Electrical Conduction in Narrow Energy Bands

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The electrical conductivity of the single-band Hubbard Hamiltonian is calculated by use of the Boltzmann-Transport-Equation. We lean on the antiferromagnetic approach to this Hamiltonian. We obtain a semiconductor with an energy gap due to the electronic correlations and a semiconductor to metal transition at the Néel temperature T_N.

1. Introduction

In the following paper we give a calculation of the electrical conductivity of the neutral Hubbard model for A-B-lattices based on the approximation given by Dichtel, Jelitto and Koppe [1,2] (DJK). As shown in a forthcoming paper by Grensing and Koppe [3], this approximation is only reasonable for sufficiently small V_0/J. The limiting value depends on the type of the lattice and is about $V_0/J < 8$. The subsequent calculations are only valid in this region.

We want to calculate the conductivity with the help of the Boltzmann-transport-equation in a constant electric field. To describe impurity-scattering we use the relaxation time-approximation. In analogy to the theory of metallic conductivity of free electrons we consider the system of free "quasiparticles", which are the elementary excitations of the narrow band system. We derive an expression for the relaxation time and obtain a semiconductor below and a temperature induced semiconductor to metal transition at the Néel temperature [4].

2. Hubbard-Hamiltonian

We start with the Hubbard-Hamiltonian:

$$\mathcal{H} = -J \sum_{nj} (u_{n+j}^{+}\, u_n + v_{n+j}^{+}\, v_n) + V_0 \sum_n u_n^{+}\, u_n\, v_n^{+}\, v_n \,. \tag{1}$$

To approximate the Coulomb-interaction by a one particle term one can introduce magnetic fields fixed at each lattice site $\boldsymbol{R}_n$. The most general form for such an operator is

$$\mathcal{H}_{\text{field}} = \sum_n \tilde{u}_n^{+} (\boldsymbol{H}_n \cdot \boldsymbol{\sigma})\, \tilde{u}_n \tag{2}$$

where $\boldsymbol{\sigma}$ means the vector build up of the Pauli-spin-matrices and $\tilde{u}_n$ the column vector (u_n, v_n).

Calculating the free energy of the Hubbard-model with the Bogoljubov inequality using the test operator

$$\mathcal{H}_{\text{test}} = -J \sum_{nj} (u_{n+j}^{+}\, u_n + v_{n+j}^{+}\, v_n) - \sum_n \tilde{u}_n^{+} (\boldsymbol{H}_n \cdot \boldsymbol{\sigma})\, \tilde{u}_n \tag{3}$$

the $\boldsymbol{H}_n$ should be variational parameters to minimize the free energy functional. But this program is too difficult to perform and therefore DJK choose

$$\mathcal{H}_{\text{field}} = \sum_n \tilde{u}_n^{+} \begin{pmatrix} \zeta & \Delta \exp\{-i\boldsymbol{Q}\cdot\boldsymbol{R}_n\} \\ \Delta \exp\{+i\boldsymbol{Q}\cdot\boldsymbol{R}_n\} & -\zeta \end{pmatrix} \tilde{u}_n \,. \tag{4}$$

After Fourier-transformation one obtains the grand canonical test Hamiltonian:

$$\mathcal{H}_{\text{test}} = \sum_k (u_k^{+}\; v_{k+Q}^{+}) \begin{pmatrix} -\mu - \zeta + \varepsilon(k) & -\Delta \\ -\Delta & -\mu + \zeta + \varepsilon(k+Q) \end{pmatrix} \begin{pmatrix} u_k \\ v_{k+Q} \end{pmatrix}. \tag{5}$$

$\boldsymbol{Q}$, μ, ζ and Δ are real variational parameters. A k-dependent rotation in spin space makes $\mathcal{H}_{\text{test}}$ diagonal:

$$\begin{pmatrix} \bar{u}_k \\ \bar{v}_k \end{pmatrix} = \begin{pmatrix} \cos(\alpha_k/2) & -\sin(\alpha_k/2) \\ \sin(\alpha_k/2) & \cos(\alpha_k/2) \end{pmatrix} \begin{pmatrix} u_k \\ v_{k+Q} \end{pmatrix} \tag{6}$$

with

$$\begin{matrix} \cos^2(\alpha_k/2) \\ \sin^2(\alpha_k/2) \end{matrix} = \frac{1}{2} \left\{ 1 \pm \frac{\varepsilon^{-}(k) - \zeta}{\sqrt{[\varepsilon^{-}(k) - \zeta]^2 + \Delta^2}} \right\} \tag{7}$$

and $\varepsilon^{\pm}(k) = \frac{1}{2}[\varepsilon(k) \pm \varepsilon(k+Q)]$. Then we find:

$$\overline{\mathcal{H}}_{\text{test}} = \sum_k [E_1(k)\, \bar{u}_k^{+}\, \bar{u}_k \;+ E_2(k)\, \bar{v}_k^{+}\, \bar{v}_k] \,. \tag{8}$$

