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INTERPLAY OF QUANTUM SIZE EFFECT AND SURFACE ELECTRON SCATTERING IN CONDUCTIVITY OF THIN FILMS

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We constructed the most general theory of the classical and quantum static electron transport for 3D films with randomly rough boundaries. The electron-surface interaction was included via approximation with mildly sloping asperities, when the rms height ξ of boundary defects is less than their mean length L. Then we analyzed influence of spatial quantization and electron-surface scattering on the film conductivity $\langle\sigma\rangle$ and their interference. Joint action of those factors leads to peculiarities (sharp dips) of $\langle\sigma\rangle$ versus the sample thickness d appearing at points where a new conducting electron channel opens. The dips have fundamental quantum origin and are caused by size quantization of electron-surface scattering rate. When studying $\langle\sigma\rangle$ versus the bulk mean free path l of electrons, we revealed that, as bulk collisions vanish ($l \to \infty$), the quantum conductivity approaches finite residual value associated with electron-surface interaction. The residual conductivity was first shown to possess either quantum or exclusively classical origin depending on d, l, and the electron wavelength. On the basis of the investigations provided, the relation between quantum and classical effects in the film conductivity was clarified. The theoretical results were successfully tested against recent experimental data concerning the conductivity of ultrathin films.

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1. Introduction

In investigation of conducting electron properties of bounded samples, a problem of size effect is known to arise. In classical systems, this effect mainly consists in a rapid increase in the resistivity as the film thickness d is reduced far below the bulk mean free path l of electrons, which is caused by intensive electron-surface interaction. In ultrathin nearly perfect samples at low temperatures, the discrete character of quasiparticle transverse movement manifests itself. The quantization of electron trajectories qualitatively changes conditions of electron-surface interaction. Therefore, for quantum microstructures, some additional indications of size effect are expected to appear. Thus, the problem of size effect in both classical and quantum approaches is mainly reduced to exploration and description of specific mechanisms of the electron scattering from surface defects.

The most widespread model of boundary defects are asperities — continuously distributed random deviations of the real surface from an ideal crystallographic plane. They are described by two microscopic parameters (rms height ξ and mean length L) and the binary correlation function of their heights. Up to now, both classical and quantum theories of

electron–surface scattering at asperities were predominantly built within the simplest Born approximation, which is based on iterations in small perturbing boundary elevations. To use this approximation, one must satisfy some restrictions, the most uncomfortable of which is the smallness of the Rayleigh parameter: $k_\perp\xi \ll 1$. Here $k_\perp$ is the absolute value of a normal (with respect to the idealized surface) component of the electron wave vector. This yields that the Born method is, in general, justified only for the electrons with small sliding angles with respect to the boundary. To avoid this delimitation, the theory of electron–surface scattering should be built, which would be independent of the Rayleigh parameter $k_\perp\xi$. Such theory was first constructed in Ref. [1]. Its only restriction is the requirement for the small slope of asperities ($\xi/L < 1$). The investigation [2] of well-treated conductor surfaces with a scanning tunneling microscope showed that the sample boundaries actually contained rather smooth asperities with the typical small slope of $\xi/L \approx 10^{-2}$–10^{-4}. This suggests that the model of mildly sloping asperities adequately reflects a profile of a real well-treated boundary.

Unfortunately, the earlier theoretical papers did not completely elucidate an important problem of relation between classical and quantum effects in the conductivity of thin specimens even for the simple Born limit.

Quite general exploration of the classical and quantum static transport in films with mildly sloping surface asperities was first provided in the recent paper [3]. The present contribution introduces principal results concerning interplay of the classical and quantum effects in the conductivity of such microstructures.

2. General classical theory

We derived the most general, for the present time, closed system of equations for the averaged classical static conductivity $\langle\sigma\rangle$ of a plate with randomly rough boundaries (see Ref. [3]). The region of validity for that system is only restricted by the small slope of surface irregularities, i.e.,

$$\xi/L < 1. \qquad (2.1)$$

The averaged classical conductivity was ascertained to be a function of three parameters: d/l, ξ/L, and $k_F L$ (k_F is the Fermi wave number). The general classical formulae are rather cumbersome but admit full numerical analysis. Such analysis disclosed, e.g., the decrease in $\langle\sigma\rangle$ with increasing k_FL. Besides, in plates with large-scale boundary defects, where $k_F L \gtrsim 10$, both the effective electron–surface scattering frequency ν_{surf} and the conductivity are slightly dependent on $k_F L$ at the constant asperity slope ξ/L. Exactly this situation gave the best explanation of recent experimental data [4] dealing with the resistivity of ultrathin ($d \approx 6\times10^{-7}$–10^{-5} cm) epitaxially grown single-crystal films of $CoSi_2$.

