha_{\vec k\sigma}$ in the lowest order in $A_{\vec q}$ and t we get [27]

$$\Phi^\alpha_{\vec k\sigma} = n^\alpha_{-\sigma} f(E^\alpha_{\vec k\sigma} - \mu), \quad \text{where} \quad E^\alpha_{\vec k\sigma} = n^\alpha_{-\sigma}\epsilon_{\vec k} + U\delta_{\alpha+} \qquad (24)$$

and $f(\omega) = (e^{\beta\omega}+1)^{-1}$. $E^\alpha_{\vec k\sigma}$ and $\Phi^\alpha_{\vec k\sigma}$ are the energies and distribution functions, respectively, of the quasi-particles in the upper ($\alpha=+$) and lower ($\alpha=-$) subbands.

By (9), (12), (19), (20) the mean values $\Phi^{(1,2)\alpha}_{\vec k\vec q\sigma}$ can be calculated from

$$\langle [n^\alpha_{i-\sigma} c^+_{i\sigma} n^\beta_{j-\sigma} c_{j\sigma} b_{\vec q}, H]_-\rangle = \langle [n^\alpha_{i-\sigma}c^+_{i\sigma} n^\beta_{j-\sigma} c_{j\sigma} b^+_{-\vec q}, H]_-\rangle = 0$$

in the same approximation as the Green functions $F^{(1,2)\alpha}_{\vec k\vec q\sigma}$ (see e.g. [31-33]):

$$\Phi^{(1)\alpha}_{\vec k\vec q\sigma} = A_{-\vec q}\frac{(1+\delta_{\alpha+} - n+\nu_{\vec q})\Phi^\alpha_{\vec k\sigma} - (n-\delta_{\alpha+}+\nu_{\vec q})\Phi^\alpha_{\vec k+\vec q\sigma}}{E^\alpha_{\vec k\sigma} - E^\alpha_{\vec k+\vec q\sigma} - \omega_{\vec q}} \equiv A_{-\vec q}\, g^\alpha_{\vec k\vec q\sigma},$$

$$\Phi^{(2)\alpha}_{\vec k\vec q\sigma} = A_{-\vec q}\, g^\alpha_{\vec k+\vec q,-\vec q\sigma}. \qquad (25)$$

Performing the indicated approximations and inserting (22), (23), (25) into (21) we obtain

$$zG^\alpha_{\vec k\sigma}(z) = -iev^\nu_{\vec k}\frac{\partial\Phi^\alpha_{\vec k\sigma}}{\partial\epsilon_{\vec k}} + \sum_{\vec q}\{w^\alpha_{\vec k,\vec k+\vec q\sigma}(z)G^\alpha_{\vec k\sigma}(z) -$$

$$- w^{\alpha}_{\vec{k}+\vec{q},\vec{k}\sigma}(z) G^{\alpha}_{\vec{k}+\vec{q}\sigma}(z) \} -$$

$$- ie \sum_{\vec{q}} |A_{\vec{q}}|^2 \{ \frac{\partial}{\partial k^{\nu}} g^{\alpha}_{\vec{k}\vec{q}\sigma} (\frac{1}{z + E^{\alpha}_{\vec{k}\sigma} - E^{\alpha}_{\vec{k}+\vec{q}\sigma} - \omega_{\vec{q}}} -$$

$$- \frac{1}{z + E^{\alpha}_{\vec{k}+\vec{q}\sigma} - E^{\alpha}_{\vec{k}\sigma} + \omega_{\vec{q}}}) +$$

$$+ \frac{\partial}{\partial k^{\nu}} g^{\alpha}_{\vec{k}+\vec{q},-\vec{q}\sigma} (\frac{1}{z + E^{\alpha}_{\vec{k}\sigma} - E^{\alpha}_{\vec{k}+\vec{q}\sigma} + \omega_{\vec{q}}} -$$

$$- \frac{1}{z + E^{\alpha}_{\vec{k}+\vec{q}\sigma} - E^{\alpha}_{\vec{k}\sigma} - \omega_{\vec{q}}}) \}, \qquad (26)$$

where

$$w^{\alpha}_{\vec{k},\vec{k}+\vec{q}\sigma}(z) = |A_{\vec{q}}|^2 (\frac{1 + \delta_{\alpha+} - n + \nu_{\vec{q}}}{z + E^{\alpha}_{\vec{k}\sigma} - E^{\alpha}_{\vec{k}+\vec{q}\sigma} - \omega_{\vec{q}}} +$$