The energy spectrum is:

$$E_{1,2}(k) = -\mu + \varepsilon^{+}(k) \pm \sqrt{[\varepsilon^{-}(k) - \zeta]^2 + \Delta^2} \,. \tag{9}$$

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It can be shown that $Q=1/a(\pi,\pi,\pi)$, going from a minimum to the maximum value of $\varepsilon(k)$, for the s. c. lattice leads to a relative minimum of the free energy. DJK showed furthermore, that the antiferromagnetic ordering always has a lower free energy than the ferromagnetic ($\Delta=0$) one in their approach. The chemical potential and magnetic field are connected with μ and ζ through the equations:

$$\begin{aligned}\zeta &= H+V_0\, s_z \\ \mu &= \mu_{\text{CHEM.}}-\tfrac{1}{2}V_0\, n\end{aligned} \qquad \text{with} \quad \begin{aligned} n &= N_e/N \\ s_z &= S_z/N\end{aligned}. \tag{10}$$

In the neutral case $n=1$, which we are interested in, the effective chemical potential μ is identically zero and without a magnetic field we obtain the energies:

$$E_{1,2}=\pm\sqrt{\varepsilon^2(k)+\Delta^2}\,. \tag{11}$$

In the following we have then:

$$\begin{matrix}\cos^2(a_k/2)\\ \sin^2(a_k/2)\end{matrix}=\frac{1}{2}\left\{1\pm\frac{\varepsilon(k)}{\sqrt{\varepsilon^2(k)+\Delta^2}}\right\}. \tag{12}$$

3. Conductivity of the Neutral Hubbard-model

Now we will calculate the electrical conductivity. Electronic motion obeys the laws:

$$\boldsymbol{v}(k)=\frac{1}{\hbar}\nabla_k\varepsilon(k)\,,\quad \frac{\partial(\hbar\boldsymbol{k})}{\partial t}=e\boldsymbol{E}\,. \tag{13), (14}$$

In cubic lattices the conductivity tensor $\sigma_{\alpha\beta}$ reduces to a scalar and with some simplifications because of symmetry we obtain from the Boltzmann equation the well-known result in relaxation time approximation:

$$\sigma=\frac{e^2}{3(2\pi)^3}\sum_{\lambda}\int_{1.\,\text{B.-Z.}}\mathrm{d}^3k\,\tau_\lambda(k)\left(-\frac{\partial f_{k\lambda}{}^0}{\partial E_\lambda(k)}\right)|\boldsymbol{v}_\lambda(k)|^2\,. \tag{15}$$

Here the index λ numerates spin states or non-degenerate bands. $f_{k\lambda}{}^0$ means the equilibrium distribution function in the absence of the electrical field. Our problem is now to calculate the relaxation time for the quasiparticles. For this purpose we add to the Hamiltonian one impurity level of energy E_J measured from the center of the band $[1/N\sum_k\varepsilon(k)=0]$ for example at the origin of the lattice:

$$\mathcal{H}_{\text{impurity}}=E_J(u_0{}^+u_0+v_0{}^+v_0)\,. \tag{16}$$

Transforming this into k-space and writing in quasiparticle operators we have

$$\begin{aligned}\overline{\mathcal{H}}_{\text{impurity}}=&\frac{E_J}{N}\sum_{kk'}\left(\cos\frac{a_k}{2}\cos\frac{a_{k'}}{2}+\sin\frac{a_k}{2}\sin\frac{a_{k'}}{2}\right)(\bar u_k{}^+\bar u_{k'}+\bar v_k{}^+\bar v_{k'})\\ &+\frac{E_J}{N}\sum_{kk'}\left(\cos\frac{a_k}{2}\sin\frac{a_{k'}}{2}-\sin\frac{a_k}{2}\cos\frac{a_{k'}}{2}\right)(\bar u_k{}^+\bar v_{k'}-\bar v_k{}^+\bar u_{k'})\,.\end{aligned} \tag{17}$$

Our approximative Hamiltonian was

$$\overline{\mathcal{H}}_{\text{test}}=\sum_k\left[E_1(k)\bar u_k{}^+\bar u_k+E_2(k)\bar v_k{}^+\bar v_k\right]. \tag{18}$$

