Phys. Status Solidi B **246**, No. 5, 989–993 (2009) / **DOI** 10.1002/pssb.200881557

physica status solidi b
www.pss-b.com
basic solid state physics

Friedel oscillations in the presence of far from equilibrium heat transport

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Received 25 November 2008, revised 9 January 2009, accepted 10 January 2009
Published online 3 April 2009

PACS 71.45.Lr, 73.63.Nm

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We investigate an inhomogeneous one-dimensional nanosystem coupled to macroscopic leads of different temperatures. In particular, we consider a system with an impurity with on-site scattering potential located in the middle of the nanowire. Such an impurity produces oscillations of the density of carriers in its vicinity, the so-called Friedel oscillations. In the equilibrium case these oscillations are symmetric with respect to the position of the impurity. Here, we demonstrate that strongly asymmetric Friedel oscillations occur if the system is far from the equilibrium. We discuss how this asymmetry depends on the model parameters and the difference of the temperatures of the leads.

1 Introduction As the size of microelectronic devices continues to decrease, the transport properties of nanosystems attract growing interest. This interest is mainly connected to their unique versatility, which results in a wide range of potential applications in, e.g., electronics, photonics and sensor production. The research focuses mainly on transport properties of nanowires, single molecules, carbon nanotubes and quantum dots [1–4]. It is common to these systems that charge carriers are distributed non-uniformly what partially is a result of a large fraction of atoms being located at the system edges. As an example, one may recall standing waves observed at the ends of carbon nanotubes [5]. Another reasons for the inhomogeneous charge distribution can be weak screening of the impurity potential or collective phenomena typical for low-dimensional systems, e.g., the charge density waves. It can also result from a finite bias voltage applied to the nanosystem [1,6,7]. Particularly in the case of nanowires, their properties may be changed significantly by inhomogeneous charge distribution. It has recently been reported for the molecular wires, that even weak diagonal disorder may seriously modify the transport currents [8].

Most of the previous researches on the Friedel oscillations in nanosytems focused on the role of the electron correlations [9–13] in the regime of the linear response to the bias-voltage. It has been demonstrated that the electronic correlations suppress the decay of oscillations [14, 15]. Here, we explore the Friedel oscillations in the far from equilibrium case. Recently, it has been shown within the formalism of the Keldysh Green functions, that finite transport currents may seriously modify the Friedel oscillations [16,17]. For a symmetric coupling between the nanowire and the leads, the wave-length of the oscillations increases with the bias voltage, but the amplitude and the spatial decay exponent of the oscillations remain intact. Similar modification of the density oscillations has been predicted for the charge density waves [18]. For an asymmetric coupling, the Friedel oscillations can either be characterized by a single wave-vector or be a superposition of oscillations with different wave-vectors. In the present paper we extend the previous analysis of the Friedel oscillations and consider the non-equilibrium steady state of a one-dimensional (1D) nanowire that is attached to two macroscopic heat reservoirs of different temperatures. Similarly to a finite bias voltage also a finite difference of temperatures between the electrodes may modify the structure of the Friedel oscillations significantly. In the latter case, the Friedel oscillations may be strongly asymmetric with respect to the position of the impurity. The mechanisms responsible for this asymmetry are discussed in the following sections.

2 Model

2.1 Hamiltonian We investigate a nanowire coupled to two macroscopic leads. Therefore, we consider a Hamiltonian, that consists of three terms $H_{\rm el}$, $H_{\rm nano}$, and $H_{\rm nano-el}$,

which describe the electrodes, nanowire and the coupling between the electrodes and the nanowire, respectively

$$H = H_{\rm el} + H_{\rm nano} + H_{\rm nano-el}. \tag{1}$$

The electrodes are modeled by the electron gas:

$$H_{\rm el} = \sum_{\mathbf{k},\sigma,\alpha} \varepsilon_{\mathbf{k},\alpha} c^{\dagger}_{\mathbf{k}\sigma\alpha} c_{\mathbf{k}\sigma\alpha}, \tag{2}$$

