EFFECT OF SCATTERING PROCESSES ON THE DYNAMICS OF ELECTRONS IN NARROW ENERGY BANDS

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We have investigated the effect of a magnetic field and the degree of filling and width of the band on the scattering processes on the basis of the Hubbard method. The electrical conductivity tensor was calculated with account taken of damping processes. It is shown that the relaxation times depend essentially on the electron spin orientations. The ordering of the electron spins under the influence of the external magnetic field leads to an increase of the electrical conductivity tensor, that in turn leads to a negative magnetoresistance.

The theoretical study of kinetic effects in crystals, which contain atoms of the transition metals and of the rare-earth compounds, presents significant difficulties that arise as a result of the necessity of a simultaneous calculation of the periodic field of the lattice acting on the electrons and of the correlated interaction between electrons. An important feature of such crystals is the existence of a narrow energy band [1-3]. Mott [4] has shown that electron correlations are important for narrow bands of the indicated compounds.

The Hubbard [5] model, describing the dynamics and interaction of electrons at one point, is a relatively simple and at the same time sufficiently realistic model which may be applied to the indicated systems. A problem arises in connection with this concerning the study of damping processes associated with the relative scattering of electrons [5, 6].

The dynamics of electrons (the electrical conductivity, in the first place), except for correlations, also depends essentially on the spin ordering. Considering the process of the ordering of electron spins under the influence of an external magnetic field, we shall obtain the mechanism of negative magnetoresistance.

Generally speaking, scattering processes of an electron with the spin \(\sigma\) take place at spatial and time fluctuations of the spin on each atom having an electron with a spin \(\sigma\). Spatial fluctuations depend on disordering by distributed electrons with a spin of \(\sigma\), that are assumed fixed. On the other hand, real systems of fixed electrons do not exist. Temporal fluctuations arise owing to the motion of electrons with spin \(\sigma\). These processes ought to be discussed all together [6]. The consideration of similar scattering processes were first assumed in [5].

Using localized Wannier functions as the basis, we write the Hubbard Hamiltonian in the presence of a weak magnetic field in the following way [7]:

\[
H = \sum_{ij} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + \frac{1}{2} \sum_{i\sigma} n_{i\sigma} n_{i\sigma} + \sum_{i\sigma} L(\sigma) n_{i\sigma},
\]

where

\[
t_{ij} = \frac{1}{N_\sigma} \sum_\epsilon e^{i\epsilon(R_i - R_j)}, \quad L(\sigma) = \frac{1}{2} g_\nu H \cdot \sigma = L \cdot \sigma.
\]

Let us assume that the Zeeman term is totally responsible for the magnetic properties. The electron correlation energy is \(I\); the magnetic field intensity is \(H = (0, 0, H)\); \(\mu_B\) is the Bohr magneton; \(N_\sigma\) is the number of atoms per unit volume; \(c_{i\sigma}^\dagger\) and \(c_{i\sigma}\) are creation and annihilation operators of electrons at the \(i\)-th point; \(n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}\); \(R_i\) is the radius vector of the \(i\)-th atom.


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The expression for the diagonal element of the electrical conductivity tensor was calculated according to Kubo's equation [8] in which the calculation by the two-body Green's function

\[ G_{ij, a}^2 = \langle n_{i\sigma}^\dagger c_{i\sigma}^{n_{j\sigma}} | P_x \rangle, \tag{2} \]

where

\[ P_x = e \sum R^I n_{i\sigma}; \ \sigma, \ \tilde{\sigma} = \pm; \ n_{i\sigma}^\dagger = n_{i\sigma}; \ n_{i\sigma}^- = 1 - n_{i\sigma} \]

are the projection operators [6, 9], was carried out with the help of the equations of motion. The uncoupling was carried out to second order. At the same time, such approximations as in [5, 6, 9] were made. It is taken into consideration that the interaction of electrons occurs at one point; we neglect the Green's functions and the averaging of higher orders obtained by virtue of the commutator \([n_{i\sigma}^\dagger H, H] \], where \(\sigma = \alpha, \beta, \gamma; \) and

