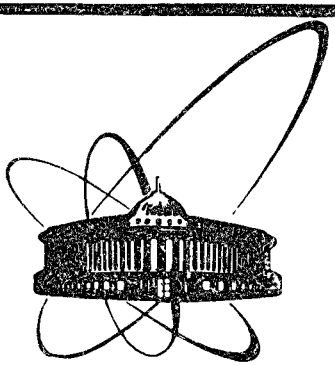

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ELECTRON-ELECTRON SCATTERING CONTRIBUTION TO THE ELECTRICAL RESISTIVITY OF A NARROW BAND

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In substances with narrow energy bands, as, e.g., transition metals, their oxides, quasi-one-dimensional charge transfer salts and mixed-valent rare-earth compounds, the electron-electron interaction substantially influences the electrical resistivity. In the calculations of the transport properties of these compounds the correlations of the conduction electrons should be included, thus invalidating the one-electron approximation of conventional band theory and requiring sophisticated many-body techniques. In spite of considerable progress in explaining the one-particle properties of the narrow band materials no explicit expression has been derived for the electron relaxation time due to electron-electron scattering processes [1]. Finite relaxation times have been obtained only by introducing an effective disorder in an alloy approximation [2-4] or by taking into account other scattering mechanisms (electron-phonon, impurity scattering [5,6]). However, the alloy approximation fails at least at low temperatures, where the electron-electron scattering processes cannot be described by a static disorder.

In the present letter the conductivity is calculated in the strong correlation limit starting from the well-known one-band Hubbard Hamiltonian

$$H = H_t + H_U = \sum_{ij\sigma} t_{ij} c^+_{i\sigma} c_{j\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} ,$$
$$t_{ij} = N^{-1} \sum_{\vec{k}} \epsilon_{\vec{k}} \exp[i\vec{k}(\vec{R}_i - \vec{R}_j)] , \qquad t_{ii} = 0, \tag{1}$$

where all symbols have their usual meaning. The calculation is carried out straightforwardly neglecting only higher-order terms in $|t|/U$. We calculate the d.c. electrical conductivity starting from the Kubo formula

$$\sigma = \frac{e^2}{3m^2\Omega} <\vec{P};\vec{P}>_{i\eta} = \frac{e^2}{3m^2\Omega} \sum_{\vec{k}\sigma} \sum_{\vec{k}'\sigma'} \frac{\partial\epsilon}{\partial\vec{k}} \frac{\partial\epsilon}{\partial\vec{k}'} <n_{\vec{k}\sigma} ; n_{\vec{k}'\sigma'}>_{i\eta} \tag{2}$$

with the correlation functions

$$<A; B>_{i\eta} = \int_0^\infty dt \exp(-\eta t) (A(t)|B) \tag{3}$$

and the scalar products

$$(A(t)|B) = \int_0^\beta d\lambda \, \mathrm{Tr}\{\rho A(t - i\lambda) B^+\}; \qquad \rho = z^{-1} \exp(-\beta H) . \tag{4}$$

For strongly correlated electrons the band splits and the occupation numbers $n_{\vec{k}\sigma} = c^+_{\vec{k}\sigma} c_{\vec{k}\sigma} = N^{-1} \sum_{ij} \exp[i\vec{k}(\vec{R}_i - \vec{R}_j)] c^+_{i\sigma} c_{j\sigma}$ should be projected onto the split bands (cf. [2]). This can be done by introducing the projection operators

$$n^\alpha_{i-\sigma} = \begin{cases} n_{i-\sigma} \\ 1 - n_{i-\sigma} \end{cases} \quad \text{for} \quad \alpha = \pm , \tag{5}$$

$$n_{\vec{k}\sigma} = \sum_{\alpha\beta} n^{\alpha\beta}_{\vec{k}\sigma} = N^{-1} \sum_{\alpha\beta} \sum_{ij} \exp[i\vec{k}(\vec{R}_i - \vec{R}_j)] c^+_{i\sigma} c_{j\sigma} \, n^\alpha_{i-\sigma} n^\beta_{j-\sigma} \tag{6}$$

and the conductivity becomes

$$\sigma = \frac{e^2}{3m^2\Omega} \sum_{ij} \sum_{mn} \sum_{\alpha\beta} \sum_{\gamma\delta} \sum_{\sigma\sigma'} <A^{\alpha\beta}_{ij\sigma} ; A^{\gamma\delta}_{mn\sigma'}>, \tag{7}$$

where

$$A^{\alpha\beta}_{ij\sigma} = N^{-1} \sum_{\vec{k}} \frac{\partial\epsilon}{\partial\vec{k}} \exp[i\vec{k}(\vec{R}_i - \vec{R}_j)] c^+_{i\sigma} \, n^\alpha_{i-\sigma} c_{j\sigma} n^\beta_{j-\sigma} . \tag{8}$$

