Short Notes

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Electrical Conductivity of a Metallic System with a Nonspherical Fermi Surface

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Investigating the electrical resistivity of transition metallic systems some peculiarities have been found, which are caused by the fairly complicated dispersion relations for the quasi-particles (electrons, phonons, etc.) involved in the transport process and the existence of nearly localized electrons (d-electrons). In particular, for transition metals it is difficult to attribute the observed temperature dependence to definite scattering mechanisms. Partially, this has been explained by the fact that the calculated temperature dependence of the resistivity depends to some extent on the assumptions used for the spectra of the quasi-particles and the interaction matrix elements. To investigate the influence of the electron dispersion on the electrical resistivity, we consider an effective single band model with tight-binding dispersion relations of the electrons

$$H_0 = \sum_{\vec{k}\sigma} E(\vec{k})\, a^+_{\vec{k}\sigma} a_{\vec{k}\sigma} \quad , \quad E(\vec{k}) = 2\sum_{\alpha} t(\vec{a}_\alpha)\cos \vec{k}\vec{a}_\alpha \quad , \tag{1}$$

where $t(\vec{a}_\alpha)$ is the hopping integral between nearest neighbours and $\vec{a}_\alpha$ ($\alpha = x, y, z$) denotes the lattice vectors in a simple lattice with an inversion centre. Furthermore we restrict our considerations to electron-phonon and electron-electron interactions, where the electron-electron interaction is described in the framework of the Hubbard model,

$$H_{ee} = \frac{U}{N} \sum_{\vec{k}_1\vec{k}_2} \sum_{\vec{k}_3\vec{k}_4} \sum_{\vec{G}} a^+_{\vec{k}_1\uparrow}\, a_{\vec{k}_2\uparrow}\, a^+_{\vec{k}_3\downarrow}\, a_{\vec{k}_4\downarrow}\, \delta(\vec{k}_1 - \vec{k}_2 + \vec{k}_3 - \vec{k}_4, \vec{G}) \,. \tag{2}$$

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The electron-phonon interaction is usually represented by the Fröhlich Hamiltonian. However, for transition metals it is difficult to estimate the interaction matrix element of this model. Therefore, a model Hamiltonian proposed by Barišić et al. /1/ will be used,

$$H_{ep} = \sum_{\vec{k}\,\vec{k}_1} \sum_{\vec{q}\,\vec{G}} \sum_{\nu\sigma} g^{\nu}_{\vec{k}\,\vec{k}_1}\, a^{+}_{\vec{k}_1\sigma}\, a_{\vec{k}\sigma}\, (b^{+}_{\vec{q}\nu} + b_{-\vec{q}\nu})\, \delta(\vec{k}_1 - \vec{k} - \vec{q} - + \vec{G}) , \quad (3)$$

where

$$g^{\nu}_{\vec{k}\,\vec{k}_1} = (2\,N\,M\,\omega_o(\vec{k},\nu))^{-1/2}\; I^{\nu}_{\vec{k}\,\vec{k}_1} , \quad (4)$$

and

$$I^{\nu}_{\vec{k}\,\vec{k}_1} = 2iq_o \sum_{\alpha} t(\vec{a}_\alpha)\, (|\vec{a}_\alpha|^{-1}\, \vec{a}_\alpha\, \vec{e}_\nu(\vec{k}_1)(\sin\vec{k}\vec{a}_\alpha - \sin\vec{k}_1\vec{a}_\alpha) . \quad (5)$$

Here M is the ion mass, $\vec{e}_\nu(\vec{k})$ are the polarization vectors of the phonons ($\nu = 1,2,3$), and q_o is the Slater coefficient originated in the exponential radial decrease of the tight-binding electron wave functions.

For the vibrating ion system we have as usually

$$H_{ph} = \sum_{\vec{q}\,\nu} \omega_o(\vec{q},\nu)\, (b^{+}_{\vec{q}\nu}\, b_{\vec{q}\nu} + \frac{1}{2}) , \quad (6)$$

where $\omega_o(\vec{q},\nu)$ are the acoustic phonon frequencies. For the calculation of the conductivity we use generalized kinetic equations which can be derived by the quasi-equilibrium statistical operator method /2, 3/. The quasi-equilibrium statistical operator is given by

$$\varrho_q = Z_q^{-1}\, \exp\left[-\beta\,(H + \sum_m P_m F_m)\right] , \quad H = H_o + H_{ph} + H_{ee} + H_{ep} , \quad (7)$$