$$+ \frac{n - \delta_{\alpha+} + \nu_{\vec{q}}}{z + E^{\alpha}_{\vec{k}\sigma} - E^{\alpha}_{\vec{k}+\vec{q}\sigma} + \omega_{\vec{q}}} + \frac{n - \delta_{\alpha+} + \nu_{\vec{q}}}{z + E^{\alpha}_{\vec{k}+\vec{q}\sigma} - E^{\alpha}_{\vec{k}\sigma} - \omega_{\vec{q}}} +$$

$$+ \frac{1 + \delta_{\alpha+} - n + \nu_{\vec{q}}}{z + E^{\alpha}_{\vec{k}+\vec{q}\sigma} - E^{\alpha}_{\vec{k}\sigma} + \omega_{\vec{q}}}).$$

This closed integral equation for $G^{\alpha}_{\vec{k}\sigma}(z)$ is analogous to the quantum kinetic equation for the nonequilibrium distribution function in the linear response approximation. However, besides the drift term $- iev_{\vec{k}} \frac{\partial \Phi^{\alpha}_{\vec{k}\sigma}}{\partial \epsilon_{\vec{k}}}$ and the collision term containing the Green functions on the right-hand side of (26) there appears an additional inhomogeneous term proportional to $|A_{\vec{q}}|^2$ discussed extensively (in the band limit $U=0$) in [31-34]. This term describes the scattering of electrons by phonons induced by the external oscillating electric field and becomes essential in the frequency region $\frac{1}{\tau} \ll \omega \ll U$ (τ electron transport relaxation time, see (38)).

In this paper our interest is confined only to the low-frequency region $\omega\tau \ll 1$. In this case the extra inhomogeneous term in (26) can be neglected since its imaginary part gives a small correction to the drift term and its real part vanishes at $\omega = 0$, as can be seen easily from (26). In order to solve the integral equation (26) we proceed along a line similar to that indicated in works by Plakida [31-33]. We define the mass operator $M^{\alpha}_{\vec{k}\sigma}$ by

$$G^{\alpha}_{\vec{k}\sigma}(z) = \frac{- iev^{\nu}_{\vec{k}} \partial \Phi^{\alpha}_{\vec{k}\sigma} / \partial \epsilon_{\vec{k}}}{z - M^{\alpha}_{\vec{k}\sigma}(z)} . \qquad (27)$$

Inserting (27) into (26) we get the nonlinear integral equation for $M^{\alpha}_{\vec{k}\sigma}$:

$$M^{\alpha}_{\vec{k}\sigma} = M^{(0)\alpha}_{\vec{k}\sigma}(z) - \sum_{\vec{q}} \frac{v^{\nu}_{\vec{k}+\vec{q}} \frac{\partial \Phi^{\alpha}_{\vec{k}+\vec{q}\sigma}}{\partial \epsilon_{\vec{k}+\vec{q}}}}{v^{\nu}_{\vec{k}} \frac{\partial \Phi^{\alpha}_{\vec{k}\sigma}}{\partial \epsilon_{\vec{k}}}} w^{\alpha}_{\vec{k}+\vec{q}\sigma}(z) \times$$

$$\times \frac{z - M^{\alpha}_{\vec{k}\sigma}(z)}{z - M^{\alpha}_{\vec{k}+\vec{q}\sigma}(z)} , \qquad (28)$$

where $M^{(0)\alpha}_{\vec{k}\sigma}(z) = \sum_{\vec{q}} w^{\alpha}_{\vec{k},\vec{k}+\vec{q}\sigma}(z)$.

We separate $M^{\alpha}_{\vec{k}\sigma}$ and $M^{(0)\alpha}_{\vec{k}\sigma}$ into the real and imaginary parts according to

$$\lim_{\epsilon\to+0} M^{\alpha}_{\vec{k}\sigma}(\omega+i\epsilon) = M'^{\alpha}_{\vec{k}\sigma}(\omega) - i\Gamma^{\alpha}_{\vec{k}\sigma}(\omega). \tag{29}$$

