JYVÄSKYLÄ STUDIES IN COMPUTING
160

Muaed Kabardov

Asymptotic and Numerical Studies of Electron Scattering in 2D Quantum Waveguides of Variable Cross-Section

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ABSTRACT

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We consider an infinite two-dimensional waveguide that far from the coordinate origin coincides with a strip. The waveguide has two narrows which play the role of effective potential barriers for the longitudinal electron motion. The part of waveguide between the narrows becomes a "resonator" and there arise conditions for electron resonant tunneling.

A magnetic field in the resonator can change the basic characteristics of this phenomenon. In the presence of a magnetic field, the tunneling phenomenon is feasible for producing spin-polarized electron flows consisting of electrons with spins of the same direction.

Taking the narrows diameter as a small parameter, we derive asymptotics for the resonant tunneling characteristics. The asymptotic formulas contain some unknown constants. We find them by solving several auxiliary boundary value problems in unbounded domains. Independently, we compute numerically the scattering matrix and compare the asymptotic and numerical results.

The operation of the resonator systems discussed before has been analyzed under the assumption that the electron energy lies between the first and the second thresholds. This condition not always can be fulfilled by modern technologies. We analyze some properties of multichannel scattering in the situation where the electron energy exceeds the second threshold.

Keywords: quantum waveguide, tunneling, resonance, spin, polarization, magnetic field, potential barrier, scattering matrix

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1 INTRODUCTION

At present the electron tunneling is being studied intensively in the systems "metallic electrode–quantum dot–metallic electrode" (e.g., see [1], [2]). A quantum dot (a conductive domain of diameter about 10 nm) is separated from the electrodes by "tunnel" intervals (vacuum gaps or dielectric layers). Due to resonant tunneling, the conductivity of the system can abruptly vary with voltage between the electrodes. There are prospects for building new nanosize electronics elements (transistors, electron energy monochromators etc.) that are based on the mentioned quantum dot systems and have frequency operating range around 10^{12}Hz. However, the tunneling probability heavily depends on inevitable electron scattering by inhomogeneities of the interfaces electrode–vacuum and quantum dot–vacuum. Therefore the production of the systems must satisfy not easily accessible accuracy conditions.

The role of resonant structures can be given to quantum wires. Instead of a system "electrode – quantum dot – electrode" one can use a quantum wire (two- or three-dimensional) with two narrows. The narrows prove to be effective potential barriers for the longitudinal electron motion and the part of the waveguide between two narrows becomes a "resonator". The fact that in such conditions resonant tunneling can occur is confirmed by numerical experiments [3], [4]. Resonant devices based on quantum wires can provide some advantages in regard to both operation properties and production technology. Such devices are homogeneous (i.e., are made of one material); when tunneling, an electron crosses no interfaces of electrodes, dielectrics, or vacuum. Therefore the operation of the devices is more stable under small perturbations of its geometry.

In [5], electron propagation was considered in a 3D waveguide with two cylindrical outlets to infinity and two narrows of small diameter ε. There were considered electrons with energy between the first and the second thresholds. For the main characteristics of resonant tunneling (electron wave function, resonant energy E_{res}, transition coefficient $T(E)$ etc.) there were obtained asymptotic formulas and estimates for the remainders as $\varepsilon \to 0$. It was assumed, that the limit waveguide in a neighborhood of each narrow coincided with two cones intersecting only at their common vertex. To construct the asymptotics the method of "compound" asymptotic expansions (the general theory of which was exposed, e.g., in [6]) was applied.

The asymptotic formulas in [5] include several unknown constant coefficients; the issue of calculation of them was not discussed. Without numerical values of the constants, the asymptotic formulas provide only a qualitative picture. When the constants are found, the asymptotics can be used as an approximate solution. It remains vague, for what band of parameters the approximation is reliable. On the other hand, one should expect numerical approach to be efficient only if the waveguide narrows are not too small in diameter, and the resonant peak of the transition coefficient is sufficiently wide. Therefore a detailed picture of resonant tunneling can be achieved when the asymptotic and numerical approaches are combined. We suggest a methodology of such a combined approach and show its application in concrete situations. In particular, we answer the questions mentioned in this paragraph.

We consider a 2D waveguide with two narrows of the same diameter ε. Independently of the article [5], we describe a new way of derivation of asymptotic formulas, which is simpler and more universal than that in [5]; it is also based on the method of compound asymptotic expansions (and can be applied to 3D waveguide). The new derivation is mainly used here to give the background of boundary value problems needed for calculation of the unknown constants in the asymptotics. These BVPs are solved numerically. Besides, independently of asymptotic approach, we approximately calculate the waveguide scattering matrix by the method from [7]. After that we can compare the asymptotics with calculated constants and the scattering matrix (the transition and reflection coefficients). It turns out, that there is an interval of values of ε, where the asymptotic and numerical results practically coincide. If ε goes outside the interval to the right, the asymptotics ceases to work, but the numerical method for calculation of the scattering matrix keeps efficient; if ε goes to the left of the interval, the numerical method becomes ill-conditioned, and the asymptotics remains reliable.

The presence of a magnetic field can essentially affect the basic characteristics of the resonant tunneling and bring new possibilities for applications in electronics. In particular, in the presence of a magnetic field, the tunneling phenomenon is feasible for producing spin-polarized electron flows consisting of electrons with spins of the same direction. We suppose that a part of the resonator is occupied by a homogeneous magnetic field. An electron wave function satisfies the Pauli equation in the waveguide and vanishes at its boundary (the work function of the waveguide is supposed to be sufficiently large, so that the boundary condition is justified). Moreover, we assume that only one incoming wave and one outgoing wave can propagate in each outlet of the waveguide. In other words, we do not discuss multichannel electron scattering and consider only electrons with energy between the first and the second thresholds. We take ε as small parameter and obtain asymptotic formulas for the aforementioned characteristics of the resonant tunneling as $\varepsilon \to 0$. The formulas depend on the limiting form of the narrows. We suppose that, in a neighborhood of each narrow, the limiting waveguide coincides with a pair of opposite angles.

As before, the asymptotic formulas contain some unknown constants. To find them, we numerically solve several boundary value problems in unbounded domains independent of ε. After that we compare the asymptotic and numerical results. We show that there is a band of ε where the results of the two approahes practically coincide.

The operation of the resonator systems discussed before has been analyzed under the assumption that the electron energy lies between the first and the second thresholds. This condition not always can be fulfilled by modern technologies. In Chapter 4 we consider some properties of multichannel scattering in the situation where the electron energy can be between the second and the fifth thresholds. These considerations show that in designing electronic devices based on the resonant tunneling in quantum waveguides of variable cross-section, it is reasonable to choose the system parameters so that electron energies do not exceed the third threshold. Some of the effects discussed in Chapter 4 have been studied by the authors of [8, 9] where they numerically analyze multichannel scattering in cylindric heterostructures. The waveguide we are studying differs from that used in [8, 9]. Also, the authors of [8, 9] do not give physical interpretation of the effects that the numerical simulation shows. In Chapter 4 we give explanations of physical phenomena coming along with multichannel scattering.

In Chapter 2 we carry out asymptotic and numerical analysis of resonant tunneling in one-channel regime, i.e. the electron energy is assumed to be between the first and the second thresholds. We study the behavior of the characteristics of the process as $\varepsilon \to 0$ in a neighborhood of one of the resonant energies. We find the range of efficiency of the asymptotic formulas by comparing it to the scattering matrix numerically found by the method in [7]. The mathematical model of the waveguide and statement of the problem are given in Section 2.1. The boundary value problems needed for the method of compound asymptotic expansions are discussed in Sections 2.2 and 2.3. We derive the asymptotics in Section 2.4 and justify the formulas in Section 2.5. Section 2.6 is devoted to numerical analysis and comparing numerical and asymptotic results.

In Chapter 3 we study the characteristics of electron flow in the presence of magnetic field. The analysis is carried out in the same way as in Chapter 2. The presence of the magnetic field changes the behavior of the asymptotic and numerical results and their proximity, though the disparities between the two approaches seen in the Chapters 2 and 3 are caused also by different openings ($\omega = 0.5\pi$ in Chapter 2 and $\omega = 0.9\pi$ in Chapter 3). The mathematical model of the waveguide and statement of the problem are in Section 3.1. The boundary value problems needed for the method of compound asymptotic expansions are discussed in Sections 3.2 and 3.3. The asymptotics derivation is given in Section 3.4 and justification of the formulas are in Section 3.5. Section 3.6 is devoted to numerical analysis and to comparison of numerical and asymptotic results.

Chapter 4 is devoted to the analysis of the same problem as in Chapter 2, but here we study multichannel scattering. We do not consider the dependence of the electron flow characteristics on the narrows diameters. On the contrary, the waveguide geometry is constant. We analyze the behavior of the transversal states of the wave function with respect to increasing electron energy and the correspondence between the waveguide resonant energies and the closed resonator eigenvalues. Section 4.1 gives some backgrounds on the problem. Section 4.2 contains the closed resonator eigenvalues and eigenfunctions which can be regarded as approximations to the corresponding values of the open resonator. The method used for calculation of the scattering matrix is described in Section 4.3. Finally, we discuss some facts which follow from the results of numerical simulations in Section 4.4.

Appendices 1 and 2 contain the description of FEM used in simulations. The computations were carried out in the environments MATLAB and COMSOL, which also have short introductions to FEM and other numerical methods mentioned in the appendices.

The results of the thesis were published as preprints in [10, 11, 12] and some results of Chapter 3 were reported to ECCOMAS [13] held in Vienna, 2012.

2 ASYMPTOTIC AND NUMERICAL STUDIES OF RESONANT TUNNELING

A waveguide coincides with a strip having two narrows of diameter ε. Electron motion is described by the Helmholtz equation with Dirichlet boundary condition. The part of the waveguide between the narrows plays the role of resonator and there can occur electron resonant tunneling. This phenomenon consists in the fact that, for an electron with energy E, the probability $T(E)$ to pass from one part of the waveguide to the other part through the resonator has a sharp peak at $E = E_{res}$, where E_{res} denotes a "resonant" energy. To analyze operation of electronic devices based on the phenomenon of resonant tunneling, it is important to know E_{res} and behavior of $T(E)$ for E close to E_{res}. In this section asymptotic formulas for resonant energy and the coefficients of transition and reflection for $\varepsilon \to 0$ are obtained. Such formulas depend on the limit shape of the narrows; we assume, that the limit waveguide in the neighborhood of each narrow coincides with a pair of vertical angles. Asymptotic results are compared with the corresponding numerical ones obtained by approximate computing the waveguide scattering matrix. This allows to determine the band of ε where the asymptotics and numerical results are in close agreement. The suggested methods are applicable to much more complicated models than that considered here. In particular, the same approach will work for asymptotic and numerical analysis of resonant tunneling in 3D quantum waveguides.

2.1 Statement of the problem

To describe the domain $G(\varepsilon)$ in $\mathbb{R}^2$ occupied by the waveguide, we first introduce two auxiliary domains G and Ω in $\mathbb{R}^2$. The domain G is the strip

$$G = \mathbb{R} \times D = \{(x, y) \in \mathbb{R}^2 : x \in \mathbb{R} = (-\infty, +\infty); y \in D = (-l/2, l/2)\}.$$

Let us define Ω. Denote by K a double cone with vertex at the origin O that contains the x-axis and is symmetric about the coordinate axes. The set $K \cap S^1$,

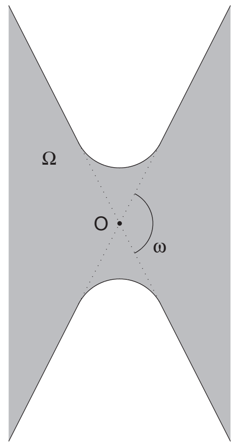


FIGURE 1 The set Ω.

where S^1 is a unit circle, consists of two simple arcs. Assume that Ω contains the cone K and a neighborhood of its vertex; moreover, outside a large disk (centered at the origin) Ω coincides with K. The boundary $\partial\Omega$ of Ω is supposed to be smooth (see Figure 1).

We now turn to the waveguide $G(\varepsilon)$. Denote by $\Omega(\varepsilon)$ the domain obtained from Ω by the contraction with center at O and coefficient ε. In other words, $(x, y) \in \Omega(\varepsilon)$ if and only if $(x/\varepsilon, y/\varepsilon) \in \Omega$. Let K_j and $\Omega_j(\varepsilon)$ stand for K and $\Omega(\varepsilon)$ shifted by the vector $\mathbf{r}_j = (x_j^0, 0)$, $j = 1, 2$. We assume that $|x_1^0 - x_2^0|$ is sufficiently large so the distance from $\partial K_1 \cap \partial K_2$ to G is positive. We put (see Figure 2)

$$G(\varepsilon) = G \cap \Omega_1(\varepsilon) \cap \Omega_2(\varepsilon).$$

The wave function of a free electron of energy k^2 satisfies the boundary value problem

$$\begin{aligned} \Delta u(x, y) + k^2 u(x, y) &= 0, \qquad (x, y) \in G(\varepsilon), \\ u(x, y) &= 0, \qquad (x, y) \in \partial G(\varepsilon). \end{aligned} \tag{2.1.1}$$

Moreover, u is subject to radiation conditions at infinity. To formulate the conditions we need the problem

$$\begin{aligned} \Delta v(y) + \lambda^2 v(y) &= 0, \qquad y \in D, \\ v(-l/2) = v(l/2) &= 0. \end{aligned} \tag{2.1.2}$$

The eigenvalues λ_q^2 of this problem, where $q = 1, 2, \ldots$ are called the thresholds; they form the sequence $\lambda_q^2 = (\pi q/l)^2$, $q = 1, 2, \ldots$. We suppose that k^2 in (2.1.1) is not a threshold. Given a real k, there exist finitely many linearly independent bounded wave functions. In the linear space spanned by such functions, a basis

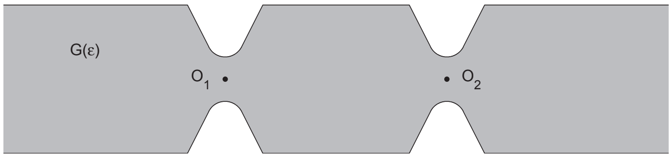


FIGURE 2 The waveguide $G(\varepsilon)$.

is formed by the wave functions subject to the radiation conditions

$$u_m(x,y) = \begin{cases} e^{i\nu_m x}\Psi_m(y) + \sum_{j=1}^{M} s_{mj}(k)\, e^{-i\nu_j x}\Psi_j(y) + O(e^{\delta x}), & x \to -\infty, \\ \sum_{j=1}^{M} s_{m,M+j}(k)\, e^{i\nu_j x}\Psi_j(y) + O(e^{-\delta x}), & x \to +\infty; \end{cases} \tag{2.1.3}$$

$$u_{M+m}(x,y) = \begin{cases} \sum_{j=1}^{M} s_{M+m,j}(k)\, e^{-i\nu_j x}\Psi_j(y) + O(e^{\delta x}), & x \to -\infty, \\ e^{-i\nu_m x}\Psi_m(y) + \\ \quad + \sum_{j=1}^{M} s_{M+m,M+j}(k)\, e^{i\nu_j x}\Psi_j(y) + O(e^{-\delta x}), & x \to +\infty; \end{cases}$$

Here M is the number of the thresholds satisfying $\lambda^2 < k^2$; $\nu_m = \sqrt{k^2 - \lambda_m^2}$; Ψ_m is an eigenfunction of the problem (2.1.2) that corresponds to the eigenvalue λ_m^2,

$$\Psi_m(y) = \begin{cases} \sqrt{2/l\nu_m}\,\sin\lambda_m y, & m \text{ even}, \\ \sqrt{2/l\nu_m}\,\cos\lambda_m y, & m \text{ odd}, \qquad m = 1,2,\dots,M. \end{cases} \tag{2.1.4}$$

In the strip G the function $U_j(x,y) = e^{i\nu_j x}\Psi_j(y),\ j = 1,\dots,M$, is a wave incoming from $-\infty$ and outgoing to $+\infty$, while $U_{M+j}(x,y) = e^{-i\nu_j x}\Psi_j(y)$ is a wave going from $+\infty$ to $-\infty$. The matrix

$$S = \|s_{mj}\|_{m,j=1,\dots,2M}$$

with entries from the conditions (2.1.3) is called the scattering matrix; it is unitary. The values

$$R_m = \sum_{j=1}^{M} |s_{mj}|^2, \qquad T_m = \sum_{j=1}^{M} |s_{m,\,M+j}|^2$$

are called the reflection and transition coefficients, relatively, for the wave U_m incoming to $G(\varepsilon)$ from $-\infty$, $m = 1,\dots,M$. (Similar definitions can be given for the wave U_{M+m} incoming from $+\infty$.)

In the present work we will discuss only the case $(\pi/l)^2 < k^2 < (2\pi/l)^2$, i.e. k^2 is between the first and the second thresholds. Then the scattering matrix is of size 2×2. We consider only the scattering of the wave incoming from $-\infty$ and denote the reflection and transition coefficients as

$$R = R(k,\varepsilon) = |s_{11}(k,\varepsilon)|^2, \qquad T = T(k,\varepsilon) = |s_{12}(k,\varepsilon)|^2. \tag{2.1.5}$$

The goal is to find a "resonant" value $k_r = k_r(\varepsilon)$ of the parameter k corresponding to the maximum of the transition coefficient, and to describe the behavior of $T(k,\varepsilon)$ for k in a neighborhood of $k_r(\varepsilon)$ as $\varepsilon \to 0$.