Taking into account $\epsilon_{\vec{k}} = \epsilon_{-\vec{k}}$ we find $A^{\alpha\beta}_{ii\sigma} = 0$. Transforming the correlation functions in (7) into Green functions and considering their equations of motion it easily can be shown that the terms $\alpha \neq \beta$ and $\gamma \neq \delta$, respectively, do not contribute to the d.c. conductivity. These terms describe interband processes between the split bands for which the energy conservation law cannot be fulfilled at $|t|/U \ll 1$.

The correlation functions in (5) can be calculated by means of the Mori projection operator technique [7]. Considering in the framework of this method a set of observables C_i, the corresponding correlation functions $<C_i ; C_j>_z$ can be calculated by the set of equations

$$\sum_k [z\delta_{ik} - \sum_\ell \omega_{i\ell} (\chi^{-1})_{\ell k} + i \sum_\ell \pi_{i\ell}(z) (\chi^{-1})_{\ell k}] <C_k ; C_j>_z = i\chi_{ij} , \tag{9}$$

where

$$\chi_{ij} = (C_i | C_j) , \qquad \sum_k \chi_{ik} (\chi^{-1})_{kj} = \delta_{ij} , \tag{10}$$

$$\omega_{ij} = i(\dot{C}_i | C_j) , \qquad \dot{C}_i = i[H, C_i] , \tag{11}$$

and

$$\pi_{ij}(z) = <\dot{C}_i Q | Q \dot{C}_j>^Q_z . \tag{12}$$

The operator $Q = 1 - P$ is a projection operator with $P = \sum_{ij} |C_i)(\chi^{-1})_{ij}(C_j|$ and $<\ldots>^Q$ denotes that in the time

evolution of the correlation function $L = i[H,...]$ is to be replaced by QLQ. For the problem considered the relevant observables are given by (8) and the system of equations (9) comprises $2N^2$ coupled equations where N is the number of lattice sites. This system of equations considerably simplifies in the limit $|t|/U \ll 1$, where the matrix of the scalar products (10) of the observables (8) reduces to

$$(A^{\alpha\alpha}_{ij\sigma} | A^{\gamma\gamma}_{mn\sigma'}) = (A^{\alpha\alpha}_{ij\sigma} | A^{\alpha\alpha}_{ij\sigma}) \delta_{\gamma\alpha} \delta_{mi} \delta_{nj} \delta_{\sigma\sigma'} =$$
$$= \tilde{\beta} N^{-2} \sum_{\vec{k}\vec{k}'} \frac{\partial\epsilon}{\partial\vec{k}} \frac{\partial\epsilon}{\partial\vec{k}'} \exp[i(\vec{k}-\vec{k}')(\vec{R}_i - \vec{R}_j)] < n_\sigma n^\alpha_{-\sigma} > < n^-_\sigma n^\alpha_{-\sigma} > \delta_{\gamma\alpha} \delta_{mi} \delta_{nj} \delta_{\sigma\sigma'} \quad (13)$$

for $i \neq j$. Using the Kubo identity we find $(\dot{A}_{ij\sigma} | A_{ij\sigma}) = 0$ and (9) becomes with $z = -i\eta \to 0$

$$< A^{\alpha\alpha}_{ij\sigma} ; A^{\alpha\alpha}_{ij\sigma} >_{i\eta} = \frac{(A^{\alpha\alpha}_{ij\sigma} | A^{\alpha\alpha}_{ij\sigma})}{(\dot{A}^{\alpha\alpha}_{ij\sigma} Q ; Q \dot{A}^{\alpha\alpha}_{ij\sigma} >^{Q}_{i\eta}} . \quad (14)$$