Because of $\omega\tau \ll 1$ we approximate $\mathrm{Re}\, w^{\alpha}_{\vec{k},\vec{k}+\vec{q}\sigma}$ and $\mathrm{Re}\, w^{\alpha}_{\vec{k}+\vec{q},\vec{k}\sigma}$ in (28) by their values at $\omega=0$ vanishing by (26). Therefore we put $\mathrm{Re}\, w^{\alpha}_{\vec{k},\vec{k}+\vec{q}}(\omega+i\epsilon) = \mathrm{Re}\, w^{\alpha}_{\vec{k}+\vec{q},\vec{k}\sigma}(\omega+i\epsilon) = 0$ and consequently look for a solution

$$M^{\alpha}_{\vec{k}\sigma}(\omega+i\epsilon) = -i\Gamma^{\alpha}_{\vec{k}\sigma}(\omega). \tag{30}$$

In accordance with (28) the damping $\Gamma^{\alpha}_{\vec{k}\sigma}(\omega)$ obeys the integral equation

$$\Gamma^{\alpha}_{\vec{k}\sigma}(\omega) = \Gamma^{(0)\alpha}_{\vec{k}\sigma}(\omega) + \sum_{\vec{q}} \frac{v^{\nu}_{\vec{k}+\vec{q}} \dfrac{\partial\Phi^{\alpha}_{\vec{k}+\vec{q}\sigma}}{\partial\epsilon_{\vec{k}+\vec{q}}}}{v^{\nu}_{\vec{k}} \dfrac{\partial\Phi^{\alpha}_{\vec{k}\sigma}}{\partial\epsilon_{\vec{k}}}} \times \mathrm{Im}\{w^{\alpha}_{\vec{k}+\vec{q},\vec{k}}(\omega+i\epsilon)\}\mathrm{Re}\left\{\frac{\omega+i\Gamma_{\vec{k}\sigma}(\omega)}{\omega+i\Gamma_{\vec{k}+\vec{q}\sigma}(\omega)}\right\}, \tag{31}$$

where

$$\Gamma^{(0)\alpha}_{\vec{k}\sigma}(\omega) = \Pi \sum_{\vec{q}} |A_{\vec{q}}|^2 \{(1+\delta_{\alpha+} - n_{+\nu_{\vec{q}}}) \times$$
$$\times(\delta(\omega + E^{\alpha}_{\vec{k}\sigma} - E^{\alpha}_{\vec{k}+\vec{q}\sigma} - \omega_{\vec{q}}) + \delta(\omega + E^{\alpha}_{\vec{k}+\vec{q}\sigma} - E^{\alpha}_{\vec{k}\sigma} + \omega_{\vec{q}})) +$$
$$+(n-\delta_{\alpha+} + \nu_{\vec{q}})(\delta(\omega + E^{\alpha}_{\vec{k}\sigma} - E^{\alpha}_{\vec{k}+\vec{q}\sigma} + \omega_{\vec{q}}) +$$
$$+\delta(\omega + E^{\alpha}_{\vec{k}+\vec{q}\sigma} - E^{\alpha}_{\vec{k}\sigma} - \omega_{\vec{q}}))\}. \tag{32}$$

Whereas $\Gamma^{(0)\alpha}_{\vec{k}\sigma}$ is connected with the damping of the single-particle excitations the second term in (31) describes the influence of the electron transport on the damping. Accordingly we solve (31) by iteration replacing the damping in the "transport term" by $\Gamma^{(0)\alpha}_{\vec{k}\sigma}$. The solution is

$$\Gamma^{\alpha}_{\vec{k}\sigma}(\omega) = \Gamma^{(0)\alpha}_{\vec{k}\sigma}(\omega) + \sum_{\vec{q}} \frac{v^{\nu}_{\vec{k}+\vec{q}} \dfrac{\partial\Phi^{\alpha}_{\vec{k}+\vec{q}\sigma}}{\partial\epsilon_{\vec{k}+\vec{q}}}}{v^{\nu}_{\vec{k}} \dfrac{\partial\Phi^{\alpha}_{\vec{k}\sigma}}{\partial\epsilon_{\vec{k}}}} \mathrm{Im}\, w^{\alpha}_{\vec{k}+\vec{q},\vec{k}\sigma}(\omega+i\epsilon) \times \mathrm{Re}\left\{\frac{\omega+i\Gamma^{(0)\alpha}_{\vec{k}\sigma}(\omega)}{\omega+i\Gamma^{(0)\alpha}_{\vec{k}+\vec{q}\sigma}(\omega)}\right\}. \tag{33}$$

As follows from (3), (6), (8), (18), (27), (30), the conductivity is given by

$$\sigma^{\nu\nu}(\omega) = -\frac{ie^2}{\Omega} \sum_{\vec{k}\sigma\alpha} (v^{\nu}_{\vec{k}})^2 \frac{\partial\Phi^{\alpha}_{\vec{k}\sigma}}{\partial\epsilon_{\vec{k}}} \frac{1}{\omega + i\Gamma^{\alpha}_{\vec{k}\sigma}(\omega)}. \tag{34}$$

The terms $\alpha=+$ and $\alpha=-$ represent the contributions to σ from the electron transition processes in the upper and lower subband, respectively.