2.2 Limit problems

We derive the asymptotics of the wave function (i.e. the solution of the problem (2.1.1) as $\varepsilon \to 0$) by use of the method of compound asymptotic expansions. To this end we introduce "limit" boundary value problems independent of the parameter ε.

2.2.1 First kind limit problems

Put $G(0) = G \cap K_1 \cap K_2$ (Figure 3); thus, $G(0)$ consists of three parts G_1, G_2, and G_3, where G_1 and G_3 are infinite domains while G_2 is a bounded resonator. The problems

$$\begin{aligned} \Delta v(x,y) + k^2 v(x,y) &= f, \qquad (x,y) \in G_j, \\ v(x,y) &= 0, \qquad (x,y) \in \partial G_j, \end{aligned} \tag{2.2.1}$$

where $j = 1,2,3$, are called the first kind limit problems.

Introduce function spaces for the problem (2.2.1) in G_2. Let ϕ_1 and ϕ_2 be smooth real functions in the closure $\overline{G}_2$ of G_2 such that $\phi_j = 1$ in a neighborhood of O_j, $j = 1,2$, and $\phi_1^2 + \phi_2^2 = 1$. For $l = 0,1,\dots$ and $\gamma \in \mathbb{R}$ the space $V^l_\gamma(G_2)$ is the completion in the norm

$$\|v; V^l_\gamma(G_2)\| = \left(\int_{G_2} \sum_{|\alpha|=0}^{l} \sum_{j=1}^{2} \phi_j^2(x,y) r_j^{2(\gamma - l + |\alpha|)} |\partial^\alpha v(x,y)|^2 \, dx\, dy \right)^{1/2} \tag{2.2.2}$$

of the set of smooth functions in $\overline{G}_2$ which vanish near O_1 and O_2; here r_j is the distance between (x,y) and O_j, $\alpha = (\alpha_1, \alpha_2)$ is a multi-index, and

$$\partial^\alpha = \frac{\partial^{|\alpha|}}{\partial x^{\alpha_1} \partial y^{\alpha_2}}.$$

Proposition 2.2.1 follows from well known general results, e.g. see [14, Chapters 2 and 4, §§1–3] or [6, v. 1, Chapter 1].

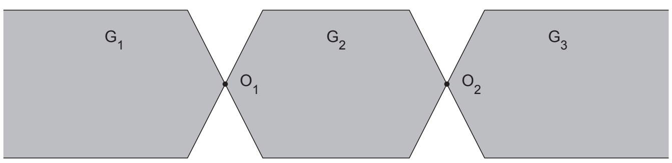


FIGURE 3 The domain $G(0)$.

Proposition 2.2.1. *Assume that $|\gamma - 1| < \pi/\omega$. Then for every $f \in V^0_\gamma(G_2)$ and any k^2 except the positive increasing sequence $\{k^2_p\}_{p=1}^\infty$ of eigenvalues, $k^2_p \to \infty$, there exists a unique solution $v \in V^2_\gamma(G_2)$ to the problem* (2.2.1) *in G_2. The estimate*

$$\|v; V^2_\gamma(G_2)\| \leq c\,\|f; V^0_\gamma(G_2)\| \tag{2.2.3}$$

holds with a constant c independent of f. If f is a smooth function in $\overline{G}_2$ vanishing near O_1 and O_2, and v is any solution in $V^2_\gamma(G_2)$ of the problem (2.2.1)*, then v is smooth in $\overline{G}_2$ except at O_1 and O_2, and admits the asymptotic representation*

$$v(x,y) = \begin{cases} b_1 \widetilde{J}_{\pi/\omega}(kr_1)\Phi(\varphi_1) + O\big(r_1^{2\pi/\omega}\big), & r_1 \to 0; \\ b_2 \widetilde{J}_{\pi/\omega}(kr_2)\Phi(\pi - \varphi_2) + O\big(r_2^{2\pi/\omega}\big), & r_2 \to 0 \end{cases}$$

near the points O_1 and O_2, where (r_j, φ_j) are polar coordinates with center at O_j, b_j are some constant coefficients, $\widetilde{J}_\mu$ stands for the Bessel function multiplied by a constant so that $\widetilde{J}_\mu(kr) = r^\mu + o(r^\mu)$, and $\Phi(\varphi) = \pi^{-1/2}\cos(\pi\varphi/\omega)$.

If $k^2 = k^2_0$ is an eigenvalue of problem (2.2.1)*, then the problem* (2.2.1) *is solvable in G_2 if and only if $(f, v_0)_{G_2} = 0$ for any eigenfunction v_0 corresponding to k^2_0. The condition being fulfilled, there exists a unique solution v to the problem* (2.2.1) *which is orthogonal to the eigenfunctions and satisfies* (2.2.3) *(i.e. the Fredholm alternative holds).*

We turn to the problems (2.2.1) for $j = 1, 3$. Let $\chi_{0,j}$ and $\chi_{\infty,j}$ be smooth real functions in the closure $\overline{G}_j$ of G_j such that $\chi_{0,j} = 1$ in a neighborhood of O_j, $\chi_{0,j} = 0$ outside of a compact set, and $\chi^2_{0,j} + \chi^2_{\infty,j} = 1$. We also assume that the support $\operatorname{supp}\chi_{\infty,j}$ is located in the cylindrical part of G_j. For $\gamma \in \mathbb{R}$, $\delta > 0$, and $l = 0, 1, \dots$ the space $V^l_{\gamma,\delta}(G_j)$ is the completion in the norm

$$\|v; V^l_{\gamma,\delta}(G_j)\| = \left(\int_{G_j} \sum_{|\alpha|=0}^{l} \big(\chi^2_{0,j} r_j^{2(\gamma - l + |\alpha|)} + \chi^2_{\infty,j}\exp(2\delta x)\big) |\partial^\alpha v|^2 \, dx\, dy \right)^{1/2} \tag{2.2.4}$$

of the set of smooth functions in $\overline{G}_j$ having compact supports and vanishing near O_j.

Recall that according to our assumption, k^2 lies between the first and the second thresholds, so in every G_j there is only one outgoing wave. Let $U^-_1 = U_2$ be the outgoing wave in G_1, and let $U^-_2 = U_1$ be the outgoing wave in G_3 (the definition of U_j in G see in Section 2.1). The next proposition follows, e.g., from [14, Theorem 5.3.5].

Proposition 2.2.2. *Let $|\gamma - 1| < \pi/\omega$ and suppose that there is no nontrivial solution to the homogeneous problem* (2.2.1) *(where $f = 0$) in $V^2_{\gamma,\delta}(G_j)$ with arbitrary small positive δ. Then for any $f \in V^0_{\gamma,\delta}(G_j)$ there exists a unique solution v to the problem* (2.2.1) *that admits the representation*

$$v = u + A_j \chi_{\infty,j} U^-_j,$$

where $A_j = const$, $u \in V^2_{\gamma,\delta}(G_j)$, and δ is sufficiently small. Furthermore, the inequality

$$\|u; V^2_{\gamma,\delta}(G_j)\| + |A_j| \le c\,\|f; V^0_{\gamma,\delta}(G_j)\| \tag{2.2.5}$$

holds with constant c independent of f. If the function f is smooth and vanishes near O_j, then the solution v in G_1 admits the representation

$$v(x,y) = a_1 \widetilde{J}_{\pi/\omega}(kr_1)\Phi(\pi - \varphi_1) + O\big(r_1^{2\pi/\omega}\big), \quad r_1 \to 0,$$

and the solution in G_3 admits the representation

$$v(x,y) = a_2 \widetilde{J}_{\pi/\omega}(kr_2)\Phi(\varphi_2) + O\big(r_2^{2\pi/\omega}\big), \quad r_2 \to 0,$$

where a_j are some constants.

2.2.2 Second kind limit problems

In the domains Ω_j, $j = 1, 2$, introduced in Section 2.1, we consider the boundary value problems

$$\begin{aligned} \Delta w(\xi_j, \eta_j) &= F(\xi_j, \eta_j), & (\xi_j, \eta_j) &\in \Omega_j, \\ w(\xi_j, \eta_j) &= 0, & (\xi_j, \eta_j) &\in \partial\Omega_j, \end{aligned} \tag{2.2.6}$$

which are called the second kind limit problems; (ξ_j, η_j) are Cartesian coordinates with origin at O_j.

Let $\rho_j = \operatorname{dist}((\xi_j, \eta_j), O_j)$ and let $\psi_{0,j}$, $\psi_{\infty,j}$ be smooth real functions in $\overline{\Omega}_j$ such that $\psi_{0,j} = 1$ for $\rho_j < N/2$, $\psi_{0,j} = 0$ for $\rho_j > N$, and $\psi^2_{0,j} + \psi^2_{\infty,j} = 1$, N being a sufficiently large positive number. For $\gamma \in \mathbb{R}$ and $l = 0, 1, \dots$ the space $V^l_\gamma(\Omega_j)$ is the completion in the norm

$$\|v; V^l_\gamma(\Omega_j)\| = \left(\int_{\Omega_j} \mathcal{S}(v)\, d\xi_j d\eta_j \right)^{1/2} \tag{2.2.7}$$

of the set $C^\infty_c(\overline{\Omega}_j)$ of compactly supported in $\overline{\Omega}_j$ smooth functions; here

$$\mathcal{S}(v) := \sum_{|\alpha|=0}^{l} \Big(\psi_{0,j}(\xi_j, \eta_j)^2 + \psi_{\infty,j}(\xi_j, \eta_j)^2 \rho_j^{2(\gamma - l + |\alpha|)} \Big) |\partial^\alpha v(\xi_j, \eta_j)|^2.$$

The next proposition is a corollary of [14, Theorem 4.3.6].

Proposition 2.2.3. *Let $|\gamma - 1| < \pi/\omega$. Then for every $F \in V^0_\gamma(\Omega_j)$ there exists a unique solution $w \in V^2_\gamma(\Omega_j)$ to the problem* (2.2.6) *and*

$$\|w; V^2_\gamma(\Omega_j)\| \le c\,\|F; V^0_\gamma(\Omega_j)\| \tag{2.2.8}$$

holds with a constant c independent of F. If $F \in C^\infty_c(\overline{\Omega}_j)$, then w is smooth in $\overline{\Omega}_j$ and admits the representation

$$w(\xi_j, \eta_j) = \begin{cases} \alpha_j \rho_j^{-\pi/\omega} \Phi(\pi - \varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j < 0, \\ \beta_j \rho_j^{-\pi/\omega} \Phi(\varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j > 0, \end{cases} \tag{2.2.9}$$

as $\rho_j \to \infty$; here (ρ_j, φ_j) are polar coordinates in Ω_j with center at O_j, and function Φ is the same as in Proposition 2.2.1*. The constant coefficients α_j and β_j are defined by*

$$\alpha_j = -(F, w_j^l)_\Omega, \qquad \beta_j = -(F, w_j^r)_\Omega,$$

where w_j^l and w_j^r are unique solutions to the homogeneous problem (2.2.6) *such that, as $\rho_j \to \infty$,*

$$w_j^l = \begin{cases} \left(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}\right)\Phi(\pi - \varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j < 0; \\ \beta\rho_j^{-\pi/\omega}\Phi(\varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j > 0; \end{cases} \tag{2.2.10}$$

$$w_j^r = \begin{cases} \beta\rho_j^{-\pi/\omega}\Phi(\pi - \varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j < 0; \\ \left(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}\right)\Phi(\varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j > 0; \end{cases} \tag{2.2.11}$$

the coefficients α and β depend only on the geometry of the set Ω and should be calculated.

2.3 Special solutions to the first kind homogeneous problems

Introduce special solutions to the homogeneous problems (2.2.1) in G_j, $j = 1, 2, 3$. These solutions are needed for construction of the asymptotics in the next section. Propositions 2.2.1 and 2.2.2 imply that the bounded solutions of homogeneous problems (2.2.1) are trivial (except the eigenfunctions of the problem in the resonator), so we consider only solutions unbounded near the points O_j.

Let us consider the problem

$$\begin{aligned} \Delta u + k^2 u &= 0 \quad \text{in} \quad K, \\ u &= 0 \quad \text{on} \quad \partial K. \end{aligned} \tag{2.3.1}$$

The function

$$v(r, \varphi) = \widetilde{N}_{\pi/\omega}(kr)\Phi(\varphi) \tag{2.3.2}$$

satisfies (2.3.1); $\widetilde{N}_{\pi/\omega}$ stands for the Neumann function multiplied by a constant such that

$$\widetilde{N}_{\pi/\omega}(kr) = r^{-\pi/\omega} + o(r^{-\pi/\omega}),$$

while Φ is the same as in Proposition 2.2.1. Let $t \mapsto \Theta(t)$ be a cut-off function on $\mathbb{R}$ equal to 1 for $t < \delta/2$ and to 0 for $t > \delta$, δ being a small positive number. Introduce a solution

$$\mathbf{v}_1(x, y) = \Theta(r_1)v(r_1, \varphi_1) + \widetilde{v}_1(x, y) \tag{2.3.3}$$

of the homogeneous problem (2.2.1) in G_1, where $\widetilde{v}_1$ solves (2.2.1) with

$$f = -[\Delta, \Theta]v,$$

the existence of $\widetilde{v}_1$ is provided by Proposition 2.2.2. Thus,

$$\mathbf{v}_1(x,y)=\begin{cases} \big(\widetilde{N}_{\pi/\omega}(kr_1)+a\widetilde{J}_{\pi/\omega}(kr_1)\big)\Phi(\pi-\varphi_1)+O(r_1^{3\pi/\omega}), & r_1\to 0,\\ AU_1^-(x,y)+O(e^{\delta x}), & x\to-\infty, \end{cases} \tag{2.3.4}$$

where $\widetilde{J}_{\pi/\omega}$ is the same as in Propositions 2.2.1 and 2.2.2, and the constant $A\neq 0$ depends only on the geometry of the domain G_1 and should be calculated.

Define the solution $\mathbf{v}_3$ to the problem (2.2.1) in G_3 by $\mathbf{v}_3(x,y)=\mathbf{v}_1(d-x,y)$, where $d=\operatorname{dist}(O_1,O_2)$. Then

$$\mathbf{v}_3(x,y)=\begin{cases} \big(\widetilde{N}_{\pi/\omega}(kr_2)+a\widetilde{J}_{\pi/\omega}(kr_2)\big)\Phi(\varphi_2)+O(r_2^{3\pi/\omega}), & r_2\to 0,\\ Ae^{-i\nu_1 d}U_2^-(x,y)+O(e^{-\delta x}), & x\to+\infty. \end{cases} \tag{2.3.5}$$

Lemma 2.3.1. *There holds the equality* $|A|^2=\operatorname{Im} a$.