where $\alpha \in \{\mathrm{L,R}\}$ indicates the left or right electrode. $c^{\dagger}_{\mathbf{k}\sigma\alpha}$ creates an electron with momentum $\mathbf{k}$ and spin σ in the electrode α. We assume that the nanowire can be described by the tight-binding Hamiltonian:

$$\mathcal{H}_{\rm nano} = -t \sum_{\langle ij\rangle\sigma} d^{\dagger}_{i\sigma} d_{j\sigma} + U \sum_{\sigma} n_{l\sigma}, \tag{3}$$

where $d^{\dagger}_{i\sigma}$ is the creation operator of an electron with spin σ at site i of the nanosystem, $n_{i\sigma}$ – occupation number operator. In order to investigate the Friedel oscillations we have introduced a single impurity of the potential U. This impurity is located in the site l. The coupling between the nanowire and the leads is given by

$$H_{\rm nano-el} = \sum_{\mathbf{k},i,\alpha,\sigma} \left(g_{\mathbf{k},i,\alpha} c^{\dagger}_{\mathbf{k}\sigma\alpha} d_{i\sigma} + \mathrm{H.c.} \right), \tag{4}$$

where the matrix elements $g_{\mathbf{k},i,\alpha}$ are nonzero only for the edge atoms of the nanowire.

2.2 Calculations scheme The electron density fluctuations have been determined by means of the nonequilibrium Keldysh Green functions. First, we have calculated the local carrier density, that is expressed by the lesser Green function,

$$\langle d^{\dagger}_{i\sigma} d_{i\sigma} \rangle = \frac{1}{2\pi i} \int \mathrm{d}\omega \, G^{<}_{i\sigma,i\sigma}(\omega). \tag{5}$$

$G^{<}_{i\sigma,i\sigma}$ is, in turn, determined by the retarded and advanced Green functions:

$$\hat{G}^{<}(\omega) = i \sum_{\alpha\in\{L,R\}} \hat{G}^{r}(\omega) \hat{\Gamma}_{\alpha}(\omega) \hat{G}^{a}(\omega) f_{\alpha}(\omega), \tag{6}$$

where

$$\left[\hat{\Gamma}_{\alpha}(\omega)\right]_{ij} = 2\pi \sum_{\mathbf{k}} g^{*}_{\mathbf{k},i,\alpha} g_{\mathbf{k},j,\alpha} \delta(\omega - \varepsilon_{\mathbf{k},\alpha}). \tag{7}$$

We have assumed that the energy bands of the leads are wide enough, and one can neglect the frequency dependence of $\hat{\Gamma}_{\alpha}$. The only non-vanishing elements of $\hat{\Gamma}$'s are $[\hat{\Gamma}_L]_{11} = [\hat{\Gamma}_R]_{NN} = \Gamma_0$, where the sites along the chain are enumerated from 1 do N.

To discuss the nonequilibrium situation we have assumed that there is a finite temperature gradient between the electrodes. Namely, we have assumed the temperatures of the left and right electrodes to be $k_B T_L$ and $k_B T_R$, respectively. Consequently, $f_{\alpha}(\omega) = [\exp((\omega - \mu_{\alpha})/k_B T_{\alpha}) + 1]^{-1}$ denotes the Fermi function of the electrode α, where μ_{α} is the chemical potential.

