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Interference of bulk and boundary scattering in ultrathin quantized systems

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Abstract

Interference of bulk and surface scattering processes is analyzed for ultrathin systems with quantized motion in the direction perpendicular to the walls. The effective relaxation time for scattering by random bulk and surface inhomogeneities is calculated, when possible analytically, beyond the Matthiessen's rule. The applications to the size effect, weak localization, transport along the walls, and boundary slip are discussed.

Keywords: localization; transport; films; surface states

1. Introduction

It is difficult to overestimate the role of boundary scattering in micro- and nanoscale systems. Though the effect of scattering by random surface inhomogeneities on transport and localization properties has been studied in detail, the interference between bulk and boundary scattering processes is often ignored. Recently, we developed a simple transport theory for ballistic particles in ultrathin quantized systems with randomly corrugated walls [1]. This diagrammatic technique can be used to analyze their combined effect of bulk and wall scattering processes on transport and localization. The first results are reported below. We consider the Born approximation for weak boundary scattering and perform the full diagrammatic summation for bulk processes.

It is assumed, often implicitly, that bulk (b) and wall (w) scattering processes are independent from each other and the effective relaxation time is described by the Matthiessen's rule, $1/\tau^{(eff)}$ = $1/\tau^{(b)} + 1/\tau^{(w)}$. In reality, the Matthiessen's rule requires more than a simple independence of individual bulk and surface scattering processes. If the scattering is *weak,* the relaxation is achieved in a series of collisions and the result depends not only on the rate of individual collisions, but also on the correlation (or lack of thereof) of consecutive and/or multiple scattering processes. The multiple wall scattering depends on whether the particle returns to the wall as a result of reflection from the opposite wall or after bulk scattering. Thus, the wall-induced relaxation τ_w itself may depend on bulk processes, $\tau^{(w)} = \tau^{(w)} (\tau^{(b)})$ and the effective relaxation becomes an entangled combination of bulk and boundary scattering processes.

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2. Effective relaxation time

We are interested in ultrathin quantized systems in which the motion in perpendicular to the walls is quantized while the motion along the walls remains quasiclassical. This quantization transforms the bulk spectrum $\epsilon(\mathbf{p})$ into a set of 2D minibands $\epsilon_j(\mathbf{q})$ and all the equations assume the matrix form. The transition probabilities between the states $(j, \mathbf{q}) \rightarrow (j', \mathbf{q}')$ are caused by correlated collisions with walls and bulk scattering. The main term in the diagrammatic expansion for the Green's function leads to the following expression for the effective relaxation time $\tau_j^{(eff)}$ in each miniband:

$$
\frac{1}{\tau_j^{(eff)}} = \frac{1}{\tau_j^{(b)}} +
$$
\n
$$
\sum_{j'=1}^{S} \int \frac{W_{jj'}(\mathbf{q}, \mathbf{q}') \tau_{j'}^{(b)-1}(\mathbf{q}') d\mathbf{q}' / (2\pi)^2}{(\epsilon_{j'}(\mathbf{q}') - \mu)^2 + 1/4\tau_{j'}^{(b)2}(\mathbf{q}')}
$$
\n(1)

where the surface-driven scattering probability [1]

$$
W_{jj'}\left(\mathbf{q},\mathbf{q}'\right) = \pi^4 j^2 j'^2 \zeta\left(\mathbf{q} - \mathbf{q}'\right) / m^2 L^6
$$

and $\zeta(\mathbf{q})$ is the Fourier image of the correlation function of surface inhomogeneities. The difference from the Matthiessen's rule with independent bulk and boundary scattering is clear: the surface scattering term (integral in $Eq.(1)$) contains inside itself the bulk scattering time and, therefore, is different from the "pure" wall relaxation time in ballistic systems. The detailed study of this effect, which has been discussed in the Introduction, is the main result of the paper.

When the bulk mean free path ℓ_b is much larger than the film thickness L or the correlation radius of surface inhomogeneities R , the denominator in Eq.(1) reduces to the δ -function and the wall and boundary scattering become independent and satisfy the Matthiessen's rule.

The deviation from the Matthiessen's rule, which is caused by the interference of bulk and boundary scattering, is noticeable for smaller ℓ_b . We calculated the effective relaxation time analytically in three different situations when $\ell_b \ll R$,

Fig. 1. Deviation from the Matthiessen's rule κ_j , Eq.(2), as a function of the bulk mean free path $x = p_F \ell_b / \hbar$ for three minibands, $j = 1; 16; 31$

when $1/L \gg 1/R$, $1/\ell_b$, and for the single-band occupancy, though the results are too cumbersome to be given here. Elsewhere, the effective relaxation time and the mean free path were calculated numerically. An example of the deviation of the effective relaxation time from the Matthiessen's rule,

$$
\kappa_j = 1 + \left[\frac{1}{\tau_j^{(eff)}} - \frac{1}{\tau_j^{(b)}} - \frac{1}{\tau_j^{(w)}} \right] \tau_j^{(w)}, \qquad (2)
$$

for the Gaussian correlation of surface inhomogeneities with $p_F R/\hbar = 50$, $p_F L/\hbar = 100$ is presented in Figure 1 (p_F is the Fermi momentum, $\tau_j^{(w)}$ is the pure wall-related relaxation time for ballistic particles in miniband j [1]). Note, that the Matthiessen's rule with independent wall and bulk contribution corresponds to $\kappa = 1$; this limit is achieved when $x \equiv p_F \ell_b / \hbar \to \infty$.

Detailed results will be published elsewhere.

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