Proof. Let $(u,v)_Q$ denote the integral $\int_Q u(x)\overline{v(x)}\,dx$ and let $G_{N,\delta}$ stand for the truncated domain $G_1\cap\{x>-N\}\cap\{r_1>\delta\}$. By the Green formula,

$$\begin{aligned} 0&=(\Delta\mathbf{v}_1+k^2\mathbf{v}_1,\mathbf{v}_1)_{G_{N,\delta}}-(\mathbf{v}_1,\Delta\mathbf{v}_1+k^2\mathbf{v}_1)_{G_{N,\delta}}\\ &=(\partial\mathbf{v}_1/\partial n,\mathbf{v}_1)_{\partial G_{N,\delta}}-(\mathbf{v}_1,\partial\mathbf{v}_1/\partial n)_{\partial G_{N,\delta}}=2i\operatorname{Im}(\partial\mathbf{v}_1/\partial n,\mathbf{v}_1)_E, \end{aligned}$$

where $E=(\partial G_{N,\delta}\cap\{x=-N\})\cup(\partial G_{N,\delta}\cap\{r_1=\delta\})$. Taking into account (2.3.4) as $x\to+\infty$ and (2.1.4), we have

$$\begin{aligned} \operatorname{Im}(\partial\mathbf{v}_1/\partial n,\mathbf{v}_1)_{\partial G_{N,\delta}\cap\{x=-N\}}&=-\operatorname{Im}\int_{-l/2}^{l/2}A\frac{\partial U_1^-}{\partial x}(x,y)\overline{AU_1^-}(x,y)\Big|_{x=-N}dy+o(1)\\ &=|A|^2\nu_1\int_{-l/2}^{l/2}|\Psi_1(y)|^2dy+o(1)=|A|^2+o(1). \end{aligned}$$

Using (2.3.4) as $r_1\to 0$ and the definition of Φ (see Proposition 2.2.1), we obtain

$$\begin{aligned} \operatorname{Im}(\partial\mathbf{v}_1/\partial n,\mathbf{v}_1)_{\partial G_{N,\delta}\cap\{r_1=\delta\}}&=\operatorname{Im}\int_{\pi-\omega/2}^{\pi+\omega/2}\Big[-\frac{\partial}{\partial r_1}\big(\widetilde{N}_{\pi/\omega}(kr_1)+a\widetilde{J}_{\pi/\omega}(kr_1)\big)\Big]\\ &\quad\times\Big(\widetilde{N}_{\pi/\omega}(kr_1)+\bar{a}\widetilde{J}_{\pi/\omega}(kr_1)\Big)|\Phi(\pi-\varphi_1)|^2r_1\Big|_{r_1=\delta}d\varphi_1+o(1)\\ &=-(\operatorname{Im} a)\frac{2\pi}{\omega}\int_{\pi-\omega/2}^{\pi+\omega/2}|\Phi(\pi-\varphi_1)|^2d\varphi_1+o(1)=-\operatorname{Im} a+o(1). \end{aligned}$$

Thus $|A|^2-\operatorname{Im} a+o(1)=0$ as $N\to\infty$ and $\delta\to 0$. □

Let k_0^2 be a simple eigenvalue for $-\Delta$ with Dirichlet boundary condition in G_2, and let v_0 be an eigenfunction corresponding to k_0^2 and normalized by $\int_{G_2}|v_0|^2dx=1$. By Proposition 2.2.1

$$v_0(x)\sim\begin{cases} b_1\widetilde{J}_{\pi/\omega}(k_0r_1)\Phi(\varphi_1), & r_1\to 0,\\ b_2\widetilde{J}_{\pi/\omega}(k_0r_2)\Phi(\pi-\varphi_2), & r_2\to 0. \end{cases} \tag{2.3.6}$$

We assume that $b_j \neq 0$; it is true, e.g. for the eigenfunction corresponding to the least eigenvalue of the resonator. Since the resonator is symmetric with respect to the mapping $(x, y) \mapsto (d - x, y)$, we have $q = b_1/b_2 = \pm 1$. For k^2 in a punctured neighborhood of k_0^2 separated from the other eigenvalues, we introduce solutions v_{0j} to the homogeneous problem (2.2.1) in G_2 by

$$v_{0j}(x, y) = \Theta(r_j)v(r_j, \varphi_j) + \widetilde{v}_{0j}(x, y), \qquad j = 1, 2, \tag{2.3.7}$$

where v is defined by (2.3.2), and $\widetilde{v}_{0j}$ is the bounded solution to the problem (2.2.1) in G_2 with

$$f_j(x, y) = -[\Delta, \Theta(r_j)]v(r_j, \varphi_j).$$

Lemma 2.3.2. *In a neighborhood $V \subset \mathbb{C}$ of k_0^2 containing no eigenvalues of the problem* (2.2.1) *in G_2 except k_0^2, the equalities $\widetilde{v}_{0j} = -b_j(k^2 - k_0^2)^{-1}v_0 + \widehat{v}_{0j}$ hold with b_j from* (2.3.6) *and functions $\widehat{v}_{0j}$ analytic in $k^2 \in V$.*

Proof. First check the equality $(v_{0j}, v_0)_{G_2} = -b_j/(k^2 - k_0^2)$, where v_{0j} are defined by (2.3.7). We have

$$(\Delta v_{0j} + k^2 v_{0j}, v_0)_{G_\delta} - (v_{0j}, \Delta v_0 + k^2 v_0)_{G_\delta} = -(k^2 - k_0^2)(v_{0j}, v_0)_{G_\delta};$$

the domain G_δ is obtained from G_2 by excluding discs with radius δ centered at points O_1 and O_2. Using the Green formula, as in Lemma 2.3.1, we get the equality

$$-(k^2 - k_0^2)(v_{0j}, v_0)_{G_\delta} = b_j + o(1).$$

It remains to let δ tend to zero.

Since k_0^2 is a simple eigenvalue, we have

$$\widetilde{v}_{0j} = \frac{B_j(k^2)}{k^2 - k_0^2} v_0 + \widehat{v}_{0j}, \tag{2.3.8}$$

where $B_j(k^2)$ does not depend on x, and $\widehat{v}_{0j}$ are some functions analytic wih respect to k^2 near the point $k^2 = k_0^2$. Multiplying (2.3.7) by v_0 and taking into account (2.3.8), the obtained formula for $(v_{0j}, v_0)_{G_2}$, and the condition $(v_0, v_0)_{G_2} = 1$, we get the equality

$$B_j(k^2) = -b_j + (k^2 - k_0^2)\widetilde{B}_j(k^2),$$

where $\widetilde{B}_j$ are some analytic functions. Together with (2.3.8) that leads to the required statement. □

In view of Lemma 2.3.2 the expressions $\mathbf{v}_{21} = (k^2 - k_0^2)v_{01}$ and $\mathbf{v}_{22} = b_2 v_{01} - b_1 v_{02}$ may be extended to functions continuous at k_0^2 with respect to k^2. According to Proposition 2.2.1,

$$\mathbf{v}_{21}(x, y) \sim \begin{cases} \big((k^2 - k_0^2)\widetilde{N}_{\pi/\omega}(kr_1) + c_1(k)\widetilde{J}_{\pi/\omega}(kr_1)\big)\Phi(\varphi_1), & r_1 \to 0, \\ c_2(k)\widetilde{J}_{\pi/\omega}(kr_2)\Phi(\pi - \varphi_2), & r_2 \to 0, \end{cases} \tag{2.3.9}$$

$$\mathbf{v}_{22}(x, y) \sim \begin{cases} \big(b_2\widetilde{N}_{\pi/\omega}(kr_1) + d_1(k)\widetilde{J}_{\pi/\omega}(kr_1)\big)\Phi(\varphi_1), & r_1 \to 0, \\ \big(-b_1\widetilde{N}_{\pi/\omega}(kr_2) + d_2(k)\widetilde{J}_{\pi/\omega}(kr_2)\big)\Phi(\pi - \varphi_2), & r_2 \to 0. \end{cases} \tag{2.3.10}$$

The proof of Lemma 2.3.2 shows that $c_j(k_0) = -b_1 b_j$.

2.4 Asymptotic formulas

This section is devoted to derivation of the asymptotic formulas. In Section 2.4.1, we present a formula for the wave function (see (2.4.1)), explain its structure, and describe the solutions of the first kind limit problems involved in the formula. Construction of formula (2.4.1) is completed in Section 2.4.2, where the solutions to the second kind limit problems are given and the coefficients in the expressions for the solutions of the first kind limit problems are calculated. In Section 2.4.3 we analyze the expression for $\widetilde{s}_{12}$ obtained in 2.4.2, and derive formal asymptotics for the characteristics of resonant tunneling. Notice, that the remainders in the formulas (2.4.20)–(2.4.22) arose in the intermediate stage of considerations while simplifying the principal part of the asymptotics; they are not the remainders in the final asymptotic formulas. The "final" remainders are estimated in the next Section 2.5, see Theorem 2.5.3. First we derive the integral estimate (2.5.13) of the remainder in the formula (2.4.1), which proves to be sufficient to obtain more simplified estimates of the remainders in the formulas for the characteristics of resonant tunneling. The formula (2.4.1) and the estimate (2.5.13) are auxiliary and are analysed only to that extent which is necessary for deriving the asymptotic expressions for the characteristics of resonant tunneling.

2.4.1 Asymptotics of the wave function

In the waveguide $G(\varepsilon)$, we consider the scattering of the wave $U = e^{i\nu_1 x}\Psi_1(y)$ incoming from $-\infty$ (see (2.1.4)). The wave function admits the representation

$$\begin{aligned} u(x,y;\varepsilon) = {} & \chi_{1,\varepsilon}(x,y)v_1(x,y;\varepsilon) \\ & + \Theta(r_1)w_1(\varepsilon^{-1}x_1,\varepsilon^{-1}y_1;\varepsilon) + \chi_{2,\varepsilon}(x,y)v_2(x,y;\varepsilon) \\ & + \Theta(r_2)w_2(\varepsilon^{-1}x_2,\varepsilon^{-1}y_2;\varepsilon) + \chi_{3,\varepsilon}(x,y)v_3(x,y;\varepsilon) + R(x,y;\varepsilon). \end{aligned} \quad (2.4.1)$$

Let us explain the notation and the structure of this formula. When composing the formula, we first describe the behavior of the wave function u outside of the narrows, where the solutions v_j to the homogeneous problems (2.2.1) in G_j serve as approximations to u. The function v_j is a linear combination of the special solutions introduced in the previous section; v_1 and v_3 are subject to the same radiation conditions as u:

$$\begin{aligned} v_1(x,y;\varepsilon) &= \frac{1}{A}\overline{\mathbf{v}}_1(x,y) + \frac{\widetilde{s}_{11}(\varepsilon)}{A}\mathbf{v}_1(x,y) \\ &\sim U_1^+(x,y) + \widetilde{s}_{11}(\varepsilon)U_1^-(x,y), \qquad x \to -\infty; \quad (2.4.2) \\ v_2(x,y;\varepsilon) &= C_1(\varepsilon)\mathbf{v}_{21}(x,y) + C_2(\varepsilon)\mathbf{v}_{22}(x,y); \quad (2.4.3) \\ v_3(x,y;\varepsilon) &= \frac{\widetilde{s}_{12}(\varepsilon)}{Ae^{-i\nu_1 d}}\mathbf{v}_3(x,y) \sim \widetilde{s}_{12}(\varepsilon)U_2^-(x,y), \qquad x \to +\infty; \quad (2.4.4) \end{aligned}$$

the approximations $\widetilde{s}_{11}(\varepsilon)$, $\widetilde{s}_{12}(\varepsilon)$ to the elements $s_{11}(\varepsilon)$, $s_{12}(\varepsilon)$ of the scattering matrix and the coefficients $C_1(\varepsilon)$, $C_2(\varepsilon)$ are yet unknown. By $\chi_{j,\varepsilon}$ we denote cut-off functions defined by

$$\chi_{1,\varepsilon}(x,y) = (1-\Theta(r_1/\varepsilon))\,\mathbf{1}_{G_1}(x,y), \qquad \chi_{3,\varepsilon}(x,y) = (1-\Theta(r_2/\varepsilon))\,\mathbf{1}_{G_3}(x,y),$$
$$\chi_{2,\varepsilon}(x,y) = (1-\Theta(r_1/\varepsilon)-\Theta(r_2/\varepsilon))\,\mathbf{1}_{G_2}(x,y),$$

where $r_j = \sqrt{x_j^2+y_j^2}$, and (x_j,y_j) are the coordinates of a point (x,y) in the system obtained by shifting the origin to the point O_j; $\mathbf{1}_{G_j}$ is the indicator of G_j (equal to 1 in G_j and to 0 outside G_j); $\Theta(\rho)$ is the same cut-off function as in (2.3.3) (equal to 1 for $0 \leqslant \rho \leqslant \delta/2$ and to 0 for $\rho \geqslant \delta$, δ being a fixed positive number). Thus, $\chi_{j,\varepsilon}$ are defined on the whole waveguide $G(\varepsilon)$ as well as the functions $\chi_{j,\varepsilon}v_3$ in (2.4.1).

Being substituted to (2.1.1), the sum $\sum_{j=1}^3 \chi_{j,\varepsilon}v_j$ gives a discrepancy in the right-hand side of the Helmholtz equation supported near the narrows. We compensate the principal part of the discrepancy by means of the second kind limit problems. Namely, the discrepancy supported in the neighborhood of the point O_j is rewritten into coordinates $(\xi_j,\eta_j) = (\varepsilon^{-1}x_j,\varepsilon^{-1}y_j)$ in the domain Ω_j and is taken as a right-hand side for the Laplace equation. The solution w_j of the corresponding problem (2.2.6) is rewritten into coordinates (x_j,y_j) and multiplied by a cut-off function. As a result, there arise the terms $\Theta(r_j)w_j(\varepsilon^{-1}x_j,\varepsilon^{-1}y_j;\varepsilon)$ in (2.4.1).

Proposition 2.2.3 provides the existence of solutions w_j decaying at infinity as $O(\rho_j^{-\pi/\omega})$ (see (2.2.9)). But those solutions will not lead us to the goal, because substitution of (2.4.1) into (2.1.1) gives a discrepancy of high order which has to be compensated again. Therefore we require the rate $w_j = O(\rho_j^{-3\pi/\omega})$ as $\rho_j \to \infty$. By Proposition 2.2.3, such a solution exists if the right-hand side of the problem (2.2.6) satisfies the additional conditions

$$(F,w_j^l)_{\Omega_j} = 0, \qquad (F,w_j^r)_{\Omega_j} = 0.$$

These conditions (two in each narrow) uniquely determine the coefficients $\widetilde{s}_{11}(\varepsilon)$, $\widetilde{s}_{12}(\varepsilon)$, $C_1(\varepsilon)$, and $C_2(\varepsilon)$. The remainder $R(x,y;\varepsilon)$ is small in comparison with the principal part of (2.4.1) as $\varepsilon \to 0$.

2.4.2 Formulas for $\widetilde{s}_{11}$, $\widetilde{s}_{12}$, C_1, and C_2

Now let us specify the right-hand sides F_j of the problems (2.2.6) and find $\widetilde{s}_{11}(\varepsilon)$, $\widetilde{s}_{12}(\varepsilon)$, $C_1(\varepsilon)$, and $C_2(\varepsilon)$. Substituting $\chi_{1,\varepsilon}v_1$ into (2.1.1), we get the discrepancy

$$(\Delta+k^2)\chi_{1,\varepsilon}v_1 = [\Delta,\chi_{\varepsilon,1}]v_1 + \chi_{\varepsilon,1}(\Delta+k^2)v_1 = [\Delta, 1-\Theta(\varepsilon^{-1}r_1)]v_1,$$

which is non-zero in a neighborhood of the point O_1, where v_1 can be replaced by asymptotics; the boundary condition in (2.1.1) is fulfilled. According to (2.4.2) and (2.3.4), as $r_1 \to 0$,

$$v_1(x,y;\varepsilon) = \big(a_1^-(\varepsilon)\widetilde{N}_{\pi/\omega}(kr_1) + a_1^+(\varepsilon)\widetilde{J}_{\pi/\omega}(kr_1)\big)\Phi(\pi-\varphi_1) + O(r_1^{3\pi/\omega}),$$

where

$$a_1^-(\varepsilon) = \frac{1}{\overline{A}} + \frac{\widetilde{s}_{11}(\varepsilon)}{A}, \quad a_1^+ = \frac{\overline{a}}{\overline{A}} + \frac{\widetilde{s}_{11}(\varepsilon)a}{A}. \tag{2.4.5}$$

Choose in each summand the leading term and take $\rho_1 = r_1/\varepsilon$, then

$$(\Delta + k^2)\chi_{\varepsilon,1}v_1 \sim [\Delta, 1 - \Theta(\varepsilon^{-1}r_1)] \left(a_1^- r_1^{-\pi/\omega} + a_1^+ r_1^{\pi/\omega}\right) \Phi(\pi - \varphi_1)$$
$$= \varepsilon^{-2}[\Delta_{(\rho_1,\varphi_1)}, 1 - \Theta(\rho_1)] \left(a_1^- \varepsilon^{-\pi/\omega}\rho_1^{-\pi/\omega} + a_1^+ \varepsilon^{\pi/\omega}\rho_1^{\pi/\omega}\right) \Phi(\pi - \varphi_1). \quad (2.4.6)$$

In the same way, by use of (2.4.3) and (2.3.9)–(2.3.10), write down the leading term of the discrepancy from $\chi_{\varepsilon,2}v_2$ supported in a neighborhood of O_1:

$$(\Delta + k^2)\chi_{\varepsilon,1}v_1 \sim \varepsilon^{-2}[\Delta_{(\rho_1,\varphi_1)}, 1 - \Theta(\rho_1)] \left(b_1^- \varepsilon^{-\pi/\omega}\rho_1^{-\pi/\omega} + b_1^+ \varepsilon^{\pi/\omega}\rho_1^{\pi/\omega}\right) \Phi(\varphi_1), \quad (2.4.7)$$

where

$$b_1^- = C_1(\varepsilon)(k^2 - k_0^2) + C_2(\varepsilon)b_2, \qquad b_1^+ = C_1(\varepsilon)c_1 + C_2(\varepsilon)d_1. \quad (2.4.8)$$

As right-hand side F_1 of the problem (2.2.6) in Ω_1, we take the function

$$F_1(\xi_1, \eta_1) = -[\Delta, \zeta^-] \left(a_1^- \varepsilon^{-\pi/\omega}\rho_1^{-\pi/\omega} + a_1^+ \varepsilon^{\pi/\omega}\rho_1^{\pi/\omega}\right) \Phi(\pi - \varphi_1)$$
$$- [\Delta, \zeta^+] \left(b_1^- \varepsilon^{-\pi/\omega}\rho_1^{-\pi/\omega} + b_1^+ \varepsilon^{\pi/\omega}\rho_1^{\pi/\omega}\right) \Phi(\varphi_1), \quad (2.4.9)$$

where ζ^+ (respectively ζ^-) stands for the function $1 - \Theta$, first restricted to the domain $\xi_1 > 0$ (respectively $\xi_1 < 0$), then extended by zero onto the whole domain Ω_1. Let w_1 be the corresponding solution and then the term

$$\Theta(r_1)w_1(\varepsilon^{-1}x_1, \varepsilon^{-1}y_1; \varepsilon)$$

in (2.4.1), being substituted in (2.1.1), compensates the discrepancies (2.4.6)–(2.4.7).

