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Quantum Kinetic Theory of the '$2k_{\mathrm{F}}$' Scattering Mechanism for Three-Dimensional Structurally Disordered Systems in the Ioffe–Regel limit

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Effect of the coherent backscattering of the conduction electrons in three-dimensional structurally disordered metals specified by the Ioffe–Regel criterion is considered within the framework of the Morgan–Howson–Šaub theory of localisation which is based on the generalised kinetic equation for the Wigner distribution function and effective medium approximation. A formula for the electrical resistivity including the weak localisation correction is expressed in terms of the dimensionless transport parameter $k_{\mathrm{F}}\ell$. The asymptotic form of the formula is derived and discussed in the context of the diagrammatic approach.

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1. Introduction

Anomalous diffusion of conduction electrons in weakly disordered metals at low temperatures is a consequence of the quantum interference phenomena which can lead to the weak localisation of the carriers. These systems can be understood as the disordered systems that are characterised by the Ioffe–Regel criterion [1]:

$$k_{\mathrm{F}}\ell \gg 1, \tag{1}$$

where k_{F} is the Fermi wavevector and ℓ is the elastic mean free path. On the other hand, the inequality (1) states a range of applicability of the Sommerfeld theory of metals based on the Boltzmann equation. Within the framework of the theory, the electrical resistivity of bulk metals can be expressed in the following form

$$\rho = (12\pi^5)^{1/3}\frac{\hbar}{\mathrm{e}^2}\frac{r_s}{k_{\mathrm{F}}\ell}, \tag{2}$$

where r_s is the Wigner–Seitz radius, and $\hbar$, e have their usual meanings. On the basis of Eq. (2) it can be concluded that the electrical resistivity increases with decreasing value of the product $k_{\mathrm{F}}\ell$ for a fixed value of the Wigner–Seitz radius. It should be mentioned that in the limiting case: $k_{\mathrm{F}}\ell \approx 1$, the semiclassical description of the electronic transport in the disordered systems breaks down, because the strong localisation phenomena emerge in the system and as a result the electrical conductivity disappears at absolute zero [2]. In fact, the situation is more complex, because the conduction electrons interact not only with an effective stochastic thermal field due to the dynamics of ions, but also with a fluctuating electric field created by other electrons [3, 4]. Both of these interaction mechanisms are a source of dephasing which randomizes the phase coherence of carriers at finite temperatures [5]. Despite these difficulties, the electrical resistivity given by the famous Drude formula [1]:

$$\rho = \frac{m\tau_{\mathrm{tr}}^{-1}}{ne^2} \tag{3}$$

is still applicable for the gas of electrons with the effective mass m and the electron density n in the disordered systems, but the transport relaxation time τ_{tr} should be determined within a framework of the quantum theory of transport.

In this short report we discuss a weak disorder limit specified by the Ioffe–Regel criterion of the Morgan–Howson–Šaub (MHŠ) theory of the '$2k_{\mathrm{F}}$' scattering mechanism. The MHŠ theory was originally formulated by Morgan et al. [6] for highly disordered systems, i.e. metallic glasses having the electrical resistivity significantly greater than 150 $\mu\Omega$ cm, and was many times applied to successfully explain the resistivity measurements in various strong or weak disordered systems, e.g. [7].

2. Theory

The general MHŠ theory of localisation is based on the linearised von Neumann equation for the density matrix which is transformed to the phase space via the Wigner–Weyl transform [6]. As a result, the generalised kinetic equation for the Wigner distribution function with the non-local potential replaced by a superposition of non-overlapping atomic pseudopotentials is derived. This equation can be reduced to a Boltzmann-like form for the averaged Wigner function $\bar{\varrho}(\boldsymbol{k})$ by applying the projection operator method of Zwanzig [6]:

$$\epsilon\bar{\varrho}(\boldsymbol{k}) + \sum_{\boldsymbol{k}'} T(\boldsymbol{k},\boldsymbol{k}')\big[\bar{\varrho}(\boldsymbol{k}) - \bar{\varrho}(\boldsymbol{k}')\big] = -\frac{e}{\hbar}\boldsymbol{E}\cdot\nabla_{\boldsymbol{k}}\varrho_0(\boldsymbol{k})\big[1+\gamma(\boldsymbol{k})\big], \tag{4}$$

where $\boldsymbol{E}$ is an adiabatically switched electric field with

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the infinitesimal ϵ, $\varrho_0(\boldsymbol{k})$ is the equilibrium distribution function for free electrons, and $\gamma(\boldsymbol{k})$ modifies the injection of electrons into the system by the electric field taking into account the local fluctuations. The generalised scattering kernel $T(\boldsymbol{k},\boldsymbol{k}')$ replaces the usual scattering probability of the conduction electrons in the ordinary Boltzmann equation and it allows one to define the inverse of the transport relaxation time in the MHŠ theory by the formula

