Physica E 73 (2015) 181–188

Contents lists available at ScienceDirect

Physica E

journal homepage: www.elsevier.com/locate/physe

Fano resonances in high energy electron transport in nanowires of variable cross-section

L.M. Baskin [a], M.M. Kabardov [a,*], N.M. Sharkova [b]

[a] The Bonch-Bruevich Saint Petersburg State University of Telecommunications, 22 - 1 Prospekt Bolshevikov, 193232 Saint-Petersburg, Russia
[b] Saint Petersburg State University, Faculty of Physics, 3 Ulyanovskaya st., 198504 Peterhof, Saint-Petersburg, Russia

HIGHLIGHTS

- An electron wave is scattered into different channels by the resonator openings.
- Some of the channels can be resonant at a given energy.
- Resonances and resonant channels are linked to the closed resonator eigenvalues.
- Resonance parameters can be found even in the case of coinciding resonances.

ARTICLE INFO

Article history:
Received 15 March 2015
Received in revised form
29 May 2015
Accepted 8 June 2015
Available online 11 June 2015

Keywords:
Nanowire
Scattering matrix
Quantum state
Fano resonance
Resonant tunneling

ABSTRACT

Electron ballistic transport in 2D quantum waveguide with two narrowings is considered. For longitudinal electron motion such narrowings play the role of effective potential barriers and conditions for resonant tunneling arise. If the electron energy is sufficiently high the electron wave can scatter into different quantum states (transverse channels of the leads) which results in complicated E-dependence of the scattering amplitudes. Numerical simulations have shown that the scattering amplitudes resonances are of Fano type. The form of the transmission probability curve is conditioned by interference of the quantum states into which the electron wave is scattered by the narrowings. The suggested interference model makes possible to find the resonance parameters with high precision and to link them to the closed resonator eigenvalues.

1. Introduction

Devices based on electron resonant tunneling can be used as field effect transistors [1], resonant tunneling diodes [2], lasers [3], and qubits [4]. Potential barriers forming a quantum resonator are usually produced by dielectric layers or by vacuum intervals between linking electrodes and a resonator (an "electrode – quantum dot – electrode" system). In both cases, incoherent electron scattering by the interfaces essentially decreases the resonator quality factor. However, the role of resonance structure can also be given to a quantum wire of variable cross-section. A waveguide narrowing is an effective potential barrier for longitudinal electron motion along a waveguide. The part of a waveguide between two narrowings becomes a resonator. Due to the absence of interfaces, there is no incoherent electron scattering in such a system. Quantum resonators of that kind can find applications as elements of nanoelectronics devices and provide some advantages in regard to operation properties and production technology.

Asymptotic theory of electron resonant tunneling in three-dimensional quantum waveguides with narrowings was developed in [5]; a ratio of the diameter of a narrowing to that of a waveguide was chosen as a small parameter ε for the asymptotics. Numerical simulation of resonant tunneling in two-dimensional waveguides in comparison with asymptotic description was presented in [6]. The impact of a magnetic field on resonant tunneling was studied in [7,8]. These papers were based on approximate computation of the waveguide scattering matrix and on asymptotic analysis of the electron wave function as $\varepsilon \to 0$. In [9], numerical simulation of electron resonant tunneling was fulfilled by approximate calculation of the waveguide R-matrix in a wide energy range.

In papers [5–8], resonant tunneling was discussed for electrons with energy between the first and the second thresholds, that is, for electrons of small energy. (Recall that the threshold energy values of a waveguide form a positive increasing sequence with limit at $+\infty$.) To analyze possibilities of using waveguides of variable cross-section in nanoelectronics, it is desirable to investigate

* Corresponding author.
E-mail address: kabardov@bk.ru (M.M. Kabardov).

http://dx.doi.org/10.1016/j.physe.2015.06.004
1386-9477/

resonant tunneling in a wider energy range.