The retarded Green function can be obtained from the following formula:

$$\hat{G}^{r}(\omega) = [\omega \hat{I} - \hat{H} - \hat{\Sigma}^{r}(\omega)]^{-1}, \tag{8}$$

where $\hat{H}$ consists of the matrix elements of $H_{\rm nano}$ and the retarded self-energy is determined by the coupling between the nanowire and the leads

$$\hat{\Sigma}^{r}(\omega) = \frac{1}{2} \sum_{\alpha\in\{L,R\}} \left[\frac{1}{\pi} P \int d\Omega \frac{\hat{\Gamma}_{\alpha}(\Omega)}{\omega - \Omega} - i \hat{\Gamma}_{\alpha}(\omega) \right]. \tag{9}$$

The particle current J_e and the energy flux J_E can be calculated from the time derivative of charge and energy operators, respectively. Since the relation between the thermal J_Q and the energy flux J_E is the following $J_Q = J_E - \mu J_e$ and we do not consider the case of a finite bias voltage V, the chemical potentials of both the leads are zero and the energy flux J_E becomes equivalent to the heat current J_Q. If we express all the currents in terms of Keldysh Green functions, we will come up with the following formulas:

$$J_e = \frac{e}{\hbar} \int \frac{d\omega}{2\pi} \big(f_L(\omega) - f_R(\omega)\big) \times \mathrm{Tr}[\hat{\Gamma}^{L}(\omega) \hat{G}^{R}(\omega) \hat{\Gamma}^{R}(\omega) \hat{G}^{A}(\omega)] \tag{10}$$

$$J_E = \frac{1}{\hbar} \int \frac{d\omega}{2\pi} \omega (f_L(\omega) - f_R(\omega)) \times \mathrm{Tr}[\hat{\Gamma}^{L}(\omega) \hat{G}^{R}(\omega) \hat{\Gamma}^{R}(\omega) \hat{G}^{A}(\omega)] \tag{11}$$

3 Results In order to analyze the structure of the Friedel oscillations we solve Eqs. (5)–(9) for a one-dimensional 129-site chain coupled to leads. We take the nearest-neighbor hopping integral t as the energy unit. As the bias voltage modifies the wave-length of the Friedel oscillations [16] we keep the chemical potential of both the leads equal, $\mu_L = \mu_R = 0$, but the temperatures can be different, i.e., $T_L \neq T_R$. The difference of temperatures may cause, as will be shown below, an asymmetry of the Friedel oscillations. It originates from the fact that wave functions lose their phase coherence due to thermal fluctuations. Consequently, the interference patterns formed by the incoming and outgoing waves, i.e. the Friedel oscillations, are exponentially damped with temperature [15]. As the nanosystem is affected by two heat reservoirs, the damping of the Friedel oscillations may by different in various parts of the nanowire. This can be inferred from Figs. 1–3.

In order to discuss the magnitude of the asymmetry in a quantitative way we have introduced the following measure

$$\delta = |(\delta_L - \delta_R)/(\delta_L + \delta_R)|, \tag{12}$$

where

$$\delta_L = \frac{1}{N_L} | \sum_{j=1}^{l-1} \langle n_{j,\sigma} \rangle \exp(iQj) |, \tag{13}$$

$$\delta_R = \frac{1}{N_R} | \sum_{j=l+1}^{N} \langle n_{j,\sigma} \rangle \exp(iQj) |, \tag{14}$$

where $N_L = N_R$ denote the number of sites on the left and right side of the impurity, respectively, and l denotes the position of the impurity. The introduced quantities δ_L and δ_R are proportional to the average amplitudes of the Friedel oscillations to the left and to the right of the impurity, respectively. Since the system under consideration is close to half-filling, the wave-length of the oscillations is close to two lattice constants and we put $Q = \pi$ in Eqs. 13 and 14. The asymmetry parameter δ is bounded. The upper bound $\delta = 1$ describes the case, when the Friedel oscillations vanish on either side of the impurity ($\delta_L = 0$ or $\delta_R = 0$), whereas the lower bound $\delta = 0$ corresponds to a symmetric charge distribution with $\delta_L = \delta_R$.