For the generalized forces we find

$$\dot{A}^{\alpha\alpha}_{ij\sigma} = i[H, A^{\alpha\alpha}_{ij\sigma}] = iN^{-1} \sum_{\vec{k}} \frac{\partial\epsilon}{\partial\vec{k}} \exp[i\vec{k}(\vec{R}_i - \vec{R}_j)] \times \quad (15)$$
$$\times \sum_{\ell} (t_{\ell i} c^+_{\ell\sigma} n^\alpha_{i-\sigma} c_{j\sigma} n^\alpha_{j-\sigma} - t_{\ell j} c^+_{i\sigma} n^\alpha_{i-\sigma} c_{\ell\sigma} n^\alpha_{j-\sigma} + \text{terms with 4 c-operators}),$$

where the last terms do not contribute in the approximation considered below. With $P\dot{A}^{\alpha\alpha}_{ij\sigma} \sim (A^{\alpha\alpha}_{ij\sigma} | \dot{A}^{\alpha\alpha}_{ij\sigma}) = 0$ the force correlation function in (13) is given by

$$< \dot{A}^{\alpha\alpha}_{ij\sigma} ; \dot{A}^{\alpha\alpha}_{ij\sigma} >_{i\eta} = N^{-2} \sum_{\ell m} \sum_{\vec{k}\vec{k}'} \sum_{\sigma\sigma'} \frac{\partial\epsilon}{\partial\vec{k}} \frac{\partial\epsilon}{\partial\vec{k}'} \exp[i(\vec{k}-\vec{k}')(\vec{R}_i - \vec{R}_j)] \times$$
$$\times < (t_{\ell i} c^+_{\ell\sigma} n^\alpha_{i-\sigma} c_{j\sigma} n^\alpha_{j-\sigma} - t_{\ell j} c^+_{i\sigma} n^\alpha_{i-\sigma} c_{\ell\sigma} n^\alpha_{j-\sigma}) ; \quad (16)$$
$$(t_{mi} c^+_{m\sigma} n^\alpha_{i-\sigma} c_{j\sigma} n^\alpha_{j-\sigma} - t_{mj} c^+_{i\sigma} n^\alpha_{i-\sigma} c_{m\sigma} n^\alpha_{j-\sigma}) >_{i\eta} .$$

For $|t|/U \ll 1$ the correlation functions can be decoupled and (15) becomes

$$< \dot{A}^{\alpha\alpha}_{ij\sigma} ; \dot{A}^{\alpha\alpha}_{ij\sigma} >_{i\eta} = n^\alpha_{-\sigma} N^{-2} \sum_{\ell} \sum_{\beta\sigma} \sum_{\vec{k}\vec{k}'} \frac{\partial\epsilon}{\partial\vec{k}} \frac{\partial\epsilon}{\partial\vec{k}'} \exp[i(\vec{k}-\vec{k}')(\vec{R}_i - \vec{R}_j)] \times$$
$$\times (|t_{\ell i}|^2 < c^+_{\ell\sigma} n^\beta_{\ell-\sigma} c_{j\sigma} n^\alpha_{j-\sigma} ; c^+_{\ell\sigma} n^\beta_{\ell-\sigma} c_{j\sigma} n^\alpha_{j-\sigma} > +$$
$$+ |t_{\ell i}|^2 < c^+_{i\sigma} n^\alpha_{i-\sigma} c_{\ell\sigma} n^\beta_{\ell-\sigma} ; c^+_{i\sigma} n^\alpha_{i-\sigma} c_{\ell\sigma} n^\beta_{\ell-\sigma} >_{i\eta}) , \quad (17)$$

where for paramagnetic systems $n^\alpha_{-\sigma} = n^\alpha_\sigma = \begin{cases} n/2 \\ 1-n/2 \end{cases}$ for $\alpha = \pm$ with n being the electron number per lattice site. As was discussed above the terms $\alpha \neq \beta$ in (17) can be neglected. Taking into account only the nearest neighbour hopping, (14) becomes