Under the influence of the impurity the system of quasiparticles as a whole can make transitions from an energy level $E_n\to E_m$ with the probability (first order perturbation theory):

$$W(n\to m)=(2\pi/\hbar)\,|\langle n|\overline{\mathcal{H}}_{\text{impurity}}|m\rangle|^2\,\delta(E_n-E_m)\,. \tag{19}$$

The state-function ψ_n has the form

$$\psi_n=\prod_{k\in A_n}\bar u_k{}^+\prod_{k\in B_n}\bar v_k{}^+|0\rangle \quad \text{with} \quad A_n,B_n\subseteq 1.\,\text{B.-Z.}$$

"$|0\rangle$" is the quasiparticle vacuum.

But only those matrix elements of $\mathcal{H}_{\text{impurity}}$ where ψ_n and ψ_m differ in one k-vector are non-zero; therefore Fermi's "Golden-rule" holds for the individual scattering process of one quasiparticle and we obtain

$$\begin{aligned}W(k,k')=&(2\pi/\hbar)\,|\langle\varphi_{k'}|\overline{\mathcal{H}}_{\text{impurity}}|\varphi_k\rangle|^2\\ &\cdot\delta[E_{\lambda'}(k')-E_\lambda(k)]\,.\end{aligned} \tag{20}$$

The first term of $\overline{\mathcal{H}}_{\text{impurity}}$ describes intra-band scattering, the second inter-band-scattering; only terms of the first kind contribute because the energy gap of 2Δ makes $E_1(k')=E_2(k)$ impossible. So we get for both bands:

$$W(k,k')=\frac{2\pi}{\hbar}\left(\frac{E_J}{N}\right)^2\left(\cos\frac{a_k}{2}\cos\frac{a_{k'}}{2}+\sin\frac{a_k}{2}\sin\frac{a_{k'}}{2}\right)^2\delta[E(k')-E(k)] \tag{21}$$

where

$$E(k)=+\sqrt{\varepsilon^2(k)+\Delta^2}\,.$$

Using the relation

$$\delta[E(k')-E(k)]=\left|\frac{E(k)}{\varepsilon(k)}\right|\{\delta[\varepsilon(k')-\varepsilon(k)]+\delta[\varepsilon(k')+\varepsilon(k)]\} \tag{22}$$

and assuming N_J impurity sites, we obtain finally for the transition probability per unit time (E_J now means the mean value of all impurity energy levels):

$$W(k,k')=\frac{2\pi}{\hbar}\frac{N_J}{N^2}E_J^2\left|\frac{E(k)}{\varepsilon(k)}\right|\left\{\delta[\varepsilon(k')-\varepsilon(k)]+\left(\frac{\Delta}{E(k)}\right)^2\delta[\varepsilon(k')+\varepsilon(k)]\right\}. \tag{23}$$

$W(k,k')$ has the properties [because $\varepsilon(k)=\varepsilon(-k)$]: $W(k,k')=W(-k,k')=W(k,-k')$ and is symmetric $W(k,k')=W(k',k)$; therefore it is possible to introduce a time of relaxation, which is well-known to be:

$$\tau(k)=\tau(-k)=1/\sum_{k'}W(k,k')\,. \tag{24}$$

We calculate $\tau(k)$ (V_c = Volume of the elementary cell of the lattice)

$$\frac{1}{\tau(k)}=\frac{2\pi}{\hbar}\frac{N_J}{N}E_J^2\frac{V_c}{(2\pi)^3}\int_{1.\,B.-Z.}\mathrm{d}^3k'\left|\frac{E(k')}{\varepsilon(k')}\right|\left\{\delta[\varepsilon(k')-\varepsilon(k)]+\left(\frac{\Delta}{E(k')}\right)^2\delta[\varepsilon(k')+\varepsilon(k)]\right\}. \tag{25}$$

With the density of states [5]

$$g(\varepsilon)=\frac{V_c}{(2\pi)^3}\int_{1.\,B.-Z.}\mathrm{d}^3k\,\delta[\varepsilon-\varepsilon(k)] \tag{26}$$

one has:

$$\frac{1}{\tau(\varepsilon)}=\frac{2\pi}{\hbar}\left(\frac{N_J}{N}\right)E_J^2\left|\frac{\sqrt{\varepsilon^2+\Delta^2}}{\varepsilon}\right|g(\varepsilon)\left(1+\frac{\Delta^2}{\varepsilon^2+\Delta^2}\right). \tag{27}$$