Analogously, using (2.4.3)–(2.4.4), (2.3.9)–(2.3.10), and (2.3.5), we find the right-hand side of the problem (2.2.6) for $j = 2$:

$$F_2(\xi_2, \eta_2) = -[\Delta, \zeta^-] \left(a_2^- \varepsilon^{-\pi/\omega}\rho_2^{-\pi/\omega} + a_2^+ \varepsilon^{\pi/\omega}\rho_2^{\pi/\omega}\right) \Phi(\pi - \varphi_2)$$
$$- [\Delta, \zeta^+] \left(b_2^- \varepsilon^{-\pi/\omega}\rho_2^{-\pi/\omega} + b_2^+ \varepsilon^{\pi/\omega}\rho_2^{\pi/\omega}\right) \Phi(\varphi_2),$$

where

$$a_2^-(\varepsilon) = -C_2(\varepsilon)b_1, \qquad a_2^+(\varepsilon) = C_1(\varepsilon)c_2 + C_2(\varepsilon)d_2,$$
$$b_2^-(\varepsilon) = \frac{\widetilde{s}_{12}(\varepsilon)}{Ae^{-i\nu_1 d}}, \qquad b_2^+(\varepsilon) = \frac{a\widetilde{s}_{12}(\varepsilon)}{Ae^{-i\nu_1 d}}. \quad (2.4.10)$$

Lemma 2.4.1. *If the solution w_j to the problem (2.2.6) with right-hand side*

$$F_j(\xi_j, \eta_j) = -[\Delta, \zeta^-] \left(a_j^- \varepsilon^{-\pi/\omega}\rho_j^{-\pi/\omega} + a_j^+ \varepsilon^{\pi/\omega}\rho_j^{\pi/\omega}\right) \Phi(\pi - \varphi_j)$$
$$- [\Delta, \zeta^+] \left(b_j^- \varepsilon^{-\pi/\omega}\rho_j^{-\pi/\omega} + b_j^+ \varepsilon^{\pi/\omega}\rho_j^{\pi/\omega}\right) \Phi(\varphi_j), \qquad j = 1, 2,$$

is $O(\rho_j^{-3\pi/\omega})$ as $\rho_j \to \infty$, then the relations

$$a_j^- \varepsilon^{-\pi/\omega} - \alpha a_j^+ \varepsilon^{\pi/\omega} - \beta b_j^+ \varepsilon^{\pi/\omega} = 0,$$
$$b_j^- \varepsilon^{-\pi/\omega} - \alpha b_j^+ \varepsilon^{\pi/\omega} - \beta a_j^+ \varepsilon^{\pi/\omega} = 0, \quad (2.4.11)$$

hold with α and β from (2.2.10) – (2.2.11).

Proof. In view of Proposition 2.2.3 we have $w_j = O(\rho_j^{-3\pi/\omega})$ as $\rho_j \to \infty$ if and only if the right-hand side of the problem (2.2.6) satisfies the conditions

$$(F_j, w_j^l)_{\Omega_j} = 0, \qquad (F_j, w_j^r)_{\Omega_j} = 0, \tag{2.4.12}$$

where w_j^l and w_j^r are solutions to the homogeneous problem (2.2.6), for which the expansions in (2.2.10)–(2.2.11) hold. Introduce the functions $f_\pm$ on Ω_j by equalities

$$f_\pm(\rho_j, \varphi_j) = \rho_j^{\pm\pi/\omega}\Phi(\varphi_j).$$

To derive (2.4.11) from (2.4.12), it suffices to check that

$$\begin{aligned}
([\Delta, \zeta^-]f_-, w_j^l)_{\Omega_j} &= ([\Delta, \zeta^+]f_-, w_j^r)_{\Omega_j} = -1,\\
([\Delta, \zeta^-]f_+, w_j^l)_{\Omega_j} &= ([\Delta, \zeta^+]f_+, w_j^r)_{\Omega_j} = \alpha,\\
([\Delta, \zeta^+]f_-, w_j^l)_{\Omega_j} &= ([\Delta, \zeta^-]f_-, w_j^r)_{\Omega_j} = 0,\\
([\Delta, \zeta^+]f_+, w_j^l)_{\Omega_j} &= ([\Delta, \zeta^-]f_+, w_j^r)_{\Omega_j} = \beta.
\end{aligned}$$

Let us prove the first equality, the rest ones are treated in a similar way. Since $[\Delta, \zeta^+]f_-$ is compactly supported, in the calculation of $([\Delta, \zeta^-]f_-, w_j^l)_{\Omega_j}$ one may replace Ω_j by

$$\Omega_j^R = \Omega_j \cap \{\rho_j < R\}$$

with sufficiently large R. Let E denote the set $\partial\Omega_j^R \cap \{\rho_j = R\} \cap \{\xi_j > 0\}$. By the Green formula

$$\begin{aligned}
([\Delta, \zeta^-]f_-, w_j^l)_{\Omega_j} =& (\Delta\zeta^- f_-, w_j^l)_{\Omega_j^R} - (\zeta^- f_-, \Delta w_j^l)_{\Omega_j^R}\\
=& (\partial f_-/\partial n, w_j^l)_E - (f_-, \partial w_j^l/\partial n)_E.
\end{aligned}$$

Taking account of (2.2.10) for $\xi_j < 0$ and the definition of Φ in Proposition 2.2.1, we arrive at

$$\begin{aligned}
([\Delta, \zeta^-]f_-, w_j^l)_{\Omega_j} =& \mathcal{S}(R)\int_{\pi-\omega/2}^{\pi+\omega/2} \Phi(\pi - \varphi_j)^2 d\varphi_j + o(1)\\
=& -\frac{2\pi}{\omega}\int_{\pi-\omega/2}^{\pi+\omega/2} \Phi(\pi - \varphi_j)^2 d\varphi_j + o(1) = -1 + o(1),
\end{aligned}$$

where $\mathcal{S}(R)$ stands for the expression

$$\rho_j\left(\frac{\partial\rho_j^{-\pi/\omega}}{\partial\rho_j}(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}) - \rho_j^{-\pi/\omega}\frac{\partial}{\partial\rho_j}(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega})\right)\Bigg|_{\rho_j=R}.$$

It remains to pass to the limit as $R \to \infty$. □

Remark 2.4.2. *The solutions w_j mentioned in Lemma 2.4.1 can be represented as linear combinations of functions independent of ε. We write down the corresponding expression* *which will be of use in the next section. Let w_j^l and w_j^r be the solutions of the problem (2.2.6) specified by conditions (2.2.10) – (2.2.11), and let ζ^+ and ζ^- be the same cut-off functions as in (2.4.9). Put*

$$\begin{aligned}\mathbf{w}_j^l &= w_j^l - \zeta^- \left(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}\right)\Phi(\pi - \varphi_j) - \zeta^+\beta\rho_j^{-\pi/\omega}\Phi(\varphi_j),\\ \mathbf{w}_j^r &= w_j^r - \zeta^-\beta\rho_j^{-\pi/\omega}\Phi(\pi - \varphi_j) - \zeta^+ \left(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}\right)\Phi(\varphi_j).\end{aligned}$$

A direct verification shows that

$$\begin{aligned}w_j &= a_j^+\varepsilon^{\pi/\omega}\mathbf{w}_j^l + \frac{1}{\beta}\left(a_j^-\varepsilon^{-\pi/\omega} - \alpha a_j^+\varepsilon^{\pi/\omega}\right)\mathbf{w}_j^r\\ &= \frac{1}{\beta}\left(b_j^-\varepsilon^{-\pi/\omega} - \alpha b_j^+\varepsilon^{\pi/\omega}\right)\mathbf{w}_j^l + b_j^+\varepsilon^{\pi/\omega}\mathbf{w}_j^r.\end{aligned} \tag{2.4.13}$$

Using (2.4.5) and (2.4.8), we transform (2.4.11) with $j = 1$ to the expressions

$$\begin{aligned}\gamma(\varepsilon)\widetilde{s}_{11}(\varepsilon) + \overline{\gamma(\varepsilon)} &= C_1(\varepsilon)c_1 + C_2(\varepsilon)d_1,\\ \delta(\varepsilon)\widetilde{s}_{11}(\varepsilon) + \overline{\delta(\varepsilon)} &= C_1(\varepsilon)(k^2 - k_0^2) + C_2(\varepsilon)b_2,\end{aligned} \tag{2.4.14}$$

where

$$\gamma(\varepsilon) = \frac{1}{A\beta}\left(\varepsilon^{-2\pi/\omega} - a\alpha\right), \qquad \delta(\varepsilon) = \frac{1}{A\beta}\left(\alpha + a(\beta^2 - \alpha^2)\varepsilon^{2\pi/\omega}\right). \tag{2.4.15}$$

For $j = 2$, taking (2.4.10) into account, reduce (2.4.11) to the equalities

$$\gamma(\varepsilon)\widetilde{s}_{12}(\varepsilon) = (C_1(\varepsilon)c_2 + C_2(\varepsilon)d_2)e^{-i\nu_1 d}, \quad \delta(\varepsilon)\widetilde{s}_{12}(\varepsilon) = -C_2(\varepsilon)b_1e^{-i\nu_1 d}. \tag{2.4.16}$$

From (2.4.14) and (2.4.16), by means of Lemma 2.3.1, we find $C_1(\varepsilon)$, $C_2(\varepsilon)$, $\widetilde{s}_{11}(\varepsilon)$, and $\widetilde{s}_{12}(\varepsilon)$:

$$\begin{aligned}C_1(\varepsilon) &= (b_1c_2)^{-1}\left(\gamma(\varepsilon)b_1 + \delta(\varepsilon)d_2\right)\widetilde{s}_{12}(\varepsilon)e^{i\nu_1 d},\\ C_2(\varepsilon) &= -b_1^{-1}\delta(\varepsilon)\widetilde{s}_{12}(\varepsilon)e^{i\nu_1 d},\end{aligned} \tag{2.4.17}$$

$$\begin{aligned}\widetilde{s}_{11}(\varepsilon) =& (2ib_1c_2)^{-1}\Big((k^2 - k_0^2)b_1|\gamma(\varepsilon)|^2 + ((k^2 - k_0^2)d_2 - b_2c_2)\overline{\gamma(\varepsilon)}\delta(\varepsilon)\\ &- b_1c_1\gamma(\varepsilon)\overline{\delta(\varepsilon)} - (c_1d_2 - c_2d_1)|\delta(\varepsilon)|^2\Big)\widetilde{s}_{12}(\varepsilon),\end{aligned} \tag{2.4.18}$$

$$\begin{aligned}\widetilde{s}_{12}(\varepsilon) =& 2ib_1c_2e^{-i\nu_1 d}\Big(-(k^2 - k_0^2)b_1\gamma(\varepsilon)^2\\ &- ((k^2 - k_0^2)d_2 - b_1c_1 - b_2c_2)\gamma(\varepsilon)\delta(\varepsilon) + (c_1d_2 - c_2d_1)\delta(\varepsilon)^2\Big)^{-1}.\end{aligned} \tag{2.4.19}$$

2.4.3 The formulas for the characteristics of resonant tunneling

The solutions of the first kind limit problems involved in (2.4.1) are defined for complex k^2 as well. The obtained expression (2.4.19) for $\widetilde{s}_{12}$ has a pole k_p^2 in the lower complex half-plane. To find k_p^2 we equate $2ib_1c_2e^{-i\nu_1 d}/\widetilde{s}_{12}$ to zero and solve the equation for $k_2 - k_0^2$:

$$k^2 - k_0^2 = \frac{(b_1c_1 + b_2c_2)\gamma(\varepsilon)\delta(\varepsilon) + (c_1d_2 - c_2d_1)\delta(\varepsilon)^2}{b_1\gamma(\varepsilon)^2 + d_2\gamma(\varepsilon)\delta(\varepsilon)}.$$

Since the right-hand side of the last equation behaves like $O(\varepsilon^{2\pi/\omega})$ as $\varepsilon \to 0$, it may be solved by the method of successive approximations. Considering the formulas (2.4.15), $c_j(k_0) = -b_1b_j$, $b_1 = \pm b_2$, and Lemma 2.3.1, and dropping the lower order terms, we get $k_p^2 = k_r^2 - ik_i^2$, where

$$\begin{aligned} k_r^2 &= k_0^2 - 2\alpha b_1^2\varepsilon^{2\pi/\omega} + O(\varepsilon^{4\pi/\omega}), \\ k_i^2 &= 2\beta^2 b_1^2|A(k_0^2)|^2\varepsilon^{4\pi/\omega} + O(\varepsilon^{6\pi/\omega}). \end{aligned} \tag{2.4.20}$$

For small $k^2 - k_p^2$ the formula (2.4.19) takes the form

$$\widetilde{s}_{12}(k,\varepsilon) = -\varepsilon^{4\pi/\omega}\frac{2i\beta^2 A(k)^2 c_2(k)e^{-i\nu_1 d}}{k^2 - k_p^2}\left(1 + O(|k^2 - k_p^2| + \varepsilon^{2\pi/\omega})\right).$$

Let $k^2 - k_0^2 = O(\varepsilon^{2\pi/\omega})$, then

$$\begin{aligned} |k^2 - k_p^2| &= O(\varepsilon^{2\pi/\omega}), & A(k) &= A(k_0^2) + O(\varepsilon^{2\pi/\omega}), \\ c_2(k^2) &= -b_1b_2 + O(\varepsilon^{2\pi/\omega}), & \nu_1(k) &= \nu_1(k_0^2) + O(\varepsilon^{2\pi/\omega}), \end{aligned}$$

and

$$\begin{aligned} \widetilde{s}_{12}(k,\varepsilon) &= \varepsilon^{4\pi/\omega}\frac{2i\beta^2 b_1b_2 A(k_0)^2 e^{-i\nu_1(k_0)d}}{k^2 - k_p^2}\left(1 + O(\varepsilon^{2\pi/\omega})\right) \\ &= \frac{q(A(k_0)/|A(k_0)|)^2 e^{-i\nu_1(k_0)d}}{1 - iP\dfrac{k^2 - k_r^2}{\varepsilon^{4\pi/\omega}}}\left(1 + O(\varepsilon^{2\pi/\omega})\right), \end{aligned}$$

where $q = b_2/b_1$ and $P = (2b_1^2\beta^2|A(k_0)|^2)^{-1}$. Thus,

$$\widetilde{T}(k,\varepsilon) = |\widetilde{s}_{12}|^2 = \frac{1}{1 + P^2\left(\dfrac{k^2 - k_r^2}{\varepsilon^{4\pi/\omega}}\right)^2}(1 + O(\varepsilon^{2\pi/\omega})). \tag{2.4.21}$$

The obtained approximation $\widetilde{T}$ to the transition coefficient has a peak at $k^2 = k_r^2$ whose width at its half-height is

$$\widetilde{\Upsilon}(\varepsilon) = \frac{2}{P}\varepsilon^{4\pi/\omega}. \tag{2.4.22}$$

2.5 Justification of the asymptotics

Introduce functional spaces for the problem

$$\Delta u + k^2 u = f \quad G(\varepsilon), \qquad u = 0 \quad \partial G(\varepsilon). \tag{2.5.1}$$

Let Θ be the same function as in (2.3.3), and let the cut-off functions η_j, $j = 1, 2, 3$, be nonzero in G_j and satisfy the relation

$$\eta_1(x, y) + \Theta(r_1) + \eta_2(x, y) + \Theta(r_2) + \eta_3(x, y) = 1$$

in $G(\varepsilon)$. For $\gamma \in \mathbb{R}$, $\delta > 0$, and $l = 0, 1, \ldots$ the space $V^l_{\gamma,\delta}(G(\varepsilon))$ is the completion in the norm

$$\left\| u; V^l_{\gamma,\delta}(G(\varepsilon)) \right\| = \left(\int_{G(\varepsilon)} \mathcal{S}(u)\, dx\, dy \right)^{1/2} \tag{2.5.2}$$

of the set of smooth functions compactly supported on $\overline{G(\varepsilon)}$; here

$$\mathcal{S}(u) := \sum_{|\alpha|=0}^{l} \left(\sum_{j=1}^{2} \Theta^2(r_j)\, (r_j^2 + \varepsilon_j^2)^{\gamma - l + |\alpha|} + \eta_1^2 e^{2\delta|x|} + \eta_2 + \eta_3^2 e^{2\delta|x|} \right) |\partial^\alpha u|^2$$

We denote by $V^{0,\perp}_{\gamma,\delta}$ the space of functions f analytic in k^2 which take values in $V^0_{\gamma,\delta}(G(\varepsilon))$ and satisfy at $k^2 = k_0^2$ the condition $(\chi_{2,\varepsilon^\sigma} f, v_0)_{G_2} = 0$ with a small positive σ.

Proposition 2.5.1. *Let k_r^2 be a resonance, $k_r^2 \to k_0^2$ as $\varepsilon \to 0$, and let*

$$|k^2 - k_r^2| = O(\varepsilon^{2\pi/\omega}).$$

Assume, that γ satisfies the condition $\pi/\omega - 2 < \gamma - 1 < \pi/\omega$, $f \in V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$, and u is the solution of the problem (2.5.1) *which admits the representation*

$$u = \widetilde{u} + \eta_1 A_1^- U_1^- + \eta_3 A_2^- U_2^-;$$

here $A_j^- = \mathrm{const}$, $\widetilde{u} \in V^2_{\gamma,\delta}(G(\varepsilon))$ for small $\delta > 0$. Then

$$\|\widetilde{u}; V^2_{\gamma,\delta}(G(\varepsilon))\| + |A_1^-| + |A_2^-| \le c \|f; V^0_{\gamma,\delta}(G(\varepsilon))\|, \tag{2.5.3}$$

where c is a constant independent of f and ε.

