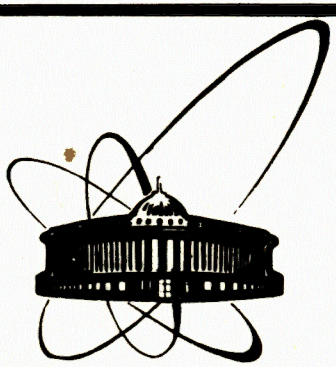

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SELF-CONSISTENT THEORY OF RESISTIVITY SATURATION

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At high temperatures the temperature dependence of the electrical resistivity ρ of some transition metals and A-15 compounds remarkably deviates from the usual $\rho \sim T$ dependence as given, e.g., by the well-known Bloch-Grüneisen law. This unusual behaviour is labelled as a resistivity saturation[1] and can be described by the following empirical formula (parallel resistor model)

$$\frac{1}{\rho(T)} = \frac{1}{\rho_{SBT}(T)} + \frac{1}{\rho_{max}} \quad , \tag{1}$$

where ρ_{SBT} is the resistivity given by the semi-classical Boltzmann transport theory ($\rho_{SBT} \sim T$), and the saturation resistivity ρ_{max} corresponds to the maximum metallic resistivity[2]. There are some attempts to explain the saturation phenomenon in the framework of the Boltzmann transport theory using special assumptions on the band structure, etc. On the other hand, the saturation phenomenon is observed in a lot of quite different substances, and it seems to be more reliable to explain the effect by deviations from the Boltzmann transport theory being valid only in the weak scattering limit. For a review of this topic see the paper of Allen[3].

Recently[4] an attempt has been undertaken to explain the resistivity saturation by calculating the resistivity starting from the force-force correlation functions and taking into account multiple scattering corrections. This has been done by introducing a temperature-dependent self-energy calculated in the lowest non-vanishing order of the electron-phonon interaction. The aim of this letter is to show that a saturation in the form given by (1) can be obtained by calculating the self-energy self-consistently within the framework of the transport theory of Christoph and Kuzemsky[5]. We start with the well-known Fröhlich Hamiltonian for the electron-phonon problem

$$H = \sum_{\vec{k}} \epsilon_{\vec{k}} a^+_{\vec{k}} a_{\vec{k}} + \sum \hbar\omega_{\vec{q}} b^+_{\vec{q}} b_{\vec{q}} + \frac{i c_{ep}}{\sqrt{\Omega}} \sum_{\vec{k},\vec{q}} F_{\vec{q}} a^+_{\vec{k}+\vec{q}} a_{\vec{k}} (b_{\vec{q}} - b^+_{-\vec{q}}) \quad , \tag{2}$$

where all symbols have their usual meaning (cf.[4]). The resistivity of a system described by the Hamiltonian (2) can be calculated very conveniently by the following expression [4-6]

$$\rho = \frac{3\Omega m^2}{e^2 (\vec{P}|\vec{P})} \cdot \frac{\lim_{\omega\to 0} \frac{1}{i\omega} (\langle\langle \vec{F}; \vec{F} \rangle\rangle_{\omega - i\eta} - \langle\langle \vec{F}; \vec{F} \rangle\rangle_{-i\eta})}{(\vec{P}|\vec{P}) + \langle\langle \vec{P}; \vec{P} \rangle\rangle_{-i\eta}} \quad , \quad \eta \to 0^+ \quad , \tag{3}$$

where $\langle\langle A; B \rangle\rangle_{-i\eta}$ are retarded Green functions and

$$(\vec{P}|\vec{P}) = -m^2 \sum_{\vec{k}} \left(\frac{\partial \epsilon_{\vec{k}}}{\partial \vec{k}}\right)^2 \frac{d}{d\epsilon_{\vec{k}}} \langle a^+_{\vec{k}} a_{\vec{k}} \rangle \quad , \quad \langle \ldots \rangle = \frac{1}{Z} \mathrm{Tr}\{ e^{-\beta H} \ldots \} . \tag{4}$$

The total momentum of the electrons is given by the expression $\vec{P} = m/h \sum_{\vec{k}} (\partial \epsilon_{\vec{k}} / \partial \vec{k}) a^+_{\vec{k}} a_{\vec{k}}$, and from $\vec{F} = i/h [H, \vec{P}]$ the total force acting on the electrons becomes

$$\vec{F} = \frac{m c_{ep}}{h^2 \sqrt{\Omega}} \sum_{\vec{k},\vec{q}} F_{\vec{q}} \left(\frac{\partial \epsilon}{\partial(\vec{k}+\vec{q})} - \frac{\partial \epsilon}{\partial \vec{k}} \right) a^+_{\vec{k}+\vec{q}} a_{\vec{k}} (b_{\vec{q}} - b^+_{-\vec{q}}) \quad . \tag{5}$$