$$\tau_{\rm tr}^{-1}(\boldsymbol{k}) = \sum_{\boldsymbol{k}'} T(\boldsymbol{k},\boldsymbol{k}')(1-\cos\vartheta_{\boldsymbol{k}'\boldsymbol{k}}), \tag{5}$$

where $\vartheta_{\boldsymbol{k}'\boldsymbol{k}}$ is the angle between $\boldsymbol{k}'$ and $\boldsymbol{k}$. The analytical form of the generalised scattering kernel is determined within the effective medium approximation. Moreover, as it was argued in [6], the weak localisation can be extracted from the generalised scattering kernel by considering the component that represents the multiple scattering processes strongly peaked in the backward direction, i.e. $\boldsymbol{k}' = -\boldsymbol{k}$. Finally, the general form of the inverse of the transport relaxation time derived within the MHŠ theory is given by the following expression [8]:

$$\tau_{\rm tr}^{-1}(\boldsymbol{k}) \approx \tau_{\rm FZ}^{-1}(\boldsymbol{k}) + \sum_{\boldsymbol{k}'} \frac{T_1(\boldsymbol{k},\boldsymbol{k}')(1-\cos\vartheta_{\boldsymbol{k}'\boldsymbol{k}})}{A_\phi + C(k,\tau)|\boldsymbol{k}+\boldsymbol{k}'|^2}, \tag{6}$$

where τ is the momentum relaxation time, $\tau_{\rm FZ}(\boldsymbol{k})$ is the transport relaxation time calculated from the Faber–Ziman theory [9], $C(k,\tau) = (\hbar k\tau)^2/(8m^2)$ in the simplest case, and A_ϕ is the dephasing term. Its form depends on microscopic mechanisms of the dephasing, but we omit this issue in the present investigation because it will be included in the forthcoming publication. The component of the generalised scattering kernel $T_1(\boldsymbol{k},\boldsymbol{k}')$ is given by the broadened delta, namely

$$T_1(\boldsymbol{k},\boldsymbol{k}') = \frac{S(|\boldsymbol{k}-\boldsymbol{k}'|)u_a^2(\boldsymbol{k}-\boldsymbol{k}')\hbar\tau^{-1}}{\pi\left\{\left[\frac{\hbar^2}{2m}\left(k^2-k'^2\right)\right]^2 + \left[\hbar\tau^{-1}\right]^2\right\}}, \tag{7}$$

where $S(|\boldsymbol{k}-\boldsymbol{k}'|)$ is the structure factor, $u_a(\boldsymbol{k}-\boldsymbol{k}')$ is the Fourier transform of the atomic pseudopotential, and τ is the momentum relaxation time which depends on $(\boldsymbol{k}+\boldsymbol{k}')/2$. The expression for the inverse transport relaxation time given by Eq. (6) allows us to look at the general MHŠ theory as a generalization of the Faber–Ziman theory by including the multiple scattering processes into consideration [10].

Short analysis of Eq. (6) shows that in the absence of the dephasing factor ($A_\phi = 0$) the second term on the left-hand side of the formula is singular for $\boldsymbol{k}' = -\boldsymbol{k}$, but the singularity is integrable in the three dimensions, so the term is strongly peaked and it gives a finite additive contribution to the electrical resistivity formula as it is shown in the next section.

3. Results and discussion

The weak localisation contribution to the inverse relaxation time formula given by the second term on the right-hand side of Eq. (6) can be converted into integral and after some lengthy calculations the relative electrical resistivity can be expressed in the following form:

$$\frac{\Delta\rho}{\rho_{\rm FZ}} \equiv \frac{\rho-\rho_{\rm FZ}}{\rho_{\rm FZ}} = 2\frac{(\tau_{\rm FZ}/\tau)}{(k_{\rm F}\ell)^2}F(k_{\rm F}\ell), \tag{8}$$

where $\rho_{\rm FZ}$ is the Faber–Ziman electrical resistivity of the system and the function $F(k_{\rm F}\ell)$ is defined by the formula:

$$F(k_{\rm F}\ell) = 2\ln\frac{g(k_{\rm F}\ell)+\sqrt{2g(k_{\rm F}\ell)}}{g(k_{\rm F}\ell)-\sqrt{2g(k_{\rm F}\ell)}}, \tag{9}$$

with $g(k_{\rm F}\ell) = 1+\sqrt{1+(2/k_{\rm F}\ell)^2}$. The form of Eq. (8) is the main result of the report and it follows directly from the combination of Eq. (3) and Eq. (6) with $A_\phi = 0$. In Fig. 1 we present the weak localisation correction to the resistivity of the three-dimensional systems as a function of the $k_{\rm F}\ell$ parameter for different values of the ratio $\tau_{\rm FZ}/\tau$.