Proof. Step A. First we construct an auxiliary function u_p. As it was mentioned before, $\widetilde{s}_{12}$ has a pole $k_p^2 = k_r^2 - ik_i^2$ (see (2.4.20)). Multiply the solutions to the limit problems, involved in (2.4.1), by $A(k) b_2 \beta \varepsilon^{2\pi/\omega} / s_{12}(\varepsilon, k) e^{i\nu_1 d}$, put $k = k_p$, and denote the resulting functions by adding the subscript p. Then

$$\begin{aligned} v_{1p}(x,y;\varepsilon) &= \varepsilon^{2\pi/\omega}(b_1\beta + O(\varepsilon^{2\pi/\omega}))\mathbf{v}_1(x,y;k_p),\\ v_{3p}(x,y;\varepsilon) &= \varepsilon^{2\pi/\omega} b_2\beta\mathbf{v}_1(x,y;k_p); \end{aligned} \tag{2.5.4}$$

$$\begin{aligned} v_{2p}(x,y;\varepsilon) = &\left(-\frac{1}{b_1} + O\big(\varepsilon^{2\pi/\omega}\big)\right)\mathbf{v}_{21}(x,y;k_p)\\ &+ \varepsilon^{2\pi/\omega}\left(-\alpha\frac{b_2}{b_1} + O\big(\varepsilon^{2\pi/\omega}\big)\right)\mathbf{v}_{22}(x,y;k_p), \end{aligned}$$

$$\begin{aligned} w_{1p}(\xi_1,\eta_1;\varepsilon) = b_1\varepsilon^{\pi/\omega}\Big(&\varepsilon^{2\pi/\omega}\Big(a(k_p)\beta + O(\varepsilon^{2\pi/\omega})\Big)\mathbf{w}_1^l(\xi_1,\eta_1)\\ &+ \Big(1 + O(\varepsilon^{2\pi/\omega})\Big)\mathbf{w}_1^r(\xi_1,\eta_1)\Big), \end{aligned} \tag{2.5.5}$$

$$\begin{aligned} w_{2p}(\xi_2,\eta_2;\varepsilon) = b_2\varepsilon^{\pi/\omega}\Big(&\Big(1 + O(\varepsilon^{2\pi/\omega})\Big)\mathbf{w}_1^l(\xi_2,\eta_2)\\ &+ a(k_p)\beta\varepsilon^{2\pi/\omega}\mathbf{w}_1^r(\xi_2,\eta_2)\Big); \end{aligned} \tag{2.5.6}$$

the dependence of k_p on ε is not shown. We set

$$\begin{aligned} u_p(x,y;\varepsilon) = \Xi(x,y)\Big[&\chi_{1,\varepsilon}(x,y)v_{1p}(x,y;\varepsilon) + \Theta(\varepsilon^{-2\sigma}r_1)w_{1p}(\varepsilon^{-1}x_1,\varepsilon^{-1}y_1;\varepsilon)\\ &+ \chi_{2,\varepsilon}(x,y)v_{2p}(x,y;\varepsilon) + \Theta(\varepsilon^{-2\sigma}r_2)w_{2p}(\varepsilon^{-1}x_2,\varepsilon^{-1}y_2;k,\varepsilon)\\ &+\chi_{3,\varepsilon}(x,y)v_{2p}(x,y;k,\varepsilon)\Big], \end{aligned} \tag{2.5.7}$$

where Ξ is a cut-off function in $G(\varepsilon)$ that is equal to 1 on the set $G(\varepsilon)\cap\{|x| < R\}$ and to 0 on $G(\varepsilon)\cap\{|x| > R+1\}$ for a large $R > 0$. The principal part of the norm of u_p is given by $\chi_{2,\varepsilon}v_{2p}$. Considering the definitions of v_{2p} and $\mathbf{v}_{21}$ (see Section 2.2) and Lemma 2.3.2, we get $\|\chi_{2,\varepsilon}v_{2p}\| = \|v_0\| + o(1)$.

Step B. Let us show that

$$\|(\Delta + k_p^2)u_p\| \le c\varepsilon^{\pi/\omega+\kappa}, \tag{2.5.8}$$

where $\kappa = \min\{\pi/\omega, 3\pi/\omega - \sigma_1, \gamma+1\}$, $\sigma_1 = 2\sigma(3\pi/\omega - \gamma + 1)$; until Step C, $\|\cdot\|$ stands for $\|\cdot\,; V^0_{\gamma,\delta}(G(\varepsilon))\|$. If $\pi/\omega < \gamma+1$ and σ is sufficiently small so that $2\pi/\omega > \sigma_1$, then $\kappa = \pi/\omega$.

In view of (2.5.7),

$$\begin{aligned} &(\Delta + k_p^2)u_p(x,y;\varepsilon)\\ &\quad=[\Delta,\chi_{1,\varepsilon}]\Big(v_1(x,y;\varepsilon) - b_1\beta\varepsilon^{2\pi/\omega}(r_1^{-\pi/\omega} + a(k_p)r_1^{\pi/\omega})\Phi(\pi-\varphi_1)\Big)\\ &\qquad+ [\Delta,\Theta]w_{1p}(\varepsilon^{-1}x_1,\varepsilon^{-1}y_1;\varepsilon) - k^2\Theta(\varepsilon^{-2\sigma}r_1)w_{1p}(\varepsilon^{-1}x_1,\varepsilon^{-1}y_1;\varepsilon)\\ &\qquad+ [\Delta,\chi_{2,\varepsilon}]\Big(v_2(x,y;\varepsilon) - \Theta(r_1)\big(b_{1p}^-(\varepsilon)r_1^{-\pi/\omega} + b_{1p}^+(\varepsilon)r_1^{\pi/\omega}\big)\Phi(\pi-\varphi_1)\\ &\qquad\qquad- \Theta(r_2)\big(a_{2p}^-(\varepsilon)r_2^{-\pi/\omega} + a_{2p}^+(\varepsilon)r_2^{\pi/\omega}\big)\Phi(\varphi_2)\Big)\\ &\qquad+ [\Delta,\Theta]w_{2p}(\varepsilon^{-1}x_2,\varepsilon^{-1}y_2;\varepsilon) - k^2\Theta(\varepsilon^{-2\sigma}r_2)w_{2p}(\varepsilon^{-1}x_2,\varepsilon^{-1}y_2;\varepsilon)\\ &\qquad+ [\Delta,\chi_{3,\varepsilon}]\Big(v_3(x,y;\varepsilon) - b_2\beta\varepsilon^{2\pi/\omega}(r_2^{-\pi/\omega} + a(k_p)r_2^{\pi/\omega})\Phi(\varphi_2)\Big)\\ &\qquad\qquad+ [\Delta,\Xi]v_1(x,y;\varepsilon) + [\Delta,\Xi]v_3(x,y;\varepsilon), \end{aligned}$$

where

$$b_{1p}^{-} = O(\varepsilon^{2\pi/\omega}), \qquad b_{1p}^{+} = b_1 + O(\varepsilon^{2\pi/\omega}),$$
$$a_{2p}^{-} = O(\varepsilon^{2\pi/\omega}), \qquad a_{2p}^{+} = b_2 + O(\varepsilon^{2\pi/\omega}).$$

Taking into account the asymptotics of $\mathbf{v}_1$ as $r_1 \to 0$ and passing to the variables $(\xi_1, \eta_1) = (\varepsilon^{-1}x_1, \varepsilon^{-1}y_1)$, we obtain

$$\left\|(x,y) \mapsto [\Delta, \chi_{1,\varepsilon}] \left(\mathbf{v}_1(x,y) - (r_1^{-\pi/\omega} + a(k_p) r_1^{\pi/\omega})\Phi(\pi - \varphi_1)\right)\right\|^2$$
$$\leq c \int_{G(\varepsilon)} (r_1^2 + \varepsilon^2)^{\gamma} \left|[\Delta, \chi_{1,\varepsilon}] r_1^{-\pi/\omega+2}\Phi(\pi - \varphi_1)\right|^2 dxdy \leq c\varepsilon^{2(\gamma - \pi/\omega+1)}.$$

This and (2.5.4) imply the estimate

$$\left\|(x,y) \mapsto [\Delta, \chi_{1,\varepsilon}] \left(v_1(x,y) - (r_1^{-\pi/\omega} + a(k_p) r_1^{\pi/\omega})\Phi(\pi - \varphi_1)\right)\right\| \leq c\varepsilon^{\gamma+\pi/\omega+1}.$$

Analogously,

$$\Big\|(x,y) \mapsto [\Delta, \chi_{2,\varepsilon}] \Big(v_2(x,y) - \Theta(r_1)\big(b_{1p}^{-}(\varepsilon) r_1^{-\pi/\omega} + b_{1p}^{+}(\varepsilon) r_1^{\pi/\omega}\big)\Phi(\pi - \varphi_1)$$
$$- \Theta(r_2)\big(a_{2p}^{-}(\varepsilon) r_2^{-\pi/\omega} + a_{2p}^{+}(\varepsilon) r_2^{\pi/\omega}\big)\Phi(\varphi_2)\Big)\Big\| \leq c\varepsilon^{\gamma+\pi/\omega+1},$$
$$\left\|(x,y) \mapsto [\Delta, \chi_{3,\varepsilon}] \left(v_3(x,y) - (r_2^{-\pi/\omega} + a(k_p) r_2^{\pi/\omega})\Phi(\varphi_2)\right)\right\| \leq c\varepsilon^{\gamma+\pi/\omega+1}.$$

It is evident, that

$$\|[\Delta, \Xi] v_l\| \leq c\varepsilon^{2\pi/\omega}, \quad l = 1, 3.$$

Further, since $\mathbf{w}_j^l$ behaves like $O(\rho_j^{-3\pi/\omega})$ at infinity, we have

$$\int_{G(\varepsilon)} (r_j^2 + \varepsilon^2)^{\gamma} \left|[\Delta, \Theta]\mathbf{w}_j^l(\varepsilon^{-1}x_j, \varepsilon^{-1}y_j)\right|^2 dx_j dy_j$$
$$\leq c \int_{K_j} (r_j^2 + \varepsilon^2)^{\gamma} \left|[\Delta, \Theta](\varepsilon^{-1}r_j)^{-3\pi/\omega}\Phi_2(\varphi_j)\right|^2 dx_j dy_j \leq c\varepsilon^{2(3\pi/\omega - \sigma_1)},$$

where $\sigma_1 = 2\sigma(3\pi/\omega - \gamma + 1)$. A similar inequality holds with $\mathbf{w}_j^l$ replaced by $\mathbf{w}_j^r$. Considering (2.5.5)–(2.5.6), we get the estimate

$$\|[\Delta, \Theta] w_{jp}\| \leq c\varepsilon^{4\pi/\omega - \sigma_1}.$$

Finally, using (2.5.5)–(2.5.6) once more, taking into account the estimate

$$\int_{G(\varepsilon)} (r_j^2 + \varepsilon^2)^{\gamma} \left|\Theta(\varepsilon^{-2\sigma} r_j)\mathbf{w}_j^l(\varepsilon^{-1}x_j, \varepsilon^{-1}y_j)\right|^2 dx_j dy_j$$
$$= \varepsilon^{2\gamma+2} \int_{\Omega} (\rho_j^2 + 1)^{\gamma} \left|\Theta(\varepsilon^{1-2\sigma}\rho_j)\mathbf{w}_j^l(\xi_j, \eta_j)\right|^2 d\xi_j d\eta_j \leq c\varepsilon^{2\gamma+2},$$

and a similar estimate for $\mathbf{w}_j^r$, we derive

$$\left\|(x,y) \mapsto \Theta(\varepsilon^{-2\sigma} r_j) w_{jp}(\varepsilon^{-1}x_j, \varepsilon^{-1}y_j)\right\| \leq c\varepsilon^{\pi/\omega+\gamma+1}.$$

Combining the obtained estimates, we arrive at (2.5.8).

Step C. This part contains somewhat modified arguments from the proof of Theorem 5.5.1 in [6]. Rewrite the right-hand side of the problem (2.5.1) in the form:

$$\begin{aligned} f(x,y) = {} & f_1(x,y;\varepsilon) + f_2(x,y;\varepsilon) + f_3(x,y;\varepsilon) \\ & + \varepsilon^{-\gamma-1}F_1(\varepsilon^{-1}x_1, \varepsilon^{-1}y_1;\varepsilon_1) + \varepsilon^{-\gamma-1}F_2(\varepsilon^{-1}x_2, \varepsilon^{-1}y_2;\varepsilon), \end{aligned} \tag{2.5.9}$$

where

$$\begin{aligned} f_l(x,y;\varepsilon) &= \chi_{l,\varepsilon^\sigma}(x,y)f(x,y), \\ F_j(\xi_j,\eta_j;\varepsilon) &= \varepsilon^{\gamma+1}\Theta(\varepsilon^{1-\sigma}\rho_j)f(x_{O_j}+\varepsilon\xi_j, y_{O_j}+\varepsilon\eta_j); \end{aligned}$$

(x,y) are arbitrary Cartesian coordinates; (x_{O_j}, y_{O_j}) stand for the coordinates of O_j in the system (x,y); x_j, y_j have been introduced in Section 2.4. From the definition of the norms it follows that

$$\|f_1; V^0_{\gamma,\delta}(G_1)\| + \|f_2; V^0_\gamma(G_2)\| + \|f_3; V^0_{\gamma,\delta}(G_3)\| + \|F_j; V^0_\gamma(\Omega_j)\| \le \|f; V^0_{\gamma,\delta}(G(\varepsilon))\|. \tag{2.5.10}$$

Consider solutions v_l and w_j to the limit problems

$$\begin{aligned} \Delta v + k^2 v = f_l \text{ in } G_l, &\qquad v = 0 \text{ on } \partial G_l, \\ \Delta w = F_j \text{ in } \Omega_j, &\qquad w = 0 \text{ on } \partial\Omega_j, \end{aligned}$$

respectively; moreover, v_l with $l = 1,3$ satisfy the intrinsic radiation conditions at infinity, and v_2 satisfies the condition $(v_2, v_0)_{G_2} = 0$. According to Propositions 2.2.1, 2.2.2, and 2.2.3, the problems in G_l and Ω_j are uniquely solvable and

$$\begin{aligned} \|v_2; V^2_\gamma(G_2)\| &\le c_2\|f_2; V^0_\gamma(G_2)\|, \\ \|v_l; V^2_{\gamma,\delta,-}(G_l)\| &\le c_l\|f_l; V^0_{\gamma,\delta}(G_l)\|,\ l = 1,3, \\ \|w_j; V^2_\gamma(\Omega_j)\| &\le C_j\|F_j; V^0_\gamma(\Omega_j)\|,\ j = 1,2, \end{aligned} \tag{2.5.11}$$

where c_l and C_j are independent of ε. We set

$$\begin{aligned} U(x,y;\varepsilon) = {} & \chi_{1,\varepsilon}(x,y)v_1(x,y;\varepsilon) + \varepsilon^{-\gamma+1}\Theta(r_1)w_1(\varepsilon^{-1}x_1, \varepsilon^{-1}y_1;\varepsilon) \\ & + \chi_{2,\varepsilon}(x,y)v_2(x,y;\varepsilon) + \varepsilon^{-\gamma+1}\Theta(r_2)w_2(\varepsilon^{-1}x_2, \varepsilon^{-1}y_2;\varepsilon) + \chi_{3,\varepsilon}(x,y)v_3(x,y;\varepsilon). \end{aligned}$$

The estimates (2.5.10) and (2.5.11) lead to

$$\|U; V^2_{\gamma,\delta,-}(G(\varepsilon))\| \le c\|f; V^0_{\gamma,\delta}(G(\varepsilon))\| \tag{2.5.12}$$

with c independent of ε. Denote the mapping $f \mapsto U$ by R_ε. Arguing as in the proof of Theorem 5.5.1 in [6], we obtain $(\Delta + k^2)R_\varepsilon = I + S_\varepsilon$, where S_ε is an operator in $V^0_{\gamma,\delta}(G(\varepsilon))$ of small norm.