where the operators P_m include all important observables which describe the reaction of the system on the external electrical field and the F_m are conjugated parameters to be determined from the kinetic equations (cf. /2/)

$$\sum_n F_n \left[\frac{1}{i}\, \mathrm{Tr}\left\{\varrho\left[P_n, P_m\right]\right\} + \langle \dot{P}_n ; \dot{P}_m \rangle\right] =$$

$$= \frac{e\vec{E}}{m}\left[\mathrm{Tr}\left\{\varrho\, \vec{P}_e(-i\lambda)\, P_m\right\} + \langle P_{\vec{e}} ; \dot{P}_m \rangle\right] , \quad (8)$$

where

$$\dot{P}_m = i\,\left[H, P_m\right] , \quad (9)$$

$$\left.\begin{aligned} \langle A ; B \rangle &= \int_{-\infty}^{0} dt\, \exp(\eta t) \int_0^{\beta} d\lambda\, \mathrm{Tr}\left\{\varrho\, A(t - i\lambda) B\right\} , \\ A(t) &= \exp(i\,Ht)\, A\, \exp(-i\,Ht) ; \quad \varrho = Z^{-1}\, \exp(-\beta H) . \end{aligned}\right\} \quad (10)$$

In (8) $\vec{P}_e$ is the total momentum of the electrons and $\vec{E}$ the external electrical field. The current density is given by (see /2, 3/)

$$\vec{j} = \frac{e}{m\Omega} \sum_m F_m \int_0^{\beta} d\lambda\, \mathrm{Tr}\left\{\varrho\, P_m(-i\lambda)\, \vec{P}_e\right\} \equiv \frac{1}{R}\, \vec{E} , \quad (11)$$

where the proportionality of the F_m to the external electrical field has been taken into account.

In the present note we consider one non-spherical Fermi body shifted in the $\vec{k}$-space and deformed by the external electrical field. Hence, the Fermi surface $E(\vec{k}) = \varepsilon_F$ is transformed into $\tilde{E}(\vec{k}) = \varepsilon_F$, where

$$\tilde{E}(\vec{k}) = E(\vec{k}) + m\vec{v}_1 \frac{\partial E}{\partial \vec{k}} + m \sum_{i=2}^{n} \vec{v}_i\, \Phi_i(\vec{k}) \frac{\partial E}{\partial \vec{k}} + \ldots . \quad (12)$$

The term proportional to $\vec{v}_1$ describes a homogeneous shift of the Fermi body in the $\vec{k}$-space and the last terms allow for deformations of the Fermi body. The polynomials $\Phi_i(\vec{k})$ have to be chosen corresponding to the symmetry of the crystal /4, 5/, and in consequence of $\tilde{E}(\vec{k} + \vec{G}) = \tilde{E}(\vec{k})$ they should satisfy the relation

$$\Phi_i(\vec{k} + \vec{G}) = \Phi_i(\vec{k}) . \quad (13)$$

Due to (12) the proper set of operators P_m in (2) is given by

$$\vec{P}_1 = \vec{P}_e = m \sum_{\vec{k}\sigma} \frac{\partial E}{\partial \vec{k}}\, a^{+}_{\vec{k}\sigma}\, a_{\vec{k}\sigma} \quad ; \quad \vec{P}_i = m \sum_{\vec{k}\sigma} \Phi_i(\vec{k}) \frac{\partial E}{\partial \vec{k}}\, a^{+}_{\vec{k}\sigma}\, a_{\vec{k}\sigma} \quad (14)$$

and the parameters F_m are replaced by generalized drift velocities. In the weak scattering limit we replace the Hamiltonian H in the operators (10) by $(H_o + H_{ph})$ and then the correlation functions in (8) can be calculated straightforwardly. Using Wick's theorem we find

$$\langle \dot{\vec{P}}_j ; \dot{\vec{P}}_i \rangle \approx \langle \dot{\vec{P}}_j^{ee} ; \dot{\vec{P}}_i^{ee} \rangle + \langle \dot{\vec{P}}_j^{ep} ; \dot{\vec{P}}_i^{ep} \rangle \,. \tag{15}$$