The total energy E of an electron moving in a cylindrical waveguide can be represented as $E = E_\perp + E_\parallel$, $E_\perp$ being the (quantized) transverse motion energy and $E_\parallel$ the longitudinal motion energy. In the dimensionless form, $E = k^2$ and $E_\perp(n) = \pi^2 n^2/D^2$, where k is the electron wave number, n is one of the positive integers such that $E_\perp(n) \le E$, and D is the waveguide width (if the waveguide is a strip). The number n is called the electron transverse quantum number and $E_\perp(n)$ is the n-th threshold. We will say that an electron is in the n-state, if its transverse quantum number is equal to n.

In the present paper, we consider multi-channel resonant tunneling. An electron wave of energy E with transverse quantum number n, incident on a resonator, is transmitted through the resonator and arises with transverse number k; shortly, the wave passes from state n to state k. We denote by $T_{nk}(E)$ the transmission coefficient of the wave, calculate the dependence $E \to T_{nk}(E)$ by computing the scattering matrix $S(E)$, and obtain $T_{nk}(E) = |S_{nk}(E)|^2$, where $S_{nk}(E)$ is the entry of $S(E)$. The curve $E \to T_{nk}(E)$ can be quite complicated and not always easily interpreted. To explain the curve, we consider $S_{nk}(E)$ as a probability amplitude and represent it in the form $S_{nk}(E) = \sum_s A_{nsk}(E)$, where $A_{nsk}(E)$ is the probability amplitude of the passage from n to k through an intermediate state s; the summation is over all intermediate states (cf. [10]).

Let $G(\varepsilon_1, \varepsilon_2)$ be a waveguide with two narrowings and let G_0 be the closed resonator, that is, the bounded part of the limit waveguide $G(0, 0)$; generally, the resonator form may be arbitrary. We denote by $k_1^2 \le k_2^2 \le \cdots$ the eigenvalues of the closed resonator. Then the resonant energies of the waveguide $G(\varepsilon_1, \varepsilon_2)$ form the sequence $\mathrm{Re}\, E_1$, $\mathrm{Re}\, E_2$, …, where $E_1, E_2, \ldots$ can be viewed as the "perturbed" $k_1^2, k_2^2, \ldots$ and $\mathrm{Im}\, E_j < 0$ for all $j = 1, 2, \ldots$. The amplitude A_{nsk} admits the representation

$$A_{nsk}(E) = H_{nk}^{(s)}(E) + \frac{R_{nk}^{(s)}(E)}{E - E_s}$$

with continuous functions $E \to H_{nk}^{(s)}(E)$ and $E \to R_{nk}^{(s)}(E)$. In a small neighborhood of $\mathrm{Re}\, E_r$,

$$|S_{nk}(E)|^2 = \left| \sum_s A_{nsk}(E) \right|^2 \approx \left| H_{nk}(E_r) + \frac{R_{nk}(E_r)}{E - E_r} \right|^2 \equiv \mathcal{T}_{nk}(E),$$

where $H_{nk}(E_r)$ and $R_{nk}(E_r)$ are constant. We take the function $\mathcal{T}_{nk}(E)$ as an approximation to the calculated $|S_{nk}(E)|^2$ and find the constants $H_{nk}(E_r)$, $R_{nk}(E_r)$, and E_r by the method of least squares.

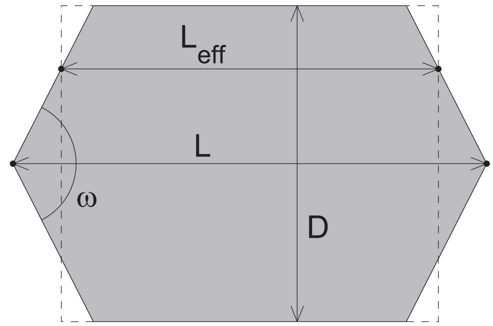


Fig. 1. The resonator.

