Electron scattering by mobile defects

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Abstract. We consider the infrared divergences caused by the electron interaction with mass–density waves (MDW) in the presence of strong static disorder localizing the states of the defects. The temperature dependence of the MDW contribution to the electrical resistance is obtained. The minimum resistance evoked by the electron–MDW scattering is found.

1. Introduction

It is generally known that light interstitials in a metal matrix (e.g. hydrogen isotopes or positive muons) can diffuse from one interstice into another. Tunnelling is the main diffusion mechanism in the low temperature region (Andreev and Lifshitz 1969). If the free path length λ of the quantum impurity (MDW) is much greater than the interatomic distance, a, the impurity is described by the Bloch eigenfunction, and the characteristic band width ε_0 for hydrogen in a metal, taking account of the polaron effect, equals 0.1/10 K (Wipf and Neumaier 1984, Fukai and Sugimoto 1985). For low temperature the value of λ is mainly determined by the MDW scattering from electrons, static imperfections and each other.

Otherwise, if $\lambda < a$, the MDW moves by hopping between interstices.

In a previous paper (Morosov and Sigov 1987) we considered the influence of infrared (IR) divergences caused by the electron–MDW interaction on the resistance of metals in the case $\lambda \gg a$ for non-interacting MDWs.

In the present paper we investigate the case of a 'strong' static disorder when the MDW band is destroyed due to the influence of lattice defects, and all the states are localized.

2. The electron–MDW interaction

The complete Hamiltonian of the electron–MDW interaction may be introduced in the form

$$\mathcal{H} = \mathcal{H}_{\text{el}} + \mathcal{H}_{\text{MDW}} + \mathcal{H}_{\text{int}} \tag{1}$$

where

$$\mathcal{H}_{\text{el}} = \sum_{k} \varepsilon(k) a^{+}(k) a(k) \tag{2}$$

$$\mathcal{H}_{\mathrm{MDW}} = \sum_n W(n)c^+(n)c(n) + t\sum_{n,\delta} c^+(n+\delta)c(n) \tag{3}$$

$$\mathcal{H}_{\mathrm{int}} = \sum_{k,k',n,\delta} V^{(0)}_{n,n+\delta}(k-k')a^+(k)a(k')c^+(n)c(n+\delta)$$

$$+ \sum_{k,k',n} V^{(0)}_{n,n}(k-k')a^+(k)a(k')c^+(n)c(n) \tag{4}$$

$$V^{(0)}_{n,n'}(k-k') = \langle n|V_0(k-k')\,\mathrm{e}^{\mathrm{i}(k'-k)R}\,|n'\rangle. \tag{5}$$

The Hamiltonian $\mathcal{H}_{\mathrm{el}}$ describes the conductivity electrons, $\varepsilon(k)$ is the dispersion law for the electrons and $a^+(k)$, $a(k)$ are the second quantization operators. The MDW Hamiltonian $\mathcal{H}_{\mathrm{MDW}}$ reflects the static disorder, $W(n)$ is the MDW energy at the nth interstice (n is the 3D integer vector), t is the tunnelling matrix element, δ runs over the nearest neighbours and $c^+(n)$ and $c(n)$ are the MDW second-quantization operators. The Hamiltonian $\mathcal{H}_{\mathrm{int}}$ describes the interaction between electrons and the MDW, $V_0(k)$ is the Fourier component of the interaction potential, $|n\rangle$ is the ψ-function of the MDW at the nth interstice defined in the coordinate space. Here and below, the MDW at an interstice is supposed to occupy the lowest oscillation level.