From (34) we obtain the dissipative part of the conductivity

$$\mathrm{Re}\,\sigma^{\nu\nu}(\omega,T) = -\frac{e^2}{\Omega} \sum_{\vec{k}\sigma\alpha} (v^{\nu}_{\vec{k}})^2 \frac{\partial\Phi^{\alpha}_{\vec{k}\sigma}(T)}{\partial\epsilon_{\vec{k}}} \frac{\Gamma^{\alpha}_{\vec{k}\sigma}(\omega,T)}{\omega^2 + \Gamma^{\alpha}_{\vec{k}\sigma}(\omega,T)^2} \tag{35}$$

and the dc conductivity

$$\sigma^{\nu\nu}(0,T) = -\frac{e^2}{\Omega} \sum_{\vec{k}\sigma\alpha} (v^{\nu}_{\vec{k}})^2 \frac{\partial\Phi^{\alpha}_{\vec{k}\sigma}(T)}{\partial\epsilon_{\vec{k}}} \tau^{\alpha}_{\vec{k}\sigma}(T), \tag{36}$$

where

$$\tau^{\alpha}_{\vec{k}\sigma} = \Gamma^{\alpha}_{\vec{k}\sigma}(0)^{-1}$$

is the transport relaxation time.

3. RESULTS AND DISCUSSION

A detailed investigation of the frequency and temperature dependence of the transport damping and the conductivity requires a numerical treatment. Here we discuss only the main qualitative features and quantitative results in different special and limiting cases. Throughout this Section we consider the paramagnetic phase $n_{\sigma} = n_{-\sigma} = n/2$ and the half-filled band case $n = 1$.

In this case we have $\mu = U/2$ (in zeroth order in $A_{\vec{q}}$) and therefore in $\frac{\partial \Phi^{\alpha}_{\vec{k}}}{\partial \epsilon_{\vec{k}}}$ the energy $\epsilon_{\vec{k}}$ can be neglected in the lowest order in t:

$$\frac{\partial \Phi^{\alpha}_{\vec{k}}}{\partial \epsilon_{\vec{k}}} = -\frac{\beta}{4}\,\frac{e^{\beta U/2}}{(1+e^{\beta U/2})^2}\,, \quad \beta = \frac{1}{k_B T}\,. \tag{37}$$

Note that this approximation is not possible for $n \neq 1$ since for $n<1$ ($n>1$) the chemical potential is of order $t(U)$ and therefore $\epsilon_{\vec{k}}$ cannot be neglected in $\frac{\partial \Phi^{-(+)}_{\vec{k}}}{\partial \epsilon_{\vec{k}}}$.

Considering a simple cubic lattice in the tight-binding approximation in which $\Sigma(v^{\nu}_{\vec{k}})^2 = 2Nt^2a^2$ (N number of sites, a lattice constant) we obtain from (36) and (37) the dc conductivity

$$\sigma^{\nu\nu}(0,T) = A\beta U\,\frac{e^{\beta U/2}}{(1+e^{\beta U/2})^2}\,\tau(T)\,, \quad \tau = \frac{1}{2}(\tau^{+}+\tau^{-})\,, \tag{38}$$

where $A = \frac{2e^2t^2a^2N}{\Omega U}$ and τ^{α} are the mean transport relaxation times

$$\tau^{\alpha} = \sum_{\vec{k}} (v^{\nu}_{\vec{k}})^2\,\tau^{\alpha}_{\vec{k}} \Big/ \sum_{\vec{k}} (v^{\nu}_{\vec{k}})^2. \tag{39}$$

3.1. Frequency Dependence

From (34), (35) we see that the conductivity shows a Drude-Lorentz type behaviour and accordingly $\mathrm{Re}\,\sigma^{\nu\nu}(\omega)$ decreases with increasing ω.