Step D. Recall that the operator S_ε is defined on the subspace $V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$. We need the image of the operator S_ε to be included in $V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$, too. To this end, replace the mapping R_ε by $\widetilde{R}_\varepsilon : f \mapsto U(f) + a(f)u_p$, where u_p has been constructed in Step **A**, $a(f)$ is a constant. Then $(\Delta + k^2)\widetilde{R}_\varepsilon = I + \widetilde{S}_\varepsilon$ with $\widetilde{S}_\varepsilon = S_\varepsilon + a(\cdot)(\Delta + k^2)u_p$. The condition $(\chi_{2,\varepsilon^\sigma}\widetilde{S}_\varepsilon f, v_0)_{G_2} = 0$ as $k = k_0$ gives

$$a(f) = -(\chi_{2,\varepsilon^\sigma} S_\varepsilon f, v_0)_{G_2} / (\chi_{2,\varepsilon^\sigma}(\Delta + k_0^2)u_p, v_0)_{G_2}.$$

Prove that $\|\widetilde{S}_\varepsilon\| \le c\|S_\varepsilon\|$, where c is independent of ε, k. We have

$$\|\widetilde{S}_\varepsilon f\| \le \|S_\varepsilon f\| + |a(f)|\, \|(\Delta + k^2)u_p\|.$$

The estimate (2.5.8) (with $\gamma > \pi/\omega - 2$ and $2\pi/\omega > \sigma_1$), the formula for k_p, and the condition $k^2 - k_0^2 = O\big(\varepsilon^{2\pi/\omega}\big)$ imply the equality

$$\|(\Delta + k^2)u_p; V^0_{\gamma,\delta}\| \le |k^2 - k_p^2|\, \|u_p; V^0_{\gamma,\delta}\| + \|(\Delta + k_p^2)u_p; V^0_{\gamma,\delta}\| \le c\varepsilon^{2\pi/\omega}.$$

Since the supports of the functions $(\Delta + k_p^2)u_p$ and $\chi_{2,\varepsilon^\sigma}$ do not intersect, we have

$$|(\chi_{2,\varepsilon^\sigma}(\Delta + k_0^2)u_p, v_0)_{G_2}| = |(k_0^2 - k_p^2)(u_p, v_0)_{G_2}| \ge c\varepsilon^{2\pi/\omega}.$$

Further, $\gamma - 1 < \pi/\omega$, so

$$|(\chi_{2,\varepsilon^\sigma} S_\varepsilon f, v_0)_{G_2}| \le \|S_\varepsilon f; V^0_{\gamma,\delta}(G(\varepsilon))\|\, \|v_0; V^0_{-\gamma}(G_2)\| \le c\|S_\varepsilon f; V^0_{\gamma,\delta}(G(\varepsilon))\|.$$

Hence,

$$|a(f)| \le c\varepsilon^{-2\pi/\omega}\|S_\varepsilon f; V^0_{\gamma,\delta}(G(\varepsilon))\|$$

and $\|\widetilde{S}_\varepsilon f\| \le c\|S_\varepsilon f\|$. Thus, the operator $I + \widetilde{S}_\varepsilon$ in $V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$ is invertible, which is also true for the operator of the problem (2.5.1):

$$A_\varepsilon : u \mapsto \Delta u + k^2 u : \mathring{V}^{2,\perp}_{\gamma,\delta,-}(G(\varepsilon)) \mapsto V^{0,\perp}_{\gamma,\delta}(G(\varepsilon));$$

here $\mathring{V}^{2,\perp}_{\gamma,\delta,-}(G(\varepsilon))$ denotes the space of elements of $V^2_{\gamma,\delta,-}(G(\varepsilon))$ that vanish on $\partial G(\varepsilon)$ and are sent by the operator $\Delta + k^2$ into $V^{0,\perp}_{\gamma,\delta}$. The inverse operator

$$A_\varepsilon^{-1} = \widetilde{R}_\varepsilon (I + \widetilde{S}_\varepsilon)^{-1}$$

is bounded uniformly with respect to ε, k. Therefore, the inequality (2.5.3) holds with c independent of ε, k. □

We consider a solution u_1 to the homogeneous problem (2.1.1) defined by

$$u_1(x,y) = \begin{cases} U_1^+(x,y) + s_{11}\, U_1^-(x,y) + O(\exp(\delta x)), & x \to -\infty, \\ s_{12}\, U_2^-(x,y) + O(\exp(-\delta x)), & x \to +\infty. \end{cases}$$

Let s_{11} and s_{12} be the elements of the scattering matrix determined by this solution. Denote by $\widetilde{u}_{1,\sigma}$ the function defined by (2.4.1) with $\Theta(r_j)$ replaced by $\Theta(\varepsilon_j^{-2\sigma} r_j)$ and with removed R; $\widetilde{s}_{11}$, $\widetilde{s}_{12}$ are the same as in (2.4.18)–(2.4.19).

Theorem 2.5.2. *Let the conjectures in Proposition* 2.5.1 *be fulfilled. Then the inequality*

$$|s_{11} - \widetilde{s}_{11}| + |s_{12} - \widetilde{s}_{12}| \leq c|\widetilde{s}_{12}|\varepsilon^{2-\delta}$$

holds with constant c independent of ε and k, δ being an arbitrarily small positive number.

Proof. The difference $R = u_1 - \widetilde{u}_{1,\sigma}$ is in the space $V^2_{\gamma,\delta,-}(G(\varepsilon))$ and

$$f_1 := (\Delta + k^2)(u_1 - \widetilde{u}_{1,\sigma})$$

is in $V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$. By Proposition 2.5.1,

$$\|R; V^2_{\gamma,\delta,-}(G(\varepsilon))\| \leq c\,\|f_1; V^0_{\gamma,\delta}(G(\varepsilon))\|. \tag{2.5.13}$$

Let us show that

$$\|f_1; V^0_{\gamma,\delta}(G(\varepsilon))\| \leq c|\widetilde{s}_{12}|(\varepsilon^{\gamma-\pi/\omega+1} + \varepsilon^{2\pi/\omega-\sigma_1}), \tag{2.5.14}$$

where $\sigma_1 = 2\sigma(3\pi/\omega - \gamma + 1)$. The required estimate is a consequence of the last two inequalities with $\gamma = \pi/\omega + 1 - \delta$ and $\sigma_1 = \delta$.

Arguing as in Step B of the proof of the previous statement, we obtain the estimate

$$\begin{aligned}\|f_1; V^0_{\gamma,\delta}(G(\varepsilon))\| &\leq c(\varepsilon^{\gamma+1} + \varepsilon^{3\pi/\omega-\sigma_1})\\ &\quad\times \max_{j=1,2}(|a_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |a_j^+(\varepsilon)|\varepsilon^{\pi/\omega} + |b_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |b_j^+(\varepsilon)|\varepsilon^{\pi/\omega}).\end{aligned}$$

From (2.4.11) it follows that

$$(|a_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |a_j^+(\varepsilon)|\varepsilon^{\pi/\omega}) \leq c(|b_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |b_j^+(\varepsilon)|\varepsilon^{\pi/\omega}).$$

Using the formulas (2.4.8) and (2.4.10) for $b_j^\pm$ and relations (2.4.17) and (2.4.15), we get

$$|b_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |b_j^+(\varepsilon)|\varepsilon^{\pi/\omega} \leq c\varepsilon^{-\pi/\omega}|\widetilde{s}_{12}(\varepsilon)|.$$

Comparing the obtained estimates, we arrive at (2.5.14). □

Theorem 2.5.2 and formulas (2.4.21) – (2.4.22) imply the next statement.

Theorem 2.5.3. *For $|k^2 - k_r^2| = O(\varepsilon^{2\pi/\omega})$ the asymptotic expansions*

$$\begin{aligned} T(k,\varepsilon) &= \frac{1}{1 + P^2\left(\dfrac{k^2 - k_r^2}{\varepsilon^{2\pi/\omega}}\right)^2}\big(1 + O(\varepsilon^{2-\delta})\big),\\ k_r^2(\varepsilon) &= k_0^2 + 2b_1^2\beta\varepsilon^{2\pi/\omega} + O\big(\varepsilon^{2\pi/\omega+2-\delta}\big),\\ \Upsilon(\varepsilon) &= \left|\frac{1}{P}\right|\varepsilon^{4\pi/\omega}\big(1 + O(\varepsilon^{2-\delta})\big)\end{aligned}$$

hold, where $\Upsilon(\varepsilon)$ is the width of the resonant peak at its half-height, δ is an arbitrarily small positive number.

2.6 Comparison of asymptotic and numerical approaches

The principal parts of the asymptotic formulas in Theorem 2.5.3 contain the constants b_1, $|A|$, α, β. To find them one has to solve numerically several boundary value problems. We state the problems and describe a way to solve them. We also outline a method for computing the waveguide scattering matrix taken from the paper [7]. Then we compare the asymptotics with calculated constants and the numerically found scattering matrix.

2.6.1 Problems and methods for numerical analysis

Calculation of b_1

To find b_1 in (2.3.6), we solve the spectral problem

$$\Delta v + k^2 v = 0 \quad \text{in } G_2, \qquad v = 0 \quad \text{on } \partial G_2,$$

by FEM (for the details see Appendix 1). Let v_0 be an eigenfunction corresponding to k_0^2 and normalized by

$$\int_{G_2} |v_0(x,y)|^2 \, dxdy = 1.$$

Then b_1 can be determined (approximately) by

$$b_1 = \varepsilon^{-\pi/\omega} \frac{v_0(\varepsilon, 0)}{\Phi(0)} = \sqrt{\pi} \varepsilon^{-\pi/\omega} v_0(\varepsilon, 0).$$

Calculation of $|A|$

The constant $A \neq 0$ has arisen in the asymptotics (2.3.4) of the solution $\mathbf{v}_1$ of homogeneous problem (2.2.1) in G_1; the solution is defined by the formula (2.3.3). To avoid difficulties related to the unboundedness of $\mathbf{v}_1$ in a neighborhood of the point O_1, introduce $\mathbf{v} = (\mathbf{v}_1 - \overline{\mathbf{v}}_1)/A$,

$$\mathbf{v}(x_1, y_1) \sim \begin{cases} \mathbf{a} r_1^{\pi/\omega} \Phi(\varphi_1) & r_1 \to 0; \\ \left(e^{-i\nu_1 x_1} + \dfrac{\overline{A}}{A} e^{i\nu_1 x_1} \right) \Psi_1(y_1) + O(e^{-\delta |x_1|}) & x_1 \to -\infty, \end{cases} \tag{2.6.1}$$

where $\mathbf{a} = 2i \operatorname{Im} a / A$. According to Lemma 2.3.1 in [5], we have $\operatorname{Im} a = |A|^2$, and hence $\mathbf{a} = 2i\overline{A}$. Thus, it suffices to calculate $\mathbf{a}$. Denote the truncated domain

$$G_1 \cap \{(x_1, y_1) : x_1 > -R\}$$

by G_1^R and put $\Gamma^R := \partial G_1^R \cap \{(x_1, y_1) : x_1 = -R\}$. Introduce the problem

$$\begin{aligned} \Delta V(x_1, y_1) + k^2 V(x_1, y_1) &= 0, & (x_1, y_1) &\in G_1^R; \\ V(x_1, y_1) &= 0, & (x_1, y_1) &\in \partial G_1^R \backslash \Gamma^R; \\ \partial_n V(x_1, y_1) + i\nu_1 V(x_1, y_1) &= 2i\nu_1 e^{i\nu_1 R} \Psi_1(y_1), & (x_1, y_1) &\in \Gamma^R; \end{aligned} \tag{2.6.2}$$

the function Ψ_1 is defined by (2.1.4). The solution V is found by FEM (for the details see Appendix 2). One may put

$$\mathbf{a} = \sqrt{\pi}\varepsilon^{-\pi/\omega} V(-\varepsilon, 0).$$

Calculation of α and β

We introduce the boundary value problem for calculation of α and β in (2.2.11), denote the truncated domain $\Omega \cap \{(r, \varphi) : r < R\}$ by Ω^R, and put

$$\Gamma^R := \partial\Omega \cap \{(r, \varphi) : r = R\}.$$

Consider the problem

$$\begin{aligned} \Delta w(\xi, \eta) &= 0, & (\xi, \eta) &\in \Omega^R; \\ w(\xi, \eta) &= 0, & (\xi, \eta) &\in \partial\Omega^R \backslash \Gamma^R; \\ \partial_n w(\xi, \eta) + \zeta w(\xi, \eta) &= g(\xi, \eta), & (\xi, \eta) &\in \Gamma^R. \end{aligned} \tag{2.6.3}$$

If w is a solution and $\zeta > 0$, then

$$\|w; L_2(\Gamma^R)\| \leqslant \zeta^{-1} \|g; L_2(\Gamma^R)\|. \tag{2.6.4}$$

Indeed, substitute $u = v = w$ to the Green formula

$$\begin{aligned} (\Delta u, v)_{\Omega^R} &= (\partial_n u, v)_{\partial\Omega^R} - (\nabla u, \nabla v)_{\Omega^R} \\ &= (\partial_n u, v)_{\partial\Omega^R \backslash \Gamma^R} + (\partial_n u + \zeta u, v)_{\Gamma^R} - \zeta(u, v)_{\Gamma^R} - (\nabla u, \nabla v)_{\Omega^R}, \end{aligned}$$

and get

$$0 = (g, w)_{\Gamma^R} - \zeta \|w; L_2(\Gamma^R)\|^2 - \|\nabla w; L_2(\Omega^R)\|^2.$$

From this and the obvious chain of inequalities

$$\begin{aligned} \zeta \|w; L_2(\Gamma^R)\|^2 &\leqslant \zeta \|w; L_2(\Gamma^R)\|^2 + \|\nabla w; L_2(\Omega^R)\|^2 = (g, w)_{\Gamma^R} \\ &\leqslant \|w; L_2(\Gamma^R)\| \, \|g; L_2(\Gamma^R)\| \end{aligned}$$

we obtain (2.6.4). Denote the left (right) part of Γ^R by Γ^R_- (Γ^R_+). Let W be the solution of (2.6.3) as $\zeta = \pi/\omega R$, $g|_{\Gamma^R_-} = 0$, and $g|_{\Gamma^R_+} = (2\pi/\omega) R^{(\pi/\omega)-1} \Phi(\varphi)$. Let, in addition, w^r be a solution to the homogeneous problem (2.2.6) in the domain Ω with asymptotics of the form (2.2.11). Since the asymptotics can be differentiated, $w_r - W$ satisfies (2.6.3) with $g = O(R^{-(3\pi/\omega)-1})$. According to (2.6.4),

$$\|w_r - W; L_2(\Gamma^R)\| \leqslant c \frac{\omega R}{\pi} R^{-(3\pi/\omega)-1} = c' R^{-3\pi/\omega}$$

as $R \to +\infty$. We find W with FEM (for the details see Appendix 2) and determine β by the equality

$$\beta = \frac{W(-R, 0)}{\Phi(0)} R^{\pi/\omega} = \sqrt{\pi} W(-R, 0) R^{\pi/\omega}.$$

Obviously, $\|(w_r - R^{\pi/\omega}\Phi(\varphi)) - (W - R^{\pi/\omega}\Phi(\varphi)); L_2(\Gamma^R)\| \leqslant c' R^{-3\pi/\omega}$, therefore we put

$$\alpha = \frac{W(R, 0) - R^{\pi/\omega}\Phi(0)}{\Phi(0)} R^{\pi/\omega} = \sqrt{\pi} W(R, 0) R^{\pi/\omega} - R^{2\pi/\omega}.$$

2.6.2 Calculation of the scattering matrix

Let us describe the method for calculation of the scattering matrix, considering only electrons of energy between the first and the second threshold. Then in (2.1.4) we have $M = 1$. Put

$$G(\varepsilon, R) = G(\varepsilon) \cap \{(x,y) : -R < x < d+R\},$$
$$\Gamma_1^R = \partial G(\varepsilon, R) \cap \{(x,y) : x = -R\}, \quad \Gamma_2^R = \partial G(\varepsilon, R) \cap \{(x,y) : x = d+R\}$$

for large R. As an approximation to the row (s_{11}, s_{12}) of the scattering matrix $S = S(k)$ we take the minimizer of a quadratic functional. To construct such a functional we consider the problem

$$\begin{aligned} \Delta \mathcal{X}^R + k^2 \mathcal{X}^R &= 0 && \text{in } G(\varepsilon, R), \\ \mathcal{X}^R &= 0 && \text{on } \partial G(\varepsilon, R) \setminus (\Gamma_1^R \cup \Gamma_2^R), \\ (\partial_n + i\zeta)\mathcal{X}^R &= i(-\nu_1 + \zeta) e^{-i\nu_1 R} \Psi_1(y) && \\ &\quad + a_1\, i(\nu_1 + \zeta) e^{i\nu_1 R} \Psi_1(y) && \text{on } \Gamma_1^R, \\ (\partial_n + i\zeta)\mathcal{X}^R &= a_2\, i(\nu_1 + \zeta) e^{i\nu_1(d+R)} \Psi_1(y) && \text{on } \Gamma_2^R, \end{aligned} \tag{2.6.5}$$

where $\zeta \in \mathbb{R} \setminus \{0\}$ is an arbitrary fixed number, and a_1, a_2 are complex numbers. As an approximation for the row (s_{11}, s_{12}) we take the minimizer $a^0(R) = (a_1^0(R), a_2^0(R))$ of the functional

$$\begin{aligned} J^R(a_1, a_2) = &\| \mathcal{X}^R - e^{-i\nu_1 R}\Psi_1 - a_1 e^{i\nu_1 R}\Psi_1; L_2(\Gamma_1^R)\|^2 \\ &+ \| \mathcal{X}^R - a_2\, e^{i\nu_1(d+R)}\Psi_1; L_2(\Gamma_2^R)\|^2, \end{aligned} \tag{2.6.6}$$

where $\mathcal{X}^R$ is a solution to the problem (2.6.5). From the results of [7] it follows that $a_j^0(R,k) \to s_{1j}(k)$ with exponential rate as $R \to \infty$. More precisely, there exist positive constants Λ and C such that $|a_j^0(R,k) - s_{1j}(k)| \leqslant C \exp(-\Lambda R)$, $j = 1, 2$, for all $k^2 \in [\mu_1, \mu_2]$ and sufficiently large R; the interval $[\mu_1, \mu_2]$ of continuous spectrum of the problem (2.1.1) lies between the first and the second thresholds and does not contain the thresholds. (Note, that application of the method is not hindered by possible presence on the interval $[\mu_1, \mu_2]$ of eigenvalues of the problem (2.1.1) corresponding to eigenfunctions exponentially decaying at infinity.) To express $\mathcal{X}^R$ by means of a_1, a_2, we consider the problems

$$\begin{aligned} \Delta v_1^{\pm} + k^2 v_1^{\pm} &= 0 && \text{in } G(\varepsilon, R), \\ v_1^{\pm} &= 0 && \text{on } \partial G(\varepsilon, R) \setminus (\Gamma_1^R \cup \Gamma_2^R), \\ (\partial_n + i\zeta) v_1^{\pm} &= i(\mp\nu_1 + \zeta) e^{\mp i\nu_1 R}\Psi_1 && \text{on } \Gamma_1^R, \\ (\partial_n + i\zeta) v_1^{\pm} &= 0 && \text{on } \Gamma_2^R, \end{aligned} \tag{2.6.7}$$

and

$$\begin{aligned} \Delta v_2^{\pm} + k^2 v_2^{\pm} &= 0 && \text{in } G(\varepsilon, R), \\ v_2^{\pm} &= 0 && \text{on } \partial G(\varepsilon, R) \setminus (\Gamma_1^R \cup \Gamma_2^R), \\ (\partial_n + i\zeta) v_2^{\pm} &= 0 && \text{on } \Gamma_1^R, \\ (\partial_n + i\zeta) v_2^{\pm} &= i(\mp\nu_2 + \zeta) e^{\mp i\nu_2(d+R)}\Psi_2 && \text{on } \Gamma_2^R. \end{aligned} \tag{2.6.8}$$