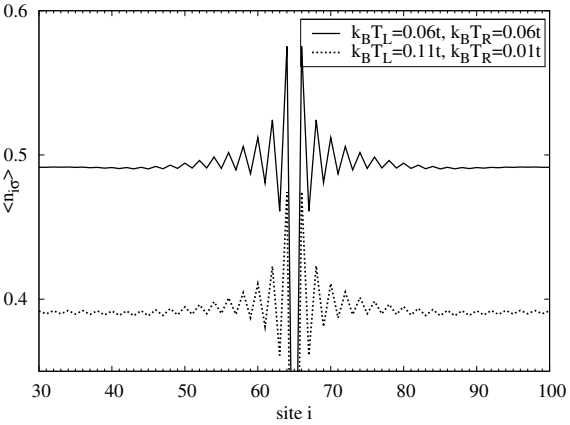

Figure 1 Occupation of sites in the vicinity of the impurity for a 129-site nanowire. The temperatures of the electrodes are indicated in the legend. We have assumed the impurity potential $U = 2t$, the zero bias voltage and the coupling between the nanowire and the electrodes $\Gamma_0 = 0.1$. For the sake of the clarity the curve for the $k_BT_L = 0.11t$ and $k_BT_R = 0.01t$ has been shifted downward by 0.1.

Within the considered model, the asymmetry of the Friedel oscillations originates from different temperatures of the leads. However, it may seriously depend on the impurity potential as well as on the coupling strength between the nanowires and the leads. It follows from the fact that these two parameters strongly influence the energy current caused by a finite temperature bias. First, we try to investigate the role of these parameters separately.

In Fig. 1 we compare the Friedel oscillations obtained in equilibrium and non-equilibrium cases for weak coupling to the leads ($\Gamma_0 = 0.1$) and for a weak impurity

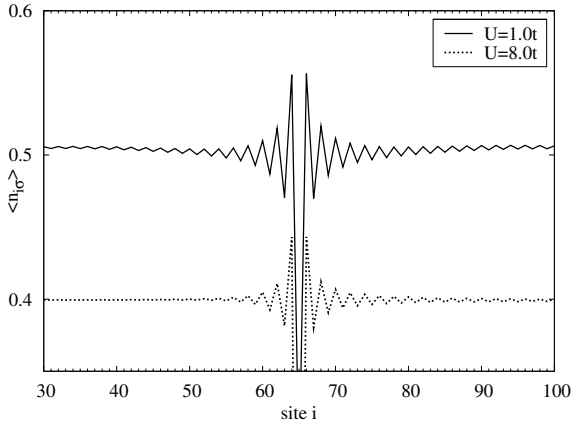

Figure 2 Occupation of sites in the vicinity of the impurity for a 129-site nanowire. The temperatures of the electrodes are $k_BT_L = 0.11t$ and $k_BT_R = 0.01t$. The values of the impurity potential are indicated in the legend. We have assumed $\Gamma_0 = 0.5$ and the zero bias voltage. The curve for the $U = 8.0t$ has been shifted downward by 0.1.

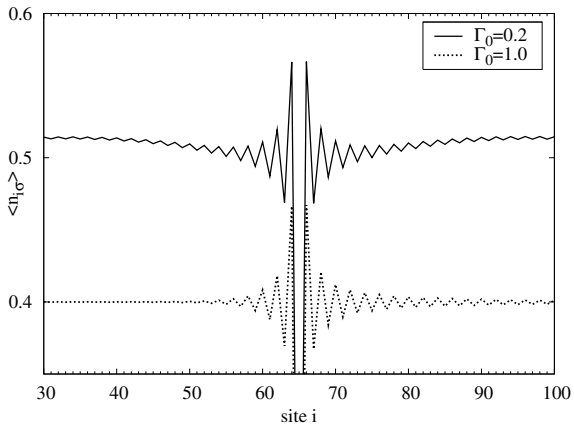

Figure 3 Occupation of sites in the vicinity of the impurity for a 129-site nanowire. The temperatures of the electrodes are $k_BT_L = 0.11t$ and $k_BT_R = 0.01t$. The values of the coupling constant are indicated in the legend. We have assumed the impurity potential $U = 4t$ and the zero bias voltage. The curve for the $\Gamma_0 = 1.0$ has been shifted downward by 0.1.