Taking the limit $\Gamma^{\alpha}_{\vec{k}} \to 0$ in (35) we obtain

$$\mathrm{Re}\,\sigma^{\nu\nu}(\omega, T) = A\beta U\,\frac{e^{\beta U/2}}{(1+e^{\beta U/2})^2}\,\pi\delta(\omega). \tag{40}$$

This result agrees with that calculated exactly in the limit $\lim_{t\to 0} \frac{\sigma}{t^2}$ in the pure Hubbard model [14,20]. The comparison of (38) and (40) shows that the singularity $\pi\delta(\omega)$ in the dc conductivity of the pure Hubbard model obtained for a half-filled band in the approximation $\lim_{t\to 0}\frac{\sigma}{t^2}$ becomes replaced by the transport relaxation time τ if both the band term and the dissipation mechanism due to electron-phonon scattering are taken into account in appropriate approximations. The results (38) and (40) give a justification of the approximation $\lim_{t\to 0}\frac{\sigma}{t^2}$ and of the assumptions concerning the δ-function peak for the half-filled band case.

On the basis of those results we guess that for another scattering mechanism we would obtain (38) with another relaxation time so that the statements concerning the δ-function peak remain valid.

As to the models including electron-phonon coupling considered in [21,22], the dc conductivity should become finite in an improved approximation just due to this coupling and not necessarily due to the imputiry scattering.

3.2. Temperature Dependence of the dc Conductivity

First consider the low-temperature region $T \ll T_D$ (T_D Debye temperature) in which $\nu_{\vec{q}} \ll 1$ and therefore can be neglected in (26), (32), (33). Accordingly, the damping

$\Gamma^{\alpha}_{0\vec{k}}(0,T)$ and the transport relaxation time $\tau(T)$ are approximated by their nonvanishing zero-temperature ($\nu_{\vec{q}}=0$) values describing the indirect electron-electron scattering. As follows from (38) the dc conductivity vanishes at $T=0$ and has a low-temperature activation energy of $\frac{U}{2}$.

Now consider the high-temperature region $T \gg T_D$. Because of $\frac{k_B T_D}{U} \simeq 10^{-2}$ (e.g. for NMP-TCNQ we have $\frac{k_B T_D}{U} \simeq \frac{1}{24}$) we also consider low temperatures with respect to the electrons ($k_B T_D \ll k_B T \ll U$).

Since $\nu_{\vec{q}} \simeq \frac{k_B T}{\omega_{\vec{q}}} \gg 1$ the terms $1+\delta_{\alpha+}-n$ and $n-\delta_{\alpha+}$ in (26), (32), (33) can be neglected. Thus we have $w^{\alpha}_{\vec{k},\vec{k}+\vec{q}} = w^{\alpha}_{\vec{k}+\vec{q},\vec{k}}$, $\Gamma^{+}_{\vec{k}} = \Gamma^{-}_{\vec{k}} = \Gamma_{\vec{k}}(0,T)$, $\tau^{+} = \tau^{-} = \tau$, and according to (33)

$$\Gamma_{\vec{k}}(0,T) = \frac{1}{\beta U}\Gamma_{o\vec{k}}. \tag{41}$$

$\Gamma_{o\vec{k}}$ does not depend on T and is given by

$$\Gamma_{o\vec{k}} = \Gamma^{(0)}_{o\vec{k}} + \sum_{\vec{q}} \frac{v^{\nu}_{\vec{k}+\vec{q}}}{v^{\nu}_{\vec{k}}} \operatorname{Im} w_{o\vec{k}+\vec{q},\vec{k}}(i\epsilon) \frac{\Gamma^{(0)}_{o\vec{k}}}{\Gamma^{(0)}_{o\vec{k}+\vec{q}}}, \tag{42}$$

where

$$\Gamma^{(0)}_{o\vec{k}} = -\operatorname{Im} \sum_{\vec{q}} w_{o\vec{k}+\vec{q},\vec{k}}(i\epsilon)$$

and

$$\operatorname{Im} w_{o\vec{k}+\vec{q},\vec{k}}(i\epsilon) = -2\pi U \frac{|A_{\vec{q}}|^2}{\omega_{\vec{q}}}\left(\delta(E^{\alpha}_{\vec{k}} - E^{\alpha}_{\vec{k}+\vec{q}} - \omega_{\vec{q}}) + \right.$$

$$\left. + \delta(E^{\alpha}_{\vec{k}} - E^{\alpha}_{\vec{k}+\vec{q}} + \omega_{\vec{q}})\right).$$