Let $v_j^{\pm} = v_{j,R}^{\pm}$ be solutions to problems (2.6.7), (2.6.8), then $\mathcal{X}^R = v_{1,R}^{+} + \sum_j a_j v_{j,R}^{-}$. Now the functional (2.6.6) can be rewritten in the form

$$J^R(a;k) = \langle a\mathcal{E}^R(k), a\rangle + 2\mathrm{Re}\,\langle \mathcal{F}_1^R(k), a\rangle + \mathcal{G}_1^R(k),$$

where $\langle\cdot,\cdot\rangle$ is the inner product on $\mathbb{C}^2$, and $\mathcal{E}^R$ stands for the 2×2-matrix with entries

$$\begin{aligned}
\mathcal{E}_{11}^R &= \Big((v_1^- - e^{i\nu_1 R}\Psi_1), (v_1^- - e^{i\nu_1 R}\Psi_1)\Big)_{\Gamma_1^R} + (v_1^-, v_1^-)_{\Gamma_2^R},\\
\mathcal{E}_{12}^R &= \Big((v_1^- - e^{i\nu_1 R}\Psi_1), v_2^-\Big)_{\Gamma_1^R} + \Big(v_1^-, (v_2^- - e^{i\nu_1 (d+R)}\Psi_1)\Big)_{\Gamma_2^R},\\
\mathcal{E}_{21}^R &= \Big(v_2^-, (v_1^- - e^{i\nu_1 R}\Psi_1)\Big)_{\Gamma_1^R} + \Big((v_2^- - e^{i\nu_1 (d+R)}\Psi_1), v_1^-\Big)_{\Gamma_2^R},\\
\mathcal{E}_{22}^R &= (v_2^-, v_2^-)_{\Gamma_1^R} + \Big((v_2^- - e^{i\nu_1 (d+R)}\Psi_1), (v_2^- - e^{i\nu_1 (d+R)}\Psi_1)\Big)_{\Gamma_2^R},
\end{aligned}$$

$\mathcal{F}^R(k)$ is the row $(\mathcal{F}_{11}^R(k), \mathcal{F}_{12}^R(k))$ and $\mathcal{G}_1^R(k)$ is the number defined by the equalities

$$\begin{aligned}
\mathcal{F}_{11}^R &= \Big((v_1^+ - e^{-i\nu_1 R}\Psi_1), (v_1^- - e^{i\nu_1 R}\Psi_1)\Big)_{\Gamma_1^R} + (v_1^+, v_1^-)_{\Gamma_2^R},\\
\mathcal{F}_{12}^R &= \Big((v_1^+ - e^{-i\nu_1 R}\Psi_1), v_2^-)\Big)_{\Gamma_1^R} + \Big(v_1^+, (v_2^- - e^{i\nu_1 (d+R)}\Psi_j)\Big)_{\Gamma_2^R},\\
\mathcal{G}_1^R &= \Big((v_1^+ - e^{-i\nu_1 R}\Psi_1), (v_1^+ - e^{-i\nu_1 R}\Psi_1)\Big)_{\Gamma_1^R} + (v_1^+, v_1^+)_{\Gamma_2^R}.
\end{aligned}$$

The minimizer $a^0 = (a_1^0(R,k), a_2^0(R,k))$ satisfies $a^0\mathcal{E}^R + \mathcal{F}_1^R = 0$. The solution to this equation serves as an approximation to the first row of the scattering matrix. In the same way one can show that the approximation to the scattering matrix $S(k)$ is the solution $S^R = S^R(k)$ to the matrix equation of the form $S^R\mathcal{E}^R + \mathcal{F}^R = 0$. If one chooses $\zeta = -\nu_1$, then $v_1^- = v_2^- = 0$, $\mathcal{E}^R = (1/\nu_1)\mathrm{Id}$, and $S^R = -\nu_1\mathcal{F}^R$.

2.6.3 Comparison of the results

Let us compare the asymptotics $k_{res,a}^2(\varepsilon)$ of resonant energy $k_{res}^2(\varepsilon)$ and the approximate value $k_{res,n}^2(\varepsilon)$ obtained numerically. Figure 4 shows good agreement of the values for $0.1 \leqslant \varepsilon \leqslant 0.5$. We have

$$|k_{res,a}^2(\varepsilon) - k_{res,n}^2(\varepsilon)|/k_{res,a}^2(\varepsilon) \leqslant 10^{-3}$$

for $0.1 \leqslant \varepsilon \leqslant 0.3$ and only for $\varepsilon = 0.5$ the ratio approaches $2\cdot 10^{-2}$. For $\varepsilon < 0.1$ the numerical method is ill-conditioned. This is caused by the fact, that the waveguide tends to the 'limit' (see Figure 3), on which the problems for calculation of the scattering matrix are incorrect (ill-posed). This means that the round-off errors cause the larger deviations in the solution and at some ε we get a random vector instead of the sought-for vector of coefficients of the piecewise polynomial function. The asymptotics moves this 'incorrectness' out of numerical part

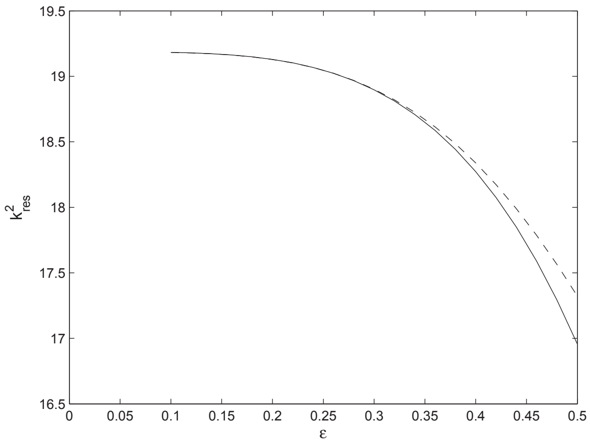


FIGURE 4 Asymptotic description $k^2_{res,a}(\varepsilon)$ (solid curve) and numerical description $k^2_{res,n}(\varepsilon)$ (dashed curve) for resonant energy $k^2_{res}(\varepsilon)$.

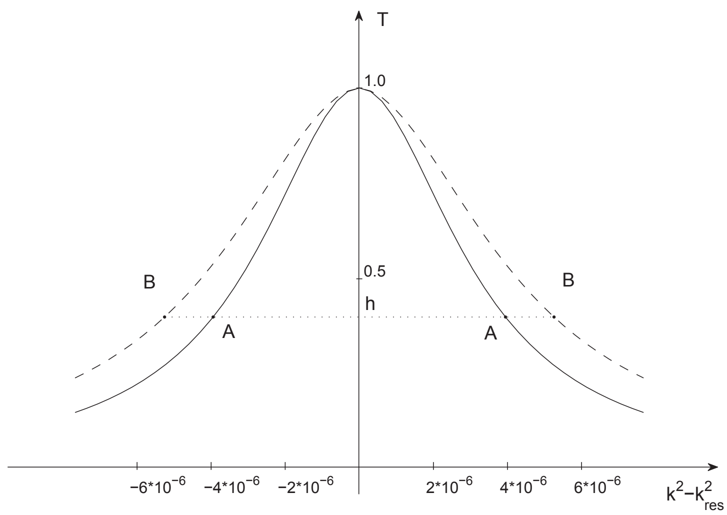


FIGURE 5 The shape of resonant peak for $\varepsilon = 0.2$: asymptotic description $T_a(k^2 - k^2_{res,a})$ (solid curve) and numerical description $T_n(k^2 - k^2_{res,n})$ (dashed curve) for transition coefficient $T(k^2 - k^2_{res})$. The width of resonant peak at height h: asymptotic $\Delta_a(h, \varepsilon) = AA$; numerical $\Delta_n(h, \varepsilon) = BB$.

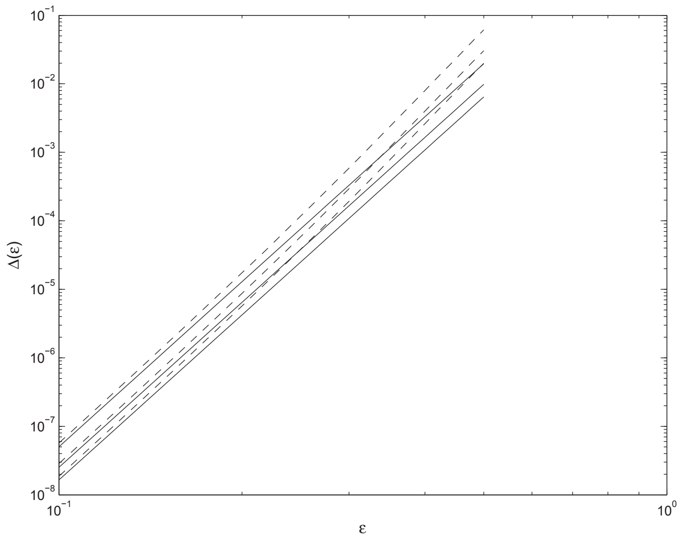


FIGURE 6 The dependence of the width $\Delta(h, \varepsilon)$ of resonant peak on ε for various heights h (dashed line for numerical description, solid line for asymptotic description): the upper pair of lines for $h = 0.2$; the middle lines for $h = 0.5$; the bottom lines for $h = 0.7$.

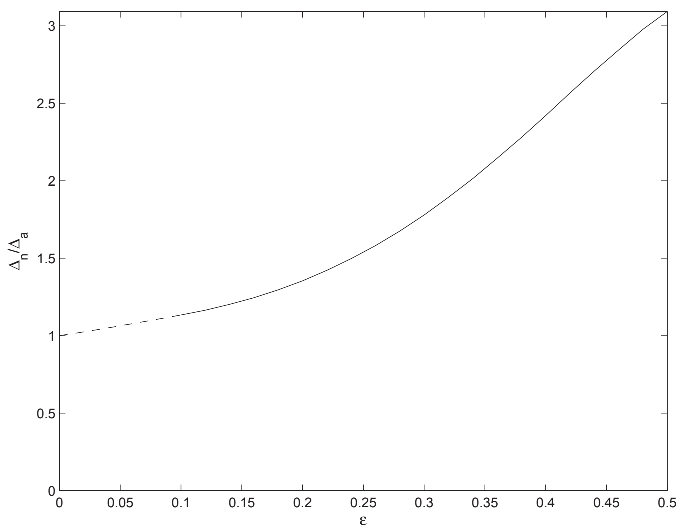


FIGURE 7 Ratio $\Delta_n(h, \varepsilon)/\Delta_a(h, \varepsilon)$ as a function of ε. The ratio is independent of h within the accuracy of the analysis.

(i.e. the problems for the constants that have to be solved numerically) and thus remains efficient at $\varepsilon \to 0$.

The difference between the asymptotic and numerical values becomes more significant as ε increases going out of the interval; the asymptotics becomes unreliable. The numerical method shows that for $\varepsilon \geq 0.5$ the resonant peak turns out to be so wide that the resonant tunneling phenomenon dies out by itself. The forms of "asymptotic" and "numerical" resonant peaks are almost the same (see Figure 5). The difference between the peaks is quantitatively depicted in Figure 6. Moreover, it turns out that the ratio of the width $\Delta_n(h, \varepsilon)$ of numerical peak at height h to $\Delta_a(h, \varepsilon)$ of asymptotic peak is independent of h. The ratio as a function in ε is displayed in Figure 7.

Note that for $\varepsilon = 0.1$ (i.e. at the left end of the band where the numerical and asymptotic results can be compared) the disparity of the results is more significant for the width of resonant peak than that for the resonant energy.

3 ELECTRON FLOW SPIN POLARIZATION IN 2D WAVEGUIDES IN THE PRESENCE OF MAGNETIC FIELD

We consider an infinite two-dimensional waveguide that far from the coordinate origin coincides with a strip. The waveguide has two narrows of diameter ε. The narrows play the role of effective potential barriers for the longitudinal electron motion. The part of waveguide between the narrows becomes a "resonator" and there can arise conditions for electron resonant tunneling. A magnetic field in the resonator can change the basic characteristics of this phenomenon. In the presence of a magnetic field, the tunneling phenomenon is feasible for producing spin-polarized electron flows consisting of electrons with spins of the same direction.

We assume that the whole domain occupied by a magnetic field is in the resonator. An electron wave function satisfies the Pauli equation in the waveguide and vanishes at its boundary. Taking ε as a small parameter, we derive asymptotics for the probability $T(E)$ of an electron with energy E to pass through the resonator, for the "resonant energy" E_{res}, where $T(E)$ takes its maximal value, and for some other resonant tunneling characteristics.

The asymptotic formulas contain some unknown constants. We find them by solving several auxiliary boundary value problems (independent of ε) in unbounded domains. Having the asymptotics with calculated constants, we can take the it as numerical approximation to the resonant tunneling characteristics. Independently, we compute numerically the scattering matrix and compare the asymptotic and numerical results.

3.1 Statement of the problem

To describe the domain $G(\varepsilon)$ in $\mathbb{R}^2$ occupied by the waveguide, we first introduce two auxiliary domains G and Ω in $\mathbb{R}^2$. The domain G is the strip

$$G = \mathbb{R} \times D = \{(x,y) \in \mathbb{R}^2 : \ x \in \mathbb{R};\ y \in D = (-l/2, l/2)\}.$$

Let us define Ω. Denote by K a pair of opposite angles with vertex at the origin O. Assume that K is symmetric about the origin and contains the axis x. The set $K \cap S^1$, where S^1 is a unit circle, consists of two simple arcs. Assume that Ω contains K and a neighborhood of its vertex. Moreover, outside a sufficiently large disc the set Ω coincides with K. The boundary $\partial\Omega$ of Ω is supposed to be smooth (see Figure 1).

We now turn to the waveguide $G(\varepsilon)$. Denote by $\Omega(\varepsilon)$ the domain obtained from Ω by contraction with center at O and coefficient ε. In other words, $(x,y) \in \Omega(\varepsilon)$ if and only if $(x/\varepsilon, y/\varepsilon) \in \Omega$. Let K_j and $\Omega_j(\varepsilon)$ stand for K and $\Omega(\varepsilon)$ shifted by the vector $\mathbf{r}_j = (x_j^0, 0)$, $j = 1, 2$. We assume that $|x_1^0 - x_2^0|$ is sufficiently large so that the distance from $\partial K_1 \cap \partial K_2$ to G is positive. We put (see Figure 8)

$$G(\varepsilon) = G \cap \Omega_1(\varepsilon) \cap \Omega_2(\varepsilon).$$

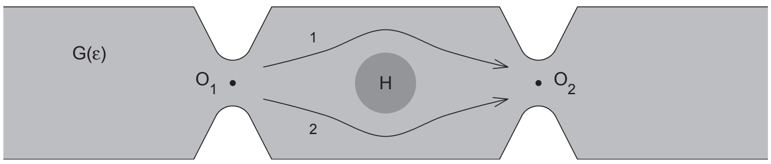


FIGURE 8 The waveguide $G(\varepsilon)$ and the support of magnetic field H in the resonator.

Consider the equations

$$(-i\nabla + \mathbf{A})^2 u \pm Hu = k^2 u, \tag{3.1.1}$$

which are 2D counterparts of the equations describing the motion of electrons of spin $\pm 1/2$ in a magnetic field parallel to z-axis. Here $\nabla = (\partial_x, \partial_y)^T$; $H = \partial_x A_y - \partial_y A_x$. Let H depend only on $\rho = ((x-x_0)^2 + (y-y_0)^2)^{1/2}$, and let $H(\rho) = 0$ as $\rho > R$, where R is a positive constant. Then we can put $\mathbf{A} = A(\rho)\mathbf{e}_\psi$, where $\mathbf{e}_\psi = \rho^{-1}(-y + y_0, x - x_0)$ and

$$A(\rho) = \frac{1}{\rho} \int_0^{\min\{\rho, R\}} tH(t)\, dt.$$

It is evident, that the equality $\partial_x A_y - \partial_y A_x = H$ defines $\mathbf{A}$ up to a summand of the form ∇f.