2. Closed resonator

A necessary condition of electron resonant tunneling consists in proximity of the incident electron energy E to one of the eigenenergies k_{ev}^2 of the closed resonator (Fig. 1). Table 1 shows the calculated values of k_{ev}^2 and the figures of the corresponding eigenfunctions.

For the rectangular resonator with unit width (i.e., $D=1$) and length L,

$$k_{ev}^2 = \pi^2 n^2 + \pi^2 m^2/L^2, \tag{1}$$

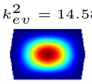
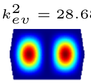
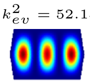
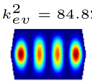
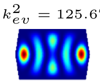
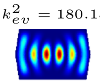
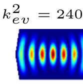
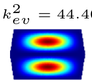
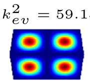
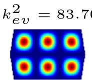
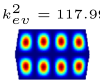
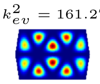
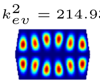
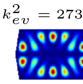
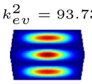
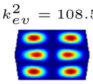
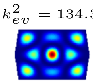
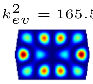
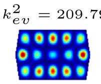
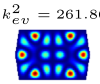
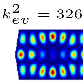
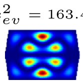
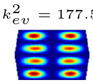
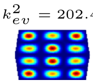
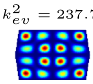
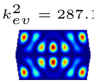
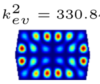
where n and m are transversal and longitudinal quantum numbers. Since the shape of the resonator is close to rectangular, the eigenvalues are well approximated by the expression (1) with L replaced by L_{eff}. For the resonator with angle $\omega = 0.9\pi$ at the vertex and with length $L=1.5$, the value of L_{eff} is approximately equal to 1.45 for $n=1$ and to 1.42 for $n > 1$.

The disparity between the calculated eigenvalues and approximations by formula (1) is less than 0.5%. Note that such an accuracy is achieved in spite of the significant difference between the considered eigenfunctions and those for the rectangular resonator (see the figures in Table 1).

3. The method for computing scattering matrix

We now describe a calculation scheme for a scattering matrix based on the method presented in [11]. The energy E of an electron moving in a cylindrical waveguide can be represented in the form $E = E_\perp + E_\parallel$, where $E_\perp$ and $E_\parallel$ are transversal and longitudinal components, respectively. The values of $E_\perp$ are quantized. In the sim-

Table 1
Eigenvalues and eigenfunctions of the closed resonator.

n \ m	1	2	3	4	5	6	7
1	$k_{ev}^2 = 14.58$ 	$k_{ev}^2 = 28.68$ 	$k_{ev}^2 = 52.15$ 	$k_{ev}^2 = 84.82$ 	$k_{ev}^2 = 125.67$ 	$k_{ev}^2 = 180.15$ 	$k_{ev}^2 = 240.35$ 
2	$k_{ev}^2 = 44.40$ 	$k_{ev}^2 = 59.15$ 	$k_{ev}^2 = 83.70$ 	$k_{ev}^2 = 117.99$ 	$k_{ev}^2 = 161.27$ 	$k_{ev}^2 = 214.93$ 	$k_{ev}^2 = 273.27$ 
3	$k_{ev}^2 = 93.73$ 	$k_{ev}^2 = 108.57$ 	$k_{ev}^2 = 134.34$ 	$k_{ev}^2 = 165.50$ 	$k_{ev}^2 = 209.79$ 	$k_{ev}^2 = 261.86$ 	$k_{ev}^2 = 326.44$ 
4	$k_{ev}^2 = 163.46$ 	$k_{ev}^2 = 177.58$ 	$k_{ev}^2 = 202.42$ 	$k_{ev}^2 = 237.73$ 	$k_{ev}^2 = 287.10$ 	$k_{ev}^2 = 330.84$ 	$k_{ev}^2 > 370$