Restricting ourselves for simplicity to a cubic system, the correlation functions of the generalized forces are given by

$$\langle \dot{\vec{P}}_j^{ee} ; \dot{\vec{P}}_i^{ee} \rangle = \frac{U^2 m^2 \beta \pi}{N^2} \sum_{\vec{k}_1 \vec{k}_2} \sum_{\vec{k}_3 \vec{k}_4} \sum_{\vec{G}} A_j(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4) \times$$

$$\times A_i(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4) f_{\vec{k}_1}(1 - f_{\vec{k}_2}) f_{\vec{k}_3}(1 - f_{\vec{k}_4}) \, \delta(E(\vec{k}_1) - E(\vec{k}_2) + E(\vec{k}_3) - E(\vec{k}_4)) \times$$

$$\times \delta(\vec{k}_1 - \vec{k}_2 + \vec{k}_3 - \vec{k}_4 + \vec{G}) \tag{16}$$

and

$$\langle \dot{P}_j^{ep} ; \dot{P}_j^{ep} \rangle = 2\pi m^2 \beta \sum_{\vec{k}_1 \vec{k}_2} \sum_{\vec{q}\vec{G}} \sum_{\nu} (g^{\nu}_{\vec{k}_1 \vec{k}_2})^2 \, B_j(\vec{k}_1, \vec{k}_2) \, B_i(\vec{k}_1, \vec{k}_2) \times$$

$$\times f_{\vec{k}_2}(1 - f_{\vec{k}_1}) \, N(\vec{q}, \nu) \, \delta(E(\vec{k}_2) - E(\vec{k}_1) + \omega_o(\vec{q}, \nu)) \, \delta(\vec{k}_2 - \vec{k}_1 - \vec{q} + \vec{G}) \,, \tag{17}$$

where

$$A_j(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_4) = \Phi_j(\vec{k}_4) \frac{\partial E}{\partial \vec{k}_4} - \Phi_j(\vec{k}_3) \frac{\partial E}{\partial \vec{k}_3} + \Phi_j(\vec{k}_2) \frac{\partial E}{\partial \vec{k}_2} - \Phi_j(\vec{k}_1) \frac{\partial E}{\partial \vec{k}_1} \,, \tag{18}$$

$$B_j(\vec{k}_1, \vec{k}_2) = \Phi_j(\vec{k}_2) \frac{\partial E}{\partial \vec{k}_2} - \Phi_j(\vec{k}_1) \frac{\partial E}{\partial \vec{k}_1} \,. \tag{19}$$

$f_{\vec{k}} \equiv f(E(\vec{k}))$ and $N(\vec{q}, \nu) \equiv N(\omega_o(\vec{q}, \nu))$ are the Fermi and Bose distribution functions, respectively. The correlation functions $\langle \dot{\vec{P}}_1, \dot{\vec{P}}_j \rangle$ vanish in the weak scattering limit, and the generalized electron numbers in (7) become

$$N_j \equiv \frac{1}{m} \mathrm{Tr} \left\{ \varrho \vec{P}_1 (-i\lambda) \vec{P}_j \right\} = m\beta \sum_{\vec{k}} \Phi_j(\vec{k}) \frac{\partial E}{\partial \vec{k}} f_{\vec{k}}(1 - f_{\vec{k}}) \,. \tag{20}$$

Because of $\beta f_{\vec{k}}(1 - f_{\vec{k}}) \to \delta(E(\vec{k}) - \varepsilon_f)$ at low temperatures the generalized electron numbers N_j (20) do not depend on temperature, and the temperature dependence of R (11) is given by the correlation functions (16) and (17). For the electron-electron scattering we find

$$\langle \dot{\vec{P}}_j^{ee} ; \dot{\vec{P}}_i^{ee} \rangle = \beta^{-2} \iiint_{-\beta\varepsilon_f}^{\beta(E_{max} - \varepsilon_f)} dx\, dy\, dz \, (\exp(x) + 1)^{-1} \times$$

$$\times (\exp(-y) + 1)^{-1} (\exp(z) + 1)^{-1} \quad (\exp(y - x - z) +$$

$$+ 1)^{-1} F_{ji}\left(\frac{x}{\beta} + \varepsilon_f, \frac{y}{\beta} + \varepsilon_f, \frac{z}{\beta} + \varepsilon_f\right) = A_{ji}^{ee} T^2 \,, \tag{21}$$

where

$$F_{ji}(E_1, E_2, E_3) = \frac{\pi m^2 U^2}{N^2} \frac{\Omega^3}{(2\pi)^9} \int d^2S_1 \int d^2S_2 \int d^2S_3 \times$$