potential $U = 2t$. Here, the upper curve shows the oscillations for equal temperatures of the leads. For this case we have obtained $\delta_L = \delta_R \simeq 3.6 \cdot 10^{-3}$ and $\delta = 0$. The lower one shows results obtained for the far from equilibrium case, when the temperature of the left lead is one order of magnitude higher than that of the right lead. Here, $\delta_L \simeq 4.25 \cdot 10^{-3}$, $\delta_R \simeq 4.31 \cdot 10^{-3}$ and $\delta = 6.05 \cdot 10^{-3}$. One can see that the Friedel oscillations are fairly symmetric despite far from equilibrium conditions, i.e., the energy current itself is insufficient to produce

asymmetric oscillations. Note that in both cases presented in Fig. 1 the average temperature of the leads is the same $k_B(T_L + T_R)/2 = 0.06t$. However, the oscillations obtained in the non-equilibrium case are more pronounced that those obtained for equilibrium conditions. It may suggest that the energy current enhances the oscillations amplitude, or equivalently, that the amplitude of the oscillations is determined predominantly by the colder lead. A similar result has recently been obtained for the Kondo effect in a quantum dot coupled to leads of different temperatures [19].

Next, we discuss the influence of the impurity potential on the asymmetry. Fig. 2 shows results obtained for $U = t$ and $U = 8t$. In both the cases we have the same non-equilibrium conditions, i.e, $k_BT_L = 0.11$, $k_BT_R = 0.01$. For a weak impurity potential $U = t$ we have found large, fairly symmetric oscillations characterized by $\delta_L \simeq 3.18 \cdot 10^{-3}$, $\delta_R \simeq 3.76 \cdot 10^{-3}$ and $\delta = 8.33 \cdot 10^{-2}$. Contrary to this case, for a strong impurity potential the oscillations become smaller and strongly asymmetric with $\delta_L \simeq 1.70 \cdot 10^{-3}$, $\delta_R \simeq 2.65 \cdot 10^{-3}$ and $\delta = 0.22$. These results clearly indicate that the asymmetry of oscillations and the energy current depend on the impurity potential in opposite ways. Impurities reduce the energy currents and drive the system closer to the equilibrium conditions. In particular, an impurity with infinite potential completely blocks the energy flow. Therefore, such an impurity splits the nanowire into two parts. Each of them is in equilibrium with the lead, that it is attached to. In this case one can straightforwardly define two different temperatures of the left and right parts of the nanowire. Then, the asymmetry of the oscillations becomes obvious since the magnitude of the Friedel oscillations in the equilibrium case decreases with the temperature [15]. Although, this picture explains the origin of asymmetry, it cannot serve as a precise description of the nonequilibrium case. Moreover, this picture may be oversimplified for the description of realistic nanowires since the phonon mechanism of the energy transport is neglected.

Finally, we discuss how the asymmetry of the Friedel oscillations depends on the strength of the coupling between the nanowire and the leads. Fig. 3. shows the Friedel oscillations obtained for relatively weak as well as for a strong coupling. We have found that for $\Gamma_0 = 0.2$ one gets $\delta_L \simeq 3.30 \cdot 10^{-3}$, $\delta_R \simeq 3.6 \cdot 10^{-3}$ and $\delta = 0.48 \cdot 10^{-1}$ whereas for $\Gamma_0 = 1$ one obtains $\delta_L \simeq 2.72 \cdot 10^{-3}$, $\delta_R \simeq 4.56 \cdot 10^{-3}$ and $\delta = 0.25$. Contrary to the case discussed in the previous paragraph, the increase of the coupling strength not only enhances the energy current but also the asymmetry of the Friedel oscillations. One can see that significant asymmetry occurs only for a nanowire that is strongly coupled to the leads.