The Green functions in (3) can be calculated by their equations of motion, where in the commutators the approximations

$$\begin{aligned} [a^+_{\vec{k}}, H] &= -\epsilon_{\vec{k}} a^+_{\vec{k}} - W^*_{\vec{k}} a^+_{\vec{k}} \quad , \quad W_{\vec{k}} = \Delta_{\vec{k}} + i\Gamma_{\vec{k}} \quad , \\ [a_{\vec{k}}, H] &= \epsilon_{\vec{k}} a_{\vec{k}} + W_{\vec{k}} a_{\vec{k}} \end{aligned} \tag{6}$$

are used, i.e., the higher order terms in the electron-phonon coupling are described by an effective shifting and damping of the one-electron states. In this approximation the Green function $\langle\langle \vec{P}; \vec{P} \rangle\rangle_{-i\eta}$ vanishes and the numerator of (3) becomes

$$\lim_{\omega\to 0} \frac{1}{i\omega} (\langle\langle \vec{F}; \vec{F} \rangle\rangle_{\omega - i\eta} - \langle\langle \vec{F}; \vec{F} \rangle\rangle_{-i\eta}) = \frac{4m^2 c_{ep}^2}{h^3} \frac{\Omega}{\Omega} \sum_{\vec{k},\vec{q}} F_{\vec{q}} \left(\frac{\partial \epsilon}{\partial(\vec{k}+\vec{q})} - \frac{\partial \epsilon}{\partial \vec{k}} \right)^2 \tag{7}$$

$$\frac{(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} + \Delta_{\vec{k}+\vec{q}} - \Delta_{\vec{k}} - \hbar\omega_{\vec{q}})(\Gamma_{\vec{k}+\vec{q}} + \Gamma_{\vec{k}})}{[(\epsilon_{\vec{k}+\vec{q}} - \epsilon_{\vec{k}} + \Delta_{\vec{k}+\vec{q}} - \Delta_{\vec{k}} - \hbar\omega_{\vec{q}})^2 + (\Gamma_{\vec{k}+\vec{q}} + \Gamma_{\vec{k}})^2]^2} [\langle a^+_{\vec{k}+\vec{q}} a_{\vec{k}+\vec{q}} \rangle \langle a^+_{\vec{k}} a_{\vec{k}} \rangle -$$

$$- 1) + (\langle a^+_{\vec{k}} a_{\vec{k}} \rangle - \langle a^+_{\vec{k}+\vec{q}} a_{\vec{k}+\vec{q}} \rangle) \nu_{\vec{q}}] \quad ,$$

where $\nu_{\vec{q}} = (\exp(\beta \hbar\omega_{\vec{q}}) - 1)^{-1}$ is the Bose distribution function of the phonons and the mean values are given by

$$\langle a^+_{\vec{k}} a_{\vec{k}} \rangle = \pi^{-1} \int_{-\infty}^{\infty} d\omega [\exp\beta(\omega - \epsilon_F) + 1]^{-1} \, \mathrm{Im} \ll a_{\vec{k}} ; a^+_{\vec{k}} \gg_{\omega + i\epsilon} . \quad (8)$$

Calculating the Green functions in (8) again within the approximation used above we find

$$\langle a^+_{\vec{k}} a_{\vec{k}} \rangle = \pi^{-1} \, \mathrm{arc\,cot}[(\epsilon_{\vec{k}} + \Delta_{\vec{k}} - \epsilon_F)/\Gamma_{\vec{k}}] , \quad (9)$$

where $\lim_{\Gamma_{\vec{k}} \to 0} \langle a^+_{\vec{k}} a_{\vec{k}} \rangle = f_{\vec{k}}$ is the Fermi distribution function. Assuming spherical symmetrical systems the quantity $W_{\vec{k}}$ should depend on the energy $\epsilon_{\vec{k}}$ only. Furthermore, it can be shown that the r.h.s. terms in (7) contribute to the sum only if $\epsilon_{\vec{k}} + \Delta_{\vec{k}} \approx \epsilon_F$ and $\epsilon_{\vec{k}+\vec{q}} + \Delta_{\vec{k}+\vec{q}} \approx \epsilon_F$ where ϵ_F is the Fermi energy. Therefore, $\Gamma(\epsilon_{\vec{k}})$ can be replaced by $\Gamma(\epsilon_F) \equiv \Gamma$ and in effect the resistivity ρ depends only on the one free parameter Γ. To determine this parameter, we use the identity

$$\rho^{-1} = \sigma_{\mathrm{KUBO}} = \frac{e^2}{3\Omega m} \ll \vec{P}; \vec{R} \gg_{-i\eta} , \quad (10)$$