In the absence of the disorder ($W(n) = W_0$) all interstices are equivalent and $\mathcal{H}_{\mathrm{MDW}}$ takes a diagonal form in the Bloch-function representation. In such a case one has

$$\mathcal{H}_{\mathrm{int}} = \sum_{k,k',q} V_0(q)a^+(k'+q)c^+(k-q)a(k')c(k). \tag{6}$$

The matrix element of $\mathcal{H}_{\mathrm{int}}$ for the transition between states with different Bloch functions does not contain the small parameter t and the complete vertex of the electron–MDW interaction $V(q)$ equals (Kondo 1984a, b)

$$V(q) = V_0(q)\,(D/\max(\varepsilon_0, T))^g \tag{7}$$

where D is the electron band width, T is temperature, and g is defined (see Morosov and Sigov 1987) as

$$g = 2\int \frac{\mathrm{d}k_1}{(2\pi)^3}\int \frac{\mathrm{d}k_2}{(2\pi)^3} \frac{|V_0(k_1-k_2)|^2}{|\nabla\varepsilon(k_1)||\nabla\varepsilon(k_2)|} \tag{8}$$

the integration is performed over the Fermi surface.

The electron–MDW interaction leads to renormalization of the MDW dispersion law and to narrowing of the MDW band width (Kondo 1984a, b):

$$\bar{\varepsilon}_0 = \varepsilon_0(\max(\varepsilon_0, T)/D)^K \qquad K \sim g. \tag{9}$$

At the same time there exists the following estimation for the renormalized effective MDW band width (Kagan and Prokof'ev 1986)

$$\bar{\varepsilon}_0 = \varepsilon_{\mathrm{ad}}(\max(T, \bar{\varepsilon}_0)/\omega)^K \tag{10}$$

where ω is the frequency of local MDW vibration at the interstice, and $\varepsilon_{\mathrm{ad}}$ is the MDW band width in the adiabatic approximation. An apparent disagreement between formulae (9) and (10) is connected with the difference in the initial expression for the band width: ε_0 corresponds to the MDW neglecting its interaction with electrons, while the interaction
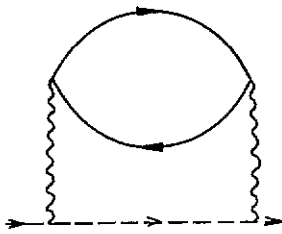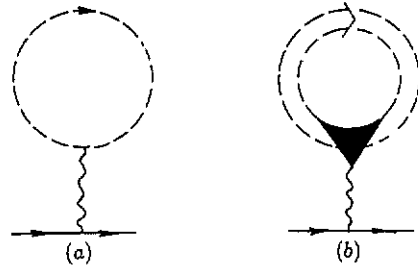
Figure 1.

Figure 2.

with electrons whose energy exceeds ω is already taken into account within the scope of the adiabatic approximation. This remark allows us to find (Leggett *et al* 1987) that

$$\varepsilon_{ad} = \varepsilon_0(\omega/D)^K. \tag{11}$$

Therefore, expressions (9) and (10) are equivalent in the framework of the parquet approximation (Nozieres *et al* 1969, Morosov and Sigov 1987). Substitution of $\bar{\varepsilon}_0$ for ε_0 in the expression $\max(T, \varepsilon_0)$ yields transformation of K into $K/(1 - K)$ for $T < \varepsilon_0$ which is *greater* than the accuracy of the parquet approximation.

3. Strong disorder

Let us consider the case when the dispersion of the MDW energy at neighbouring interstices caused by lattice imperfections (dislocations, heavy point defects) considerably exceeds ε_0:

$$\xi = \langle |W(n) - W(n + \delta)| \rangle \gg \varepsilon_0 \tag{12}$$

where the symbol $\langle \ldots \rangle$ denotes averaging over n and δ. At the same time we suppose that $\xi \ll D$ and the conductivity electrons are delocalized and described by the Bloch functions.

In this case, the eigenstates of the Hamiltonian $\mathcal{H}_{MDW}$ are localized and the integral intersection of the wave functions of states centred at neighbouring interstices containing the small parameter t/ξ. Thus, the main contribution to IR divergencies comes from the term in $\mathcal{H}_{int}$ that is diagonal with respect to n. Indeed, let us examine the quadratic in $V_{n,n'}^{(0)}$ correction to the MDW Green function