$$\times \frac{A_j(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_1 - \vec{k}_2 + \vec{k}_3 + \vec{G}) \cdot A_i(\vec{k}_1, \vec{k}_2, \vec{k}_3, \vec{k}_1 - \vec{k}_2 + \vec{k}_3 + \vec{G})}{\left|\frac{\partial E}{\partial \vec{k}_1}\right| \left|\frac{\partial E}{\partial \vec{k}_2}\right| \left|\frac{\partial E}{\partial \vec{k}_3}\right|} \times$$

$$\times \delta(E(\vec{k}_1) - E(\vec{k}_2) + E(\vec{k}_3) - E(\vec{k}_1 - \vec{k}_2 + \vec{k}_3 + \vec{G})) \,. \tag{22}$$

$\int d^2S_1$ denotes an integration on the surface $E(\vec{k}) = E_1$. In (17) at low temperatures only phonons with small q are excited and we find with $\omega_o(\vec{q}, \nu) \approx v_o^{\nu} q$

$$\langle \dot{\vec{P}}_j^{ep} ; \dot{\vec{P}}_i^{ep} \rangle = \beta^{-5} \frac{m\Omega^2}{(2\pi)^6} \sum_{\nu} \frac{1}{(v_o^{\nu})^6} \int_0^{\beta v_o^{\nu} q_{max}} \frac{x^5 \, dx}{\exp(x) - 1} \times$$

$$\times \int \sin\Theta_q \, d\Theta_q \int d\varphi_q \, \tilde{F}_{ji}(\Theta_q, \varphi_q) = A_{ji}^{ep} T^5 \,, \tag{23}$$

where

$$\tilde{F}_{ji} = \int d\vec{k} \left[\left(\frac{\vec{q}}{q} \frac{\partial}{\partial \vec{k}'} \right) g^{\nu}_{\vec{k}\,\vec{k}'} \Big|_{\vec{k}'=\vec{k}} \right]^2 \left[\left(\frac{\vec{q}}{q} \frac{\partial}{\partial \vec{k}'} \right) B_j(\vec{k}, \vec{k}') \Big|_{\vec{k}'=\vec{k}} \right] \times$$

$$\times \left[\left(\frac{\vec{q}}{q} \frac{\partial}{\partial \vec{k}'} \right) B_i(\vec{k}, \vec{k}') \Big|_{\vec{k}'=\vec{k}} \right] f_{\vec{k}}(1 - f_{\vec{k}}) \, \delta\left(\frac{\vec{q}}{q} \frac{\partial E}{\partial \vec{k}} + v_o^{\nu} \right) . \qquad (24)$$

Hence at low temperatures the electron-electron and the electron-phonon contributions are proportional to T^2 and T^5, respectively, for any polynomial $\Phi_i(k)$. It is worth noting that for open Fermi surfaces these proportionalities follow for normal and Umklapp processes either. For a closed Fermi surface the electron-phonon Umklapp processes freeze out at sufficiently low temperatures and only the electron-phonon normal processes contribute to the electrical resistivity. With (21) and (23) the generalized kinetic equations (8) become

$$\sum_{j=1}^{n} \vec{v}_j \left(A^{ee}_{ji} T^2 + A^{ep}_{ji} T^5 \right) = e \vec{E} N_i . \qquad (25)$$

For simplicity we restrict our consideration to two parameters $\vec{v}_1$ and $\vec{v}_2$ describing the homogeneous shift and one type of deformation of the Fermi body. Taking into consideration more parameters is straightforward but does not yield any qualitatively new results. With (25) and (11) the electrical resistivity becomes

$$R = \frac{\Omega}{3e^2} \frac{(A^{ee}_{11} T^2 + A^{ep}_{11} T^5)(A^{ee}_{22} T^2 + A^{ep}_{22} T^5) - (A^{ee}_{12} T^2 + A^{ep}_{12} T^5)^2}{N_1^2 (A^{ee}_{22} T^2 + A^{ep}_{22} T^5) + N^2 (A^{ee}_{11} T^2 + A^{ep}_{11} T^5) - 2N_1 N_2 (A^{ee}_{12} T^2 + A^{ep}_{12} T^5)} \qquad (26)$$

and in general a simple dependence $R \sim T^n$ can be expected only if one of the scattering mechanisms is much more effective than the other. Expressions $R(T) \approx AT^2 + BT^5$ frequently used to fit the experimental R(T) dependences can be justified for nearly spherical Fermi surfaces only where the deformation of the Fermi body is negligible.

References

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