where $\vec{R} = -i \sum_{\vec{k},\vec{k}_1} a^+_{\vec{k}} a_{\vec{k}_1} \frac{\partial}{\partial \vec{k}_1} \delta(\vec{k},\vec{k}_1)$ is the position operator of the electrons. Using the same approximations for the calculation of the Green functions in both sides of (10), the identity becomes a very convenient equation for the determination of free parameters used in the approximated calculation of the Green functions. With the approximation used above the r.h.s. Green function in (10) reads

$$\ll \vec{P}; \vec{R} \gg_{-i\eta} = -\frac{m}{2\Gamma} \sum_{\vec{k}} \left(\frac{\partial \epsilon}{\partial \vec{k}}\right)^2 \frac{\partial}{\partial \epsilon_{\vec{k}}} \langle a^+_{\vec{k}} a_{\vec{k}} \rangle , \quad (11)$$

and (10) becomes an equation for the determination of the damping parameter Γ. For temperatures high compared to the Debye temperature the phonon distribution function is given by $\nu_{\vec{q}} = k_B T/\hbar\omega_{\vec{q}}$, and the resistivity given by (3), (7) and (9) can be written as

$$\rho(T,\Gamma) = aT + f(\Gamma) \cdot T \quad (12)$$

where $f(0) = 0$. The first term is the well-known Bloch-Grüneisen result, and by (10) it follows that Γ increases with increasing temperatures. Restricting ourselves to the lowest order in Γ from equations (10) to (12) we obtain the following equation for determination of Γ

$$b/\Gamma = (aT + f'(0)\Gamma T)^{-1} , \quad (13)$$

where a and b easily can be obtained from (7) and (10), respectively. As shown below, the quantity $f'(0)$ is negative, and then conductivity (10) becomes

$$\sigma = \rho^{-1} = 1/aT + (b/a)|f'(0)| . \quad (14)$$

The expression (14) has the form of the empirical formula (1), where, however, in the higher orders of Γ correction terms will be obtained.

To estimate the order of magnitude of the saturation resistivity, the coefficients a, b, and $f'(0)$ are calculated for a system of quasi-free electrons with $\epsilon_{\vec{k}} = \hbar^2\vec{k}^2/2m^*$ and acoustical phonons with $\omega_{\vec{q}} = \hbar v_0 q$. For this model the integrations in (7) and (11) can be carried out analytically, and we obtain

$$a = \frac{3}{8}\pi \frac{m^{*2} c_{ep}^2 q_D^4 k_B}{e^2 \hbar^4 k_F^6 v_0} , \quad (15)$$

$$b = \frac{e^2 \hbar k_F^3}{6 m^{*} \pi^2} , \quad (16)$$

$$f'(0) = -24 \frac{m^{*3} c_{ep}^2 k_B}{e^2 \hbar^6 k_F^4 v_0} \left| P\left(\frac{q_D}{2k_F}\right) \right| , \qquad q_D < 2k_F , \quad (17)$$

where $P(x) = 2x + \ln|(1-x)/(1+x)|$. Comparing (1) and (14) we find for the saturation resistivity ρ_{max} the formula

$$\rho_{max} = \frac{3}{32}\pi^3 \frac{\hbar}{e^2} \cdot \frac{q_D^4}{k_F^5} \left| P\left(\frac{q_D}{2k_F}\right) \right|^{-1} , \quad (18)$$

where $\hbar k_F$ is the Fermi momentum of the electrons and $\hbar q_D$ the Debye momentum of the phonons. For one electron per lattice site we have $k_F = \sqrt[3]{2}\, q_D$ [7], and using the reasonable value $q_D \approx 2 \cdot 10^{10}\ \mathrm{m}^{-1}$ we find for the saturation resistivity $\rho_{max} \approx 840 \mu\Omega$ cm. This value is too large in comparison with experimental ones (100 ... 300 $\mu\Omega$ cm), but it is smaller than Mott's estimate [8] and has the order of magnitude of the estimate given by Gurvitch [9]. Hence, in the present paper the parellel resistor formula (1) was explained by taking into

consideration higher-order terms in the electron-phonon interaction and by determing the self-energy describing these higher order terms self-consistently. For an improved theory using more realistic dispersion relations for electrons and phonons the momentum dependence of the self-energy has to be taken into account, but the qualitative saturation behaviour described by the theory given above should remain unchanged.

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Самосогласованная теория насыщения электросопротивления

Выводится формула для модели параллельных сопротивлений, с помощью которой можно описывать насыщение электросопротивления в веществах с сильным электрон-фононным взаимодействием. Вклады высших порядков по электрон-фононному взаимодействию учитываются в затухании одночастичных состояний электронов, которое вычисляется самосогласованно.

Работа выполнена в Лаборатории теоретической физики ОИЯИ.

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Self-Consistent Theory of Resistivity Saturation

The parallel resistor formula describing the saturation phenomenon of the electrical resistivity in systems with strong electron-phonon interaction is derived. Higher-order terms in the electron-phonon interaction are described by a self-energy which is determined self-consistently.

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

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