It should be mentioned, that the relaxation time approximation doesn't contradict to particle conservation in first order of the perturbation; we used the Ansatz:

$$f_{k\lambda}=f_{k\lambda}^0-\tau_\lambda(k)\boldsymbol{v}_\lambda(k)\cdot e\boldsymbol{E}\frac{\partial f_{k\lambda}^0}{\partial E_\lambda(k)}\,.$$

Summing over the whole Brillouin-zone one gets:

$$n=\frac{1}{N}\sum_{k\lambda}f_{k\lambda}=\frac{1}{N}\sum_{k\lambda}f_{k\lambda}^0=n^0 \tag{28}$$

because it is

$$e\boldsymbol{E}\cdot\frac{1}{N}\sum_{k\lambda}\tau_\lambda(k)\boldsymbol{v}_\lambda(k)\frac{\partial f_{k\lambda}^0}{\partial E_\lambda(k)}=0\,.$$

The equilibrium distribution functions are given by:

$$f_{k1,2}^0=1/[\exp\{\pm\sqrt{\varepsilon^2(k)+\Delta^2}\}+1]\,. \tag{29}$$

The velocities are:

$$|\boldsymbol{v}(k)|=\frac{|\varepsilon(k)|}{\sqrt{\varepsilon^2(k)+\Delta^2}}\frac{1}{\hbar}|\nabla_k\varepsilon(k)| \tag{30}$$

for both bands; therefore we have total hole-particle symmetry and the conductivities for both bands are equal.

At this point we are able to calculate the conductivity:

$$\sigma=\frac{e^2N\beta}{(2\pi)^4N_JE_J^2\,2\hbar}\int_{1.\,B.-Z.}\mathrm{d}^3k\,\frac{|\varepsilon(k)|^2}{[\sqrt{\varepsilon^2(k)+\Delta^2}]^2}\tfrac{1}{3}|\nabla_k\varepsilon(k)|^2\frac{|\varepsilon(k)|\sqrt{\varepsilon^2(k)+\Delta^2}}{\cosh^2\left(\frac{\beta}{2}\sqrt{\varepsilon^2(k)+\Delta^2}\right)g[\varepsilon(k)][\varepsilon^2(k)+2\Delta^2]}\,. \tag{31}$$

Finally we have

$$\sigma=\sigma_0\int_0^B\mathrm{d}\varepsilon\,\frac{\varepsilon^3h(\varepsilon)\beta}{\sqrt{\varepsilon^2+\Delta^2}\,(\varepsilon^2+2\Delta^2)\,g(\varepsilon)\cosh^2\left(\frac{\beta}{2}\sqrt{\varepsilon^2+\Delta^2}\right)} \tag{32}$$

with $A = \begin{cases} 2J \\ 8J \end{cases}$ $B = \begin{cases} 3 \text{ for s.c} \\ 1 \text{ for b.c.c.} \end{cases}$ lattice

and (a = lattice constant):

$$\sigma_0 = \frac{e^2}{2\pi\hbar a}\left(\frac{N}{N_J}\right)\left(\frac{A}{E_J}\right)^2$$

$$h(\varepsilon) = \frac{V_c}{(2\pi)^3}\int_{1.\,B.-Z.} \mathrm{d}^3k\,\delta \cdot \left(\varepsilon - \frac{\varepsilon(k)}{A}\right)\frac{1}{3}\,|\nabla_k \varepsilon(k)|^2 \frac{1}{(aA)^2}\,. \qquad (33)$$

$\Delta, \beta = 1/k_B T$ are measured in units of A.

The function $h(\varepsilon)$ is the mean value of the ordinary band velocity over the energy surface $\varepsilon(k)/A = \varepsilon$, which was calculated numerically.

The factor $e^2/(2\pi\hbar a)$ has the dimension of a conductivity and about the value $\approx 10^6\,\Omega^{-1}\,\mathrm{cm}^{-1}$.

We need the gap equation too (DJK):

$$1 = V_0 \int_0^B \mathrm{d}\varepsilon\, \frac{g(\varepsilon)}{\sqrt{\varepsilon^2+\Delta^2}} \tanh\left(\frac{\beta}{2}\sqrt{\varepsilon^2+\Delta^2}\right). \qquad (34)$$

We can now calculate σ as a function of temperature and for fixed temperature as a function of the ratio V_0/J. This will be done in the last chapter.