$$< A^{\alpha\alpha}_{ij\sigma} ; A^{\alpha\alpha}_{ij\sigma} >_{i\eta} = (A^{\alpha\alpha}_{ij\sigma} | A^{\alpha\alpha}_{ij\sigma}) \; [n^\alpha_\sigma t^2 N^{-2} \sum_{\vec{k}\vec{k}'} \frac{\partial\epsilon}{\partial\vec{k}} \frac{\partial\epsilon}{\partial\vec{k}'} \exp[i(\vec{k}-\vec{k}')(\vec{R} - \vec{R})] \times$$
$$\times (\sum'_{\ell \neq i} < c^+_{\ell\sigma} n^\alpha_{\ell-\sigma} c_{j\sigma} n^\alpha_{j-\sigma} ; c^+_{\ell\sigma} n^\alpha_{\ell-\sigma} c_{j\sigma} n^\alpha_{j-\sigma} > + \quad (18)$$
$$+ \sum'_{\ell \neq j} < c^+_{i\sigma} n^\alpha_{i-\sigma} c_{\ell-\sigma} n^\alpha_{\ell-\sigma} ; c^+_{i\sigma} n^\alpha_{i-\sigma} c_{\ell\sigma} n^\alpha_{\ell-\sigma} >_{i\eta})]^{-1} ,$$

where t is the nearest neighbour hopping element and $\sum'_{\ell \neq i}$ denotes a summation over the z nearest neighbour. The system of equations can be solved by the simple expressions for the correlation functions

$$< A^{\alpha\alpha}_{ij\sigma} ; A^{\alpha\alpha}_{ij\sigma} >_{i\eta} = (\sqrt{2 n^\alpha_\sigma z} \, |t|)^{-1} \; (A^{\alpha\alpha}_{ij\sigma} | A^{\alpha\alpha}_{ij\sigma}) \quad (19)$$

and the conductivity reads

$$\sigma = \frac{e^2 \tilde{\beta}}{3m^2 \Omega} \frac{1}{\sqrt{2z}} \frac{1}{|t|} \sum_{\vec{k}} (\frac{\partial\epsilon}{\partial\vec{k}})^2 \sum_{\alpha} (n^\alpha_\sigma)^{-1/2} < n^\alpha_\sigma n^\alpha_{-\sigma} > (n^\alpha_\sigma - < n^\alpha_\sigma n^\alpha_{-\sigma} >) =$$
$$= AT^{-1} \sum_{\alpha} (n^\alpha_\sigma)^{-1/2} < n^\alpha_\sigma n^\alpha_{-\sigma} > (n^\alpha_\sigma - < n^\alpha_\sigma n^\alpha_{-\sigma} >) . \quad (20)$$

With $< n_\sigma n_{-\sigma} > = \frac{1}{2} n f(U) = \frac{1}{2} n (1 + \exp \tilde{\beta}(U - \phi))^{-1}$ and $\tilde{\beta}U \gg 1$ we find the conductivity in dependence on the electron number

$0 \leq n < 1$	$\tilde{\beta}\phi = \ln \frac{n/2}{1-n}$	$\sigma = AT^{-1} \frac{1}{2} \frac{n(1-n)}{\sqrt{1-n/2}}$
$n = 1$	$\phi = \frac{U}{2}$	$\sigma = \frac{A}{\sqrt{2}} T^{-1} \exp(-\frac{\tilde{\beta}U}{2})$
$2 \geq n > 1$	$\tilde{\beta}\phi = \tilde{\beta}U + \ln \frac{n-1}{1-n/2}$	$\sigma = AT^{-1} \sqrt{2} \frac{(1-n/2)(n-1)}{\sqrt{n}}$.

We see that for $n \neq 1$ the system is a metal with vanishing resistivity at $T=0$, where for $n=1$ it behaves like an intrinsic semiconductor. However, this can be understood already by the difference in the effective electron numbers being available for the electronic transport process (cf. [1,2,5]). It would be desirable to generalize (20) to any bandwidths in order to compare the expression for σ with that obtained in the Born approximation for a weak electron-electron interaction. For this the Hubbard I approximation fails because it breaks the translational symmetry of the problem and yields unphysical results.

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Влияние электрон-электронного столкновения на электросопротивление веществ с узкими зонами

С помощью формализма Мори вычисляется электросопротивление в рамках модели Хаббарда вблизи атомного предела. Показано, что сопротивление ρ пропорционально T при $n \neq 1$ /число электронов на узел/. Для $n = 1$ имеется экспоненциальная зависимость как в случае собственных полупроводников.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Christoph V.
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Electron-Electron Scattering Contribution to the Electrical Resistivity of a Narrow Band

The d.c. electrical conductivity of the Hubbard model is calculated near the atomic limit using the Mori projection operator technique.

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

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