1. \(\langle c_{n_{i\sigma}}^\dagger n_{n_{i\sigma}}^\dagger (n_{i\sigma}^\dagger - n_{i\sigma}^-) c_{j\sigma} n_{j\sigma}^\dagger | P_x \rangle \approx n_{i\sigma}^\dagger \langle c_{n_{i\sigma}}^\dagger (n_{i\sigma}^\dagger - n_{i\sigma}^-) c_{j\sigma} n_{j\sigma}^\dagger | P_x \rangle ; \)

2. \(\langle n_{n_{m\sigma}} n_{m\sigma}^\dagger c_{m\sigma} (n_{i\sigma}^\dagger - n_{i\sigma}^-) c_{j\sigma} n_{j\sigma}^\dagger | P_x \rangle \approx E_1 \langle n_{n_{m\sigma}} n_{m\sigma}^\dagger c_{m\sigma} (n_{i\sigma}^\dagger - n_{i\sigma}^-) c_{j\sigma} n_{j\sigma}^\dagger | P_x \rangle , \)

where

\[ E_1 = \begin{cases} 1, & \gamma = + \\ 0, & \gamma = - \end{cases} \]

3. \(\langle n_{n_{m\sigma}} c_{n_{m\sigma}}^\dagger c_{n_{m\sigma}}^\dagger c_{i\sigma} n_{j\sigma}^\dagger | P_x \rangle \approx n_{n_{m\sigma}} \langle c_{n_{m\sigma}}^\dagger c_{j\sigma} n_{j\sigma}^\dagger | P_x \rangle . \)

The Green's functions of second order

\[ \bar{R}_{ij, k}^2 (w) = \langle c_{m\sigma}^\dagger n_{n_{m\sigma}}^\dagger (n_{i\sigma}^\dagger - n_{i\sigma}^-) c_{i\sigma} n_{j\sigma}^\dagger | P_x \rangle w, \tag{3} \]

describing the scattering processes at disordered spins (scattering at spatial fluctuations), and

\[ D_{ij, k}^2 (w) = \langle c_{m\sigma}^\dagger n_{n_{m\sigma}}^\dagger c_{i\sigma} c_{j\sigma} n_{j\sigma}^\dagger | P_x \rangle w, \tag{4} \]

describing the dynamic processes (scattering at temporal fluctuations of the spins), were calculated with the use of methods proposed in [5 and 9].

The equations of motion for the Green's functions were written as

\[ G_{k, a}^\dagger (w) = \frac{\sigma}{i} \nabla_k \bar{G}_{k, a}^\dagger (w) + (E_k - E_0) \bar{G}_{k, a}^\dagger (w) + \]

\[ + n_{k\sigma} [\epsilon (k) + L (w)] \sum_{t=1}^{\tilde{t}} G_{k, a}^\dagger (w) - n_{k\sigma} \sum_{t=1}^{\tilde{t}} \bar{G}_{k, a}^\dagger (w) + \]

\[ + \sum_{k'} \bar{R}_{k, a}^1 \left[ G_{k, a}^\dagger (w) - n_{k\sigma} \sum_{a'} G_{k, a'}^\dagger (w) \right] - \sum_{k'} \bar{R}_{k, a}^1 \left[ G_{k, a}^\dagger (w) - n_{k\sigma} \sum_{a'} \bar{G}_{k, a'} (w) \right] + \]

\[ + \sum_{t=1}^{\tilde{t}} \bar{D}_{k, a}^1 \left[ n_{-k\sigma} G_{k, a}^\dagger - n_{-k\sigma} \bar{G}_{k, a}^\dagger \right] - \sum_{t=1}^{\tilde{t}} \bar{D}_{k, a}^1 \left[ n_{-k\sigma} \bar{G}_{k, a}^\dagger - n_{-k\sigma} G_{k, a}^\dagger \right] \tag{5} \]