4. Discussion of Results

For very high temperatures and $\Delta = 0$ the formula (32) would lead to $\sigma \sim 1/T$. This is of course a consequence of the fact, that a one-band model becomes unphysical at high temperatures. As soon as kT is much larger than the width of the band, all states are occupied with equal probability, and the band behaves as if fully occupied.

For low temperatures, (32) leads to

$$\sigma \sim (1/T)\exp\{-\Delta_0/k_B T\} \qquad (35)$$

where Δ_0 is the gap at $T = 0$.

Results of a detailed calculation are shown in Figs. 1 and 2 for the s. c. lattice (the b. c. c. lattice shows qualitatively the same behaviour). As can be seen, the disappearance of the gap causes a very sudden increase of the conductivity.

In Fig. 3, the conductivity has been plotted as a function of Δ for β fixed. The dependence is almost exponential.

As it should be, for $E_J \to 0$ the conductivity tends to infinity and just so for vanishing impurity concentration $N_J/N \to 0$.

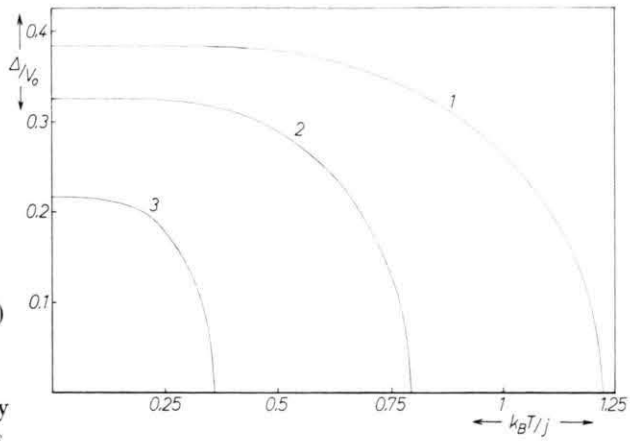

Fig. 1. Energy gap Δ as a function of temperature for s.c. lattice. **1**: $V_0/J=6$; **2**: $V_0/J=4.5$; **3**: $V_0/J=3$.

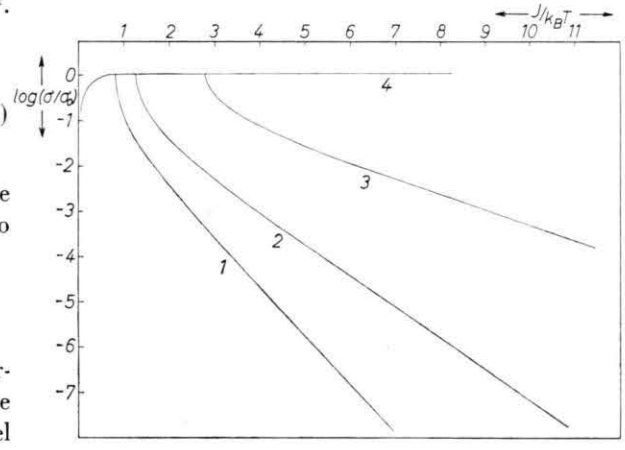

Fig. 2. Conductivity as a function of temperature for s.c. lattice. **1**: $V_0/J=6$; **2**: $V_0/J=4.5$; **3**: $V_0/J=3$; **4**: $\Delta=0$.

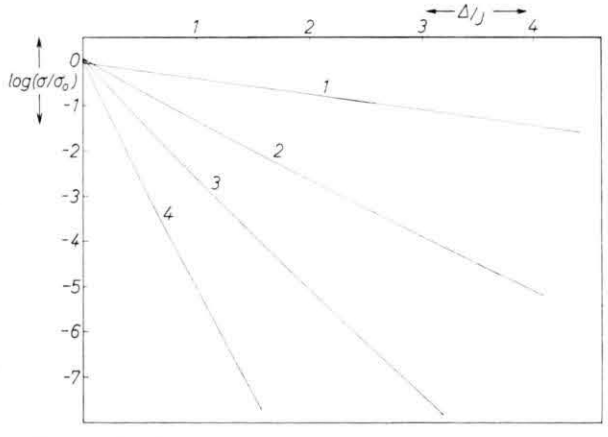

Fig. 3. Conductivity as a function of the energy gap for some temperature values ($\beta = J/k_B T$) and for the s.c. lattice. **1**: $\beta=0.5$; **2**: $\beta=2.5$; **3**: $\beta=5$; **4**: $\beta=10$.

A remark is necessary about the range of temperature. Only for low temperatures the resistance is dominated by impurities; the high (room) temperature dependence of the conductivity is due to electron-phonon interaction. This fact is not considered in our model.

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