As expected, the asymmetry of the Friedel oscillations becomes stronger when the difference between the temperatures of the leads increases. However, the role of the remaining parameters, i.e., the coupling strength and the impurity potential, is by far less obvious. In Fig. 4 we present δ as a function of these two parameters, whereas in Fig. 5 we show how these parameters influence the energy current. Comparison of these figures indicates that the largest asymmetry does not occur for the parameters, which maximize the energy flow. The maximal energy current occurs for the conditions when neither the contacts between the nanowire nor the impurity block the energy flow. The strongest asymmetry of the Friedel oscillations takes place when the contacts themselves would enable a significant energy flow, however, this flow is blocked by the impurity.

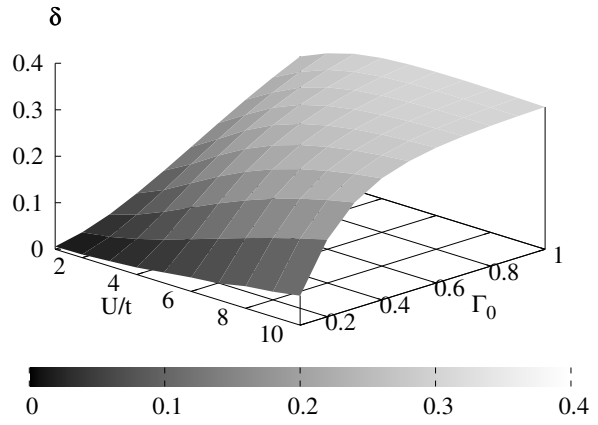

Figure 4 The asymmetry of the occupation of sites (Eq. 12) for a 129-site nanowire as a function of the coupling constant Γ_0 and the impurity potential U. The temperatures of the electrodes are $k_BT_L = 0.11t$ and $k_BT_R = 0.01t$. The bias voltage in the system is zero.

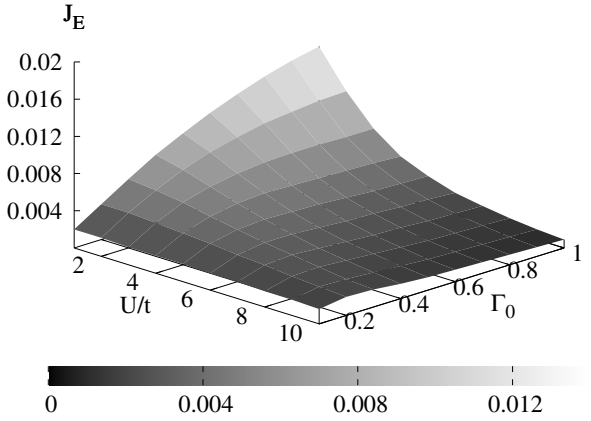

Figure 5 Energy flow Eq. (12) through a 129-site nanowire as a function of the coupling constant Γ_0 and the impurity potential U. The temperatures of the electrodes are $k_BT_L = 0.11t$ and $k_BT_R = 0.01t$.The bias voltage in the system is zero. The energy flow is expressed in $(t^2/\hbar)$ units.

The discussed numerical results have been obtained for $U > 0$. Similar results occur also for negative values of U. This can be easily checked with the help of the particle–hole transformation applied to the Hamiltonian (1).

4 Conclusions To summarize, we have discussed how the energy current caused by a finite temperature bias affects the Friedel oscillations in a nanowire. The presented results combined with those reported in Refs. [16] and [17] show that under nonequilibrium conditions the Friedel oscillations may be modified by various parameters. The resulting profiles of the oscillations depend on the bias voltage, the gradient of the temperature, strength and symmetry of the coupling to the leads. Therefore, the experimental observations of the Friedel oscillations should allow one to get insight into many crucial parameters of the experimental setup.

Acknowledgements This work has been supported by the Polish Ministry of Education and Science under Grant No. 1 P03B 071 30.

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