3. Small-scale asperities

For films with small-scale boundary asperities, when

$$k_F L < 1, \tag{3.1}$$

we built not only classical but also the most general quantum theory of the conductivity (see Ref. [3]). Therewith we assumed the constant electron concentration and took into account quantization of the electron chemical potential, which leads to its dependence on the sample thickness d. While classical $\langle\sigma\rangle$ is a universal function of the single parameter d/l, the quantum conductivity depends on d and l separately. Comparing the quantum and classical results, we can conclude that the quantum or classical nature of the electron transport in films is, in addition, determined by a method of measuring $\langle\sigma\rangle$, i.e., either it is measured versus the plate thickness d or the electron mean free path l.

The conductivity as a function of l has essentially quantum origin only in ultrathin samples with a small number n_d of conducting electron channels ($n_d < 5$). Starting from $n_d = 5$, the static conductivity is adequately described by the quasiclassical theory and at $n_d \gtrsim 400$ one may use classical results. When bulk collisions vanish ($l \to \infty$), quantum $\langle\sigma\rangle$, unlike the diverging classical conductivity, approaches the finite residual value σ_{res} associated with the electron–surface scattering. Its quasiclassical asymptotics is given by

$$\sigma_{\text{res}} \approx (\pi^2/4)(k_F d/\pi)^2 \sigma_i, \tag{3.2}$$

where $\sigma_i \propto (k_F\xi)^{-2}(k_F L)^{-2}(k_F e^2/\hbar)$ is the "intrinsic" sample conductivity depending on neither d nor l.

As studying the quantum conductivity versus the film thickness d, we revealed peculiarities (sharp dips) appearing at points where a new propagating electron mode opens (see Fig. 1). Those dips have fundamental quantum origin and are provoked by the size quantization of the electron–surface scattering frequency ν_{surf}. Note that similar peculiarities (but of another form) also take place in films with idealized boundaries within the regime of the constant chemical po-

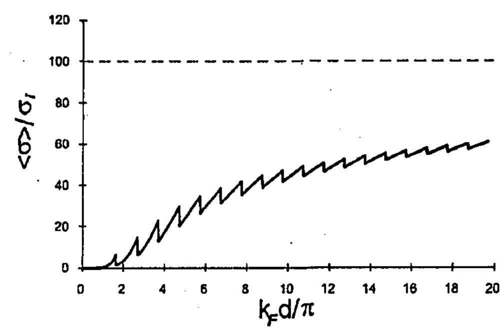

Fig. 1. The quantum conductivity vs. $k_F d/\pi$ at a fixed mean free path l and weak bulk electron scattering as compared to surface one. The dashed line describes the conductivity of a bulk sample.

tential (see, e.g., Ref. [5]). However, in that case the dips are just originated from the quantization of the electron concentration. All this confirms the necessity to account for the electron–surface interaction at the quantum size effect. We emphasize that the classical conductivity does not coincide with the quantum one averaged over the dips. The quantum conductivity always turns out to be less than the classical one for same values of external parameters. This distinction is particularly striking in thin nearly perfect films.

4. Large-scale asperities

The case with large-scale boundary asperities, when

$$k_\mathrm{F} L \gg 1, \tag{4.1}$$

is the most typical of both metals and semiconductors, but is much more complicated to analyze, since the problem of correlations between neighboring collisions of electrons with the surface arises. We demonstrated that the strong correlations are only essential in ultra-quantum films with a few propagating electron modes and constructed the quasiclassical theory of the conductivity (see Ref. [3]). The nonmonotonous dependence of ν_surf on an electron momentum was revealed. This gives rise to competition between the quasiparticles flatly and steeply impinging on the sample surface. If the flatly impinging electrons dominate, the residual conductivity has the quantum origin and is described by the asymptotics

$$\sigma^q_\mathrm{res} \sim (k_\mathrm{F}\xi)^{-2}(k_\mathrm{F}L)^{1/2}(k_\mathrm{F}d/\pi)^2(k_\mathrm{F}e^2/\hbar). \tag{4.2}$$

This type of the residual conductivity can be observed in relatively thick films with $k_\mathrm{F}d/\pi \gg (k_\mathrm{F}L)^{3/2} \gg 1$ at reasonably low temperatures. However, in sufficiently thin films with $k_\mathrm{F}d/\pi \ll (k_\mathrm{F}L)^{3/2}$ the conductivity mainly arises from the steeply impinging particles, for which the size quantization is insignificant. In this case the residual conductivity has the exclusively classical origin and is of the order

$$\sigma^\mathrm{cl}_\mathrm{res} \sim (\xi/L)^{-2}(k_\mathrm{F}d/\pi)(k_\mathrm{F}e^2/\hbar). \tag{4.3}$$

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