In accordance with (41) we write

$$\tau = \beta U \tau_0 \quad \text{where} \quad \tau_0 = \sum_{\vec{k}} (v^{\nu}_{\vec{k}})^2 \Gamma^{-1}_{o\vec{k}} / \sum_{\vec{k}} (v^{\nu}_{\vec{k}})^2. \tag{43}$$

Inserting (43) into (38) we get

$$\sigma^{\nu\nu}(0,T) = A(\beta U)^2 \frac{e^{\beta U/2}}{(1+e^{\beta U/2})^2}\tau_0. \tag{44}$$

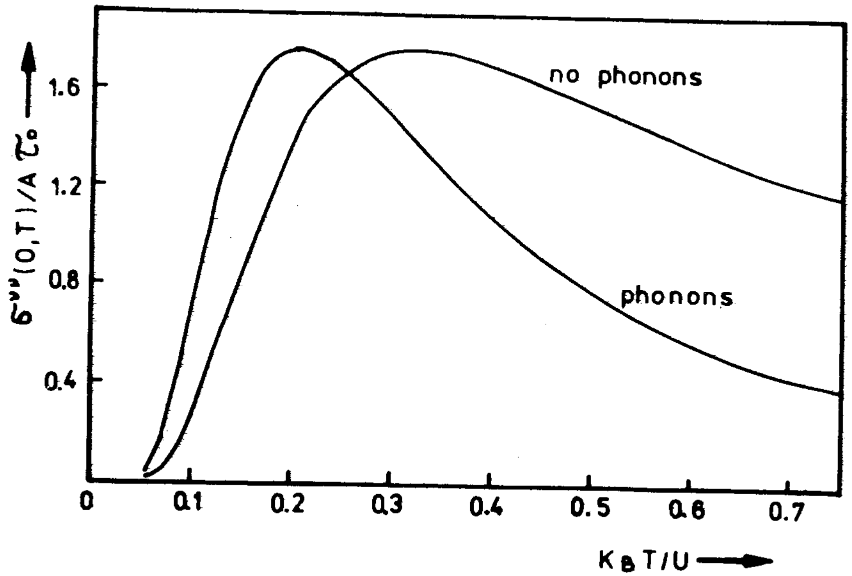
In order to see the effects of phonons on the conductivity (44) we compare it with the conductivity in the phononless Hubbard model including some temperature-independent scattering mechanism. Reasoning as in Section 3.1 we obtain the conductivity in this case by replacing $\pi\delta(\omega)$ in (40) by some temperature-independent relaxation time τ_1:

$$\sigma^{\nu\nu}(0,T) = A\beta U \frac{e^{\beta U/2}}{(1+e^{\beta U/2})^2}\tau_1. \tag{45}$$

Comparing the temperature dependence of (44) and (45) we see that, due to the additional factor βU in (44), the effects of phonons consist in a shift of the conductivity maximum temperature to a lower value, in the sharpening of the maximum, and in the decrease of $\sigma^{\nu\nu}(0,T)$ for high T according to T^{-2}. The conductivities (44) and (45) are plotted in *Fig. 1* where for convenience we have put $\tau_1 = 3.92\,\tau_0$ (yielding equal maximum values). The maximum temperatures of (44) and (45) are given by $k_B T_m = 0.21U$ and $0.33U$, respectively.

Because the Hubbard model is analogous to the Cullen-Callen model (CC model) of Fe_3O_4 /4/, an analogous conductivity calculation could be performed for this model including electron-phonon interaction. Lorentz and the present author [6] have calculated the conductivity in the phononless CC model in the strong coupling region above and below the Verwey transition temperature $T_v = 120K$ in the approximation $\lim_{t\to 0} \frac{\sigma}{t^2}$ in which the occuring δ -

function peak was replaced by a temperature-independent quantity as in (45). As to the dc conductivity above T_v the calculated and measured temperature dependences (*fig. 2* in [6]) resemble qualitatively the curves shown in *Fig. 1*. Especially the conductivity maximum observed experimentally at 305K is calculated to be a smooth maximum at 380K. From the results of this paper and the analogy of the two models under consideration we guess that the difference between the theoretical and measured temperature dependences of $\sigma''(0,T)$ in Fe_3O_4 reflects the effects of phonons and is reduced by their inclusion into the CC model.



Temperature dependence of the dc conductivity in the Hubbard model including electron-phonon interaction and in the phononless Hubbard model.

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