$$\Psi_{n,n}^{(0)} = [i\varepsilon_m - \bar{W}(n) + \zeta]^{-1}. \tag{13}$$

Here $\bar{W}(n)$ is the eigenvalue of the Hamiltonian $\mathcal{H}_{MDW}$, ζ is the MDW chemical potential, and $\varepsilon_m = (2m + 1)\pi T$, where $m = 0, \pm 1, \pm 2, \ldots$. The diagram in figure 1 corresponds to this correction term. The broken line represents the function $\Psi_{n,n}^{(0)}(\varepsilon_m)$, the wavy line denotes $V_{n,n'}^{(0)}$, and the full curve is the electron Green function

$$G^{(0)}(k, \varepsilon_m) = [i\varepsilon_m - \varepsilon(k) + \mu]^{-1} \tag{14}$$

where μ is the chemical potential of electrons. The contribution of terms with $n' = n + \delta$ to the self-energy part of MDW, $\chi_{n,n}(\varepsilon_m)$, contains the square of the matrix element
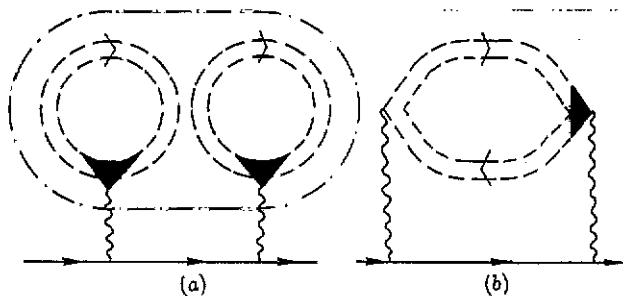
Figure 3.

$V_{n,n+\delta}^{(0)} \sim t/\xi$ and the logarithmic divergence is cut off at $\max(\varepsilon_0, T, \xi)$. Hence for $\xi \gg \varepsilon_0$ the term with $n' = n$ is much greater than the others. Neglecting them, one finds

$$\Psi_{n,n}(\varepsilon) = \Psi_{n,n}^{(0)}(\varepsilon)(T/D)^g$$

$$V_{n,n}(\varepsilon) = V_{n,n}^{(0)}(\varepsilon)(D/T)^g \tag{15}$$

where $\Psi_{n,n}(\varepsilon)$ and $V_{n,n}(\varepsilon)$ are the results of analytic extrapolation of the corresponding expressions from points $\varepsilon = i\varepsilon_m$ to the real axis.

4. MDW contribution to the resistance

When the MDWs are described by the Bloch waves, the diagram displayed in figure 2(a) does not contribute to the relaxation of electrons and gives rise to renormalization of μ only. The situation changes drastically in the case of localized MDWs. The process displayed in figure 2(a) leads to a change in the electron momentum. If the IR divergencies are accounted for, one has to replace $\Psi_{n,n}^{(0)}$ by $\Psi_{n,n}$ and $V_{n,n}^{(0)}(q)$ by $V_{n,n}(q)$ (figure 2(b)). The double broken circle and the full triangle with a wavy line correspond to the elements $\Psi_{n,n}$ and $V_{n,n}(q)$, respectively. Renormalizations of the vertex and of the Green function cancel each other. Therefore, the contribution described by this diagram has the form

$$G^{(0)}(p, \varepsilon_m)G^{(0)}(p', \varepsilon_m) \sum_n V_{n,n}^{(0)}(p - p')f(n) \, e^{i(p-p')R} \tag{16}$$

where $f(n)$ is the Fermi–Dirac function for the MDW distribution between the eigenstates of the Hamiltonian $\mathcal{H}_{MDW}$. It can be easily seen that equation (16) with the exception of the factor $f(n)$ coincides with the analogous expression for the scattering of electrons from frozen-in defects in the 'cross' technique (Abricosov *et al* 1963). In the latter case the summation is performed over the impurities.

If one neglects the interaction between the MDWs (since their concentration is low) and assumes the absence of correlation between the deviations of $\bar{W}(n)$ from its mean value, then the averaging over the realizations of static disorder is completely analogous to that in the 'cross' technique. As a result, in the framework of our approximation, one obtains a general diagram (figure 3(a)) for a full contribution of diagrams of this type to the relaxation of electrons. All MDW loops within the chain curve correspond to the same $|n\rangle$.