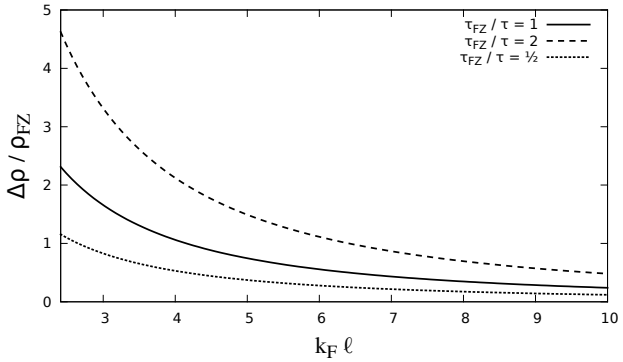

Fig. 1. The weak localisation correction to electrical resistivity of the bulk disordered systems as a function of the dimenionless transport parameter $k_{\rm F}\ell$ for different values of the ratio $\tau_{\rm FZ}/\tau$.

For $\tau_{\rm FZ}/\tau = 1$, the minimal value of the parameter $k_{\rm F}\ell$ is equal to 2.41 (not ≈ 1). It is an important result of the MHŠ theory of the strong localisation, because the critical value of parameter $k_{\rm F}\ell$ determines the Anderson localisation at $T = 0$ K within the framework of the MHŠ theory [11].

In the limit of weak disorder in the sense of the Ioffe–Regel criterion, the function $F(k_{\rm F}\ell)$ can be expanded into a power series with respect to the dimensionless parameter $k_{\rm F}\ell$. For simplicity we assume that the Ioffe–Regel condition is realised by the condition $k_{\rm F}\ell \to \infty$. However it should be noted that in real disordered systems the limit $k_{\rm F}\ell \to \infty$ cannot be achieved, because the samples have finite dimensions and therefore the mean free path is always finite, although it may be very large.

Taking into account the limiting case of the Ioffe–Regel condition we obtain the asymptotic form of the relative electrical resistivity as follows:

$$\frac{\Delta\rho}{\rho_{\rm FZ}} \approx 4\frac{(\tau_{\rm FZ}/\tau)}{(k_{\rm F}\ell)^2}\left[\ln(2k_{\rm F}\ell)^2 + \frac{3}{(k_{\rm F}\ell)^2} + \frac{35}{16(k_{\rm F}\ell)^4}\right]. \tag{10}$$

The asymptotic formula differs from the exact results by about $10^{-5} \div 10^{-8}$ in the range $4 < k_F\ell < 10$, which is seen as typical for disordered metallic conductors [12]. In principle, we received the same result as the author of paper [12], i.e. the terms are of the same order with respect to the dimenionless transport parameter $1/(k_F\ell)$, as obtained after the application of the diagrammatic perturbation theory to the solution of the Bethe–Salpeter equation for the probability of the quantum diffusion within the Kubo–Greenwood formula [12]. The only exception is the emergence of the non-singular term $2\ln(k_F\ell)/(k_F\ell)^2$ in the expression for the asymptotic formula for the electrical resistivity given by Eq. (10). It is very likely that this difference is due to the non-perturbative formulation of the MHŠ theory.

4. Conclusions

We have investigated the weak localisation correction due to the quantum interference phenomena to the electrical conductivity derived within the framework of the quantum kinetic theory of the Morgan–Howson–Šaub in the weakly disordered limit of the bulk systems specified by the Ioffe–Regel criterion. We have expressed the electrical resistivity formula in terms of the dimensionless parameter $k_F\ell$ and we have found its asymptotic form in the limit $k_F\ell \to \infty$. The presented result differs from the commonly used expression derived within the diagrammatic method, because it contains an additional non-singular term in the form $2\ln(k_F\ell)/(k_F\ell)^2$ in the considered limit. In real bulk disordered samples the parameter $k_F\ell$ is finite, because the anomalous diffusion processes of the conduction electrons in the limit of the weak disorder are determined by the following length-scale hierarchy in the absence of the dephasing processes: $\lambda_F \ll \ell \ll L$, where λ_F is the Fermi wavelength and L is the size of the sample.

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