The second contribution to the electron relaxation time τ_{el} comes from the processes introduced in figure 3(b), and is analogous to that considered by Morosov and Sigov
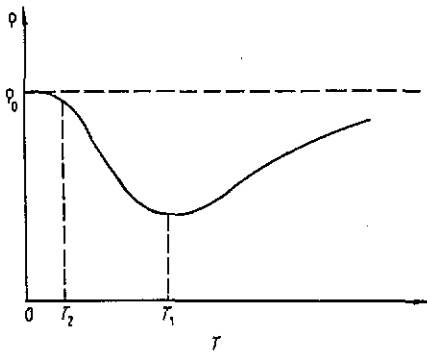
Figure 4. Temperature dependence of the MDW contribution to the resistance of the disordered crystal.

(1987). In addition to elastic processes, when both MDW lines in the loop correspond to the same n, the relaxation of electrons is influenced by the inelastic processes, for which $n' \neq n$. The contribution of the latter processes is smaller by the parameter $(\varepsilon_0/\xi)^2$. Neglecting it we obtain the following expression for τ_{el}

$$\tau_{el}^{-1}(p) = \frac{1}{(2\pi)^2} \int \frac{dp'}{|\nabla\varepsilon(p')|} \sum_n |V_{n,n}^{(0)}(p - p')|^2 \{f^2(n) + [f(n) - f^2(n)](T/D)^g\} \tag{17}$$

where the integration is performed over the Fermi surface. The expression for τ_{el} becomes very simple when the value $V_{n,n}(q)$ is independent of n. Then one finds

$$\tau_{el}^{-1} = \tau_0^{-1}x^{-1} \sum_n \{f^2(n) + [f(n) - f^2(n)](T/D)^g\} \tag{18}$$

where τ_0 is the electron relaxation time in the case of scattering from the 'frozen-in' impurities of identical chemical nature and equal concentration x.

Considering the two-particle Green function we have (analogously) for the MDW contribution into the resistance

$$\rho = \rho_0 x^{-1} \sum_n \{f^2(n) + [f(n) - f^2(n)](T/D)^g\} \tag{19}$$

where ρ_0 is the residual resistance in the case of the 'frozen-in' impurities.

In the region of high temperature, $f(n)$ appears to be so small that

$$\sum_n f^2(n) \ll \sum_n f(n)(T/D)^g. \tag{20}$$

Then one obtains

$$\rho(T) = \rho_0(T/D)^g \tag{21}$$

as in the case of the absence of the diagonal disorder (Morosov and Sigov 1987). This is evidence for the universality of such a dependence on temperature. Because of the absence of a $\rho(T)$ dependence upon ε_0 we have no crossover to the 'cross' technique in the limit $\varepsilon_0 \to 0$. In the 'cross' technique one considers impurities as the external field, but here we treat them as internal degrees of freedom of the crystal. With increasing

impurity mass (diminishing ε_0) there is an exponentially increasing MDW system relaxation time, τ_{MDW}. Its value equals (Kagan and Prokof'ev 1986)

$$\tau_{MDW}^{-1} = (g\, \bar\varepsilon_0^2/\xi)\exp(-\xi/T). \tag{22}$$

Hence heavy impurities are practically always in the non-equilibrium 'frozen-in' state.

With decreasing temperature at $T = T_1$ the inequality (20) changes its sign. At $T < T_1$ the value of $\rho(T)$ increases with decreasing temperature. This process continues down to the temperature T_2 of degeneration of the MDW gas. At $T < T_2$ the resistance $\rho = \rho_0$. The characteristic temperature dependence of the MDW contribution to the resistance is introduced in figure 4. The values of T_1 and T_2 depend upon the character of the MDW density of states $\nu(\bar W(n))$.

5. Conclusions

We found the contribution to the electrical resistance of crystals of scattering from the MDW. Unlike in the case of the 'frozen-in' impurities in which residual resistance remains constant, the MDW contribution in the case of 'strong' static disorder appears to be non-monotonic and the resistance displays a minimum at $T = T_1$. At higher temperatures one has $\rho(T) \propto T^g$, therefore the index of the temperature dependence is non-universal and reflects specific properties of a given material.

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