Let (ρ, ψ) be polar coordinates in the plane xy with center at (x_0, y_0), the angle ψ being measured from a ray parallel to x-axis. Introduce $f(x,y) = c\psi$, where

$$c = \int_0^R tH(t)\,dt.$$

We assume that $-\pi/2 < \psi < 3\pi/2$. The function f is uniquely determined in the waveguide for $|x - x_0| > 0$, moreover, $\nabla f = \mathbf{A}$ for $|x - x_0| > R$. Let $\tau(t)$ be a cut-off function on $\mathbb{R}_+$, equal to 1 as $t > R + 2\delta$ and to 0 as $t < R + \delta$, δ being a positive constant. Put $\mathbf{A}'(x,y) = \mathbf{A}(x,y) - \nabla(\tau(|x - x_0|)f(x,y))$. Then

$$\partial_x A'_y - \partial_y A'_x = \partial_x A_y - \partial_y A_x = H$$

and $\mathbf{A}' = 0$ as $|x - x_0| > R + 2\delta$. The wave function $u' = u\exp\{i\tau f\}$ satisfies (3.1.1) with $\mathbf{A}$ replaced by $\mathbf{A}'$. As $|x - x_0| > R + 2\delta$ the equation (3.1.1) with new potential $\mathbf{A}'$ reduces to the Helmholtz equation

$$-\Delta u' = k^2 u'.$$

In what follows we omit the primes in the notations. We look for solutions to (3.1.1) satisfying the homogeneous Dirichlet boundary condition

$$u = 0 \quad \text{on } \partial G(\varepsilon). \tag{3.1.2}$$

The obtained boundary value problems are self-adjoint with respect to the Green formulas

$$\begin{aligned}((-i\nabla + \mathbf{A})^2 u \pm Hu - k^2 u, v)_{G(\varepsilon)} &+ ((\partial_n + iA_n)u, v)_{\partial G(\varepsilon)} \\ &= (u, (-i\nabla + \mathbf{A})^2 v \pm Hv - k^2 v)_{G(\varepsilon)} + (u, (\partial_n + iA_n)v)_{\partial G(\varepsilon)},\end{aligned}$$

where A_n is a projection of $\mathbf{A}$ onto the outward normal to $\partial G(\varepsilon)$; $u, v \in C_0^\infty(G(\varepsilon))$. Additionally, we require u to satisfy some radiation conditions at infinity. To formulate the conditions, we consider the problem

$$\begin{aligned}\Delta v(y) + \lambda^2 v(y) = 0, &\qquad y \in (-l/2, l/2), \\ v(-l/2) = v(l/2) = 0.&\end{aligned} \tag{3.1.3}$$

The eigenvalues λ_q^2 of this problem are called thresholds; they form the sequence

$$\lambda_q^2 = (\pi q/l)^2, \qquad q = 1, 2, \dots$$

Assume that k^2 in (3.1.1) does not coincide with any of the thresholds. Let us consider the equation (3.1.1) with "$+$". For a fixed real k there exist finitely many linearly independent bounded wave functions. In the linear space spanned by such functions, a basis is formed by the wave functions subject to the radiation conditions

$$u_m^+(x,y) = \begin{cases} e^{i\nu_m x}\Psi_m(y) + \sum_{j=1}^{M} s_{mj}^+(k)\, e^{-i\nu_j x}\Psi_j(y) + O(e^{\delta x}), & x \to -\infty, \\ \sum_{j=1}^{M} s_{m,M+j}^+(k)\, e^{i\nu_j x}\Psi_j(y) + O(e^{-\delta x}), & x \to +\infty; \end{cases} \tag{3.1.4}$$

$$u_{M+m}^+(x,y) = \begin{cases} \sum_{j=1}^{M} s_{M+m,j}^+(k)\, e^{-i\nu_j x}\Psi_j(y) + O(e^{\delta x}), & x \to -\infty, \\ e^{-i\nu_m x}\Psi_m(y) + \sum_{j=1}^{M} s_{M+m,M+j}^+(k)\, e^{i\nu_j x}\Psi_j(y) + O(e^{-\delta x}), & x \to +\infty. \end{cases}$$

Here M is the number of thresholds not exceeding k^2; $\nu_m = \sqrt{k^2 - \lambda_m^2}$; Ψ_m is an eigenfunction to the problem (3.1.3) that corresponds to λ_m^2, i.e.

$$\Psi_m(y) = \begin{cases} \sqrt{2/l\nu_m}\sin\lambda_m y, & m \text{ even}, \\ \sqrt{2/l\nu_m}\cos\lambda_m y, & m \text{ odd}; \qquad m = 1, 2, \ldots, M. \end{cases} \tag{3.1.5}$$

The function $U_j(x,y) = e^{i\nu_j x}\Psi_j(y)$, $j = 1, \ldots, M$, in the strip G is a wave incoming from $-\infty$ and outgoing to $+\infty$, while $U_{M+j}(x,y) = e^{-i\nu_j x}\Psi_j(y)$ is a wave going from $+\infty$ to $-\infty$. The matrix

$$S^+ = \|s_{mj}^+\|_{m,j=1,\ldots,2M}$$

with entries from (3.1.4) is called the scattering matrix; it is unitary. The values

$$R_m^+ = \sum_{j=1}^{M} |s_{mj}^+|^2, \qquad T_m^+ = \sum_{j=1}^{M} |s_{m,\,M+j}^+|^2$$

are called the reflection and transition coefficients, respectively, for the wave U_m incoming to $G(\varepsilon)$ from $-\infty$, $m = 1, \ldots, M$. Similar definitions can be given for the wave U_{M+m} coming from $+\infty$. The scattering matrix S^- and the reflection and transition coefficients R_m^-, T_m^- for the equation (3.1.1) with "$-$" are introduced in the same way.

In the present work, we consider only the case when k^2 lies between the first and the second thresholds. Thereby, the scattering matrix is of size 2×2. We discuss only the scattering of the wave coming from $-\infty$ and denote the reflection and transition coefficients by

$$R^\pm = R^\pm(k,\varepsilon) = |s_{11}^\pm(k,\varepsilon)|^2, \qquad T^\pm = T^\pm(k,\varepsilon) = |s_{12}^\pm(k,\varepsilon)|^2. \tag{3.1.6}$$

The goal is to find a "resonant" value $k_r^\pm = k_r^\pm(\varepsilon)$ of the parameter k, where the transition coefficient takes its maximum, and to describe the behavior of $T^\pm(k,\varepsilon)$ in a neighborhood of $k_r^\pm(\varepsilon)$ as $\varepsilon \to 0$.

3.2 The limit problems

We construct the asymptotics of the wave function (i.e. the solution of (3.1.1)) as $\varepsilon \to 0$ by the compound asymptotics method. To this end, we introduce "limit" boundary value problems independent of the parameter ε. We suppose the domain occupied by the magnetic field to be localized in the resonator, the part of the waveguide between the narrows. Furthermore, we assume that $|x_j - x_0| > R + 2\delta$, $j = 1, 2$, so the vector potential $\mathbf{A}$ differs from zero only on a domain inside the resonator. Then outside the resonator and, in particular, near the narrows the sought wave function satisfies the Helmholtz equation.

3.2.1 First kind limit problems

Let $G(0) = G \cap K_1 \cap K_2$ (Figure 9); therefore, $G(0)$ consists of three parts G_1, G_2 and G_3, where G_1 and G_3 are infinite domains, and G_2 is a bounded resonator.

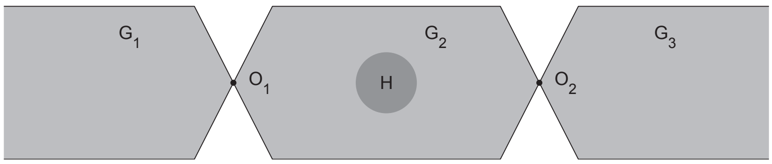


FIGURE 9 The domain $G(0) = G_1 \cup G_2 \cup G_3$.

The boundary value problems

$$\begin{aligned} \Delta v(x,y) + k^2 v(x,y) &= f(x,y), \qquad (x,y) \in G_j, \\ v(x,y) &= 0, \qquad (x,y) \in \partial G_j, \end{aligned} \tag{3.2.1}$$

where $j = 1, 3$, and

$$\begin{aligned} (-i\nabla + \mathbf{A}(x,y))^2 v(x,y) \pm H(\rho) v(x,y) &= k^2 v(x,y), \qquad (x,y) \in G_2, \\ v(x,y) &= 0, \qquad (x,y) \in \partial G_2, \end{aligned} \tag{3.2.2}$$

are called the first kind limit problems.

We introduce function spaces for the problem (3.2.2) in G_2. Let ϕ_1 and ϕ_2 be smooth real functions in the closure $\overline{G}_2$ of G_2 such that $\phi_j = 1$ in a neighborhood of O_j, $j = 1, 2$, and $\phi_1^2 + \phi_2^2 = 1$. For $l = 0, 1, \dots$ and $\gamma \in \mathbb{R}$ the space $V^l_\gamma(G_2)$ is the completion in the norm

$$\|v; V^l_\gamma(G_2)\| = \left(\int_{G_2} \sum_{|\alpha|=0}^{l} \sum_{j=1}^{2} \phi_j^2(x,y) r_j^{2(\gamma - l + |\alpha|)} |\partial^\alpha v(x,y)|^2 \, dx\, dy \right)^{1/2} \tag{3.2.3}$$

of the set of smooth functions in $\overline{G}_2$ vanishing near O_1 and O_2; here r_j is the distance from (x,y) to the origin O_j, $\alpha = (\alpha_1, \alpha_2)$ is a multi-index, and $\partial^\alpha = \partial^{|\alpha|}/\partial x^{\alpha_1} \partial y^{\alpha_2}$. Proposition 3.2.1 follows from the well-known general results; e.g., see [14, Chapters 2 and 4, Sections 1–3] or [6, vol. 1, Chapter 1].

Proposition 3.2.1. *Assume that* $|\gamma - 1| < \pi/\omega$. *Then for* $f \in V^0_\gamma(G_2)$ *and arbitrary* k^2, *except the positive increasing sequence* $\{k^2_p\}^\infty_{p=1}$ *of eigenvalues,* $k^2_p \to \infty$, *there exists a unique solution* $v \in V^2_\gamma(G_2)$ *to the problem* (3.2.1) *in* G_2. *The estimate*

$$\|v;\, V^2_\gamma(G_2)\| \le c\|f;\, V^0_\gamma(G_2)\| \tag{3.2.4}$$

holds with a constant c *independent of* f. *If* f *is a smooth function in* $\overline{G}_2$ *vanishing near* O_1 *and* O_2, *and* v *is any solution in* $V^2_\gamma(G_2)$ *to the problem* (3.2.1), *then* v *is smooth in* $\overline{G}_2$ *except at* O_1 *and* O_2 *and admits the asymptotic representation*

$$v(x,y) = \begin{cases} b_1\widetilde{J}_{\pi/\omega}(kr_1)\Phi(\varphi_1) + O\big(r_1^{2\pi/\omega}\big), & r_1 \to 0, \\ b_2\widetilde{J}_{\pi/\omega}(kr_2)\Phi(\pi - \varphi_2) + O\big(r_2^{2\pi/\omega}\big), & r_2 \to 0, \end{cases}$$

near the points O_1 *and* O_2, *where* (r_j, φ_j) *are polar coordinates centered at* O_j, b_j *are some constants coefficients,* $\widetilde{J}_\mu$ *stands for the Bessel function multiplied by a constant such that* $\widetilde{J}_\mu(kr) = r^\mu + o(r^\mu)$, *and* $\Phi(\varphi) = \pi^{-1/2}\cos(\pi\varphi/\omega)$.

Let $k^2 = k^2_0$ *be an eigenvalue of the problem* (3.2.1). *Then the problem* (3.2.1) *in* G_2 *is solvable if and only if* $(f, v_0)_{G_2} = 0$ *for any eigenfunction* v_0 *corresponding to* k^2_0. *These conditions being fulfilled, there exists a unique solution* v *to the problem* (3.2.1) *that is orthogonal to the eigenfunctions and satisfies* (3.2.4) *(i.e., the Fredholm alternative holds).*

We turn to the problems (3.2.1) for $j = 1, 3$. Let $\chi_{0,j}$ and $\chi_{\infty,j}$ be smooth real functions in the closure $\overline{G}_j$ of G_j such that $\chi_{0,j} = 1$ in a neighborhood of O_j, $\chi_{0,j} = 0$ outside a compact set, and $\chi^2_{0,j} + \chi^2_{\infty,j} = 1$. We also assume that the support $\operatorname{supp}\chi_{\infty,j}$ is located in the strip G. For $\gamma \in \mathbb{R}$, $\delta > 0$, and $l = 0, 1, \dots$ the space $V^l_{\gamma,\delta}(G_j)$ is the completion in the norm

$$\|v;\, V^l_{\gamma,\delta}(G_j)\| = \left(\int_{G_j} \sum_{|\alpha|=0}^{l} \big(\chi^2_{0,j} r_j^{2(\gamma-l+|\alpha|)} + \chi^2_{\infty,j}\exp(2\delta x)\big)|\partial^\alpha v|^2\, dx\, dy\right)^{1/2} \tag{3.2.5}$$

of the set of smooth functions with compact supports on $\overline{G}_j$ vanishing near O_j.

Recall that, by assumption, k^2 is between the first and the second thresholds, therefore in each domain G_j there exists only one outgoing wave. Let $U_1^- = U_2$ be the outgoing wave in G_1 and let $U_2^- = U_1$ be the outgoing wave in G_3 (the definitions of U_j and G are given in Section 3.1). The next proposition follows, e.g., from Theorem 5.3.5 in [14].

Proposition 3.2.2. *Let* $|\gamma - 1| < \pi/\omega$ *and suppose that there is no nontrivial solution to the homogeneous problem* (3.2.1) *(where* $f = 0$*) in* $V^2_{\gamma,\delta}(G_j)$ *with arbitrarily small positive* δ. *Then for any* $f \in V^0_{\gamma,\delta}(G_j)$ *there exists a unique solution* v *to* (3.2.1) *that admits the representation*

$$v = u + A_j\chi_{\infty,j}U_j^-,$$

where $A_j = \text{const}$, $u \in V^2_{\gamma,\delta}(G_j)$, *and* δ *is sufficiently small; herewith the estimate*

$$\|u; V^2_{\gamma,\delta}(G_j)\| + |A_j| \le c\|f; V^0_{\gamma,\delta}(G_j)\|, \tag{3.2.6}$$

holds with a constant c *independent of* f. *If* f *is smooth and vanishes near* O_j, *then the solution* v *to the problem in* G_1 *satisfies*

$$v(x,y) = a_1 \widetilde{J}_{\pi/\omega}(kr_1)\Phi(\pi - \varphi_1) + O\big(r_1^{2\pi/\omega}\big), \quad r_1 \to 0,$$

and the solution to the problem in G_3 *satisfies*

$$v(x,y) = a_2 \widetilde{J}_{\pi/\omega}(kr_2)\Phi(\varphi_2) + O\big(r_2^{2\pi/\omega}\big), \quad r_2 \to 0,$$

where a_j *are some constants.*

3.2.2 Second kind limit problems

In the domains Ω_j, $j = 1, 2$, introduced in Section 3.1, we consider the boundary value problems

$$\begin{aligned} \Delta w(\xi_j,\eta_j) &= F(\xi_j,\eta_j), \qquad &(\xi_j,\eta_j) \in \Omega_j, \\ w(\xi_j,\eta_j) &= 0, &(\xi_j,\eta_j) \in \partial\Omega_j, \end{aligned} \tag{3.2.7}$$

which are called the second kind limit problems; (ξ_j,η_j) stands for Cartesian coordinates with origin at O_j.

Let $\rho_j = \operatorname{dist}((\xi_j,\eta_j), O_j)$ and let $\psi_{0,j}$, $\psi_{\infty,j}$ be smooth real functions in $\overline{\Omega}_j$ such that $\psi_{0,j} = 1$ for $\rho_j < N/2$, $\psi_{0,j} = 0$ for $\rho_j > N$, and $\psi^2_{0,j} + \psi^2_{\infty,j} = 1$, where N is a sufficiently large positive number. For $\gamma \in \mathbb{R}$ and $l = 0, 1, \dots$ the space $V^l_\gamma(\Omega_j)$ is the completion in the norm

$$\|v;\, V^l_\gamma(\Omega_j)\| = \left(\int_{\Omega_j} \mathcal{S}(v)\, d\xi_j d\eta_j\right)^{1/2} \tag{3.2.8}$$

of the set $C^\infty_c(\overline{\Omega}_j)$ of smooth functions compactly supported in $\overline{\Omega}_j$; here

$$\mathcal{S}(v) = \sum_{|\alpha|=0}^{l} \big(\psi_{0,j}(\xi_j,\eta_j)^2 + \psi_{\infty,j}(\xi_j,\eta_j)^2 \rho_j^{2(\gamma - l + |\alpha|)}\big)|\partial^\alpha v(\xi_j,\eta_j)|^2.$$

The next proposition is a corollary of Theorem 4.3.6 in [14].

Proposition 3.2.3. *Let* $|\gamma - 1| < \pi/\omega$. *Then for* $F \in V^0_\gamma(\Omega_j)$ *there exists a unique solution* $w \in V^2_\gamma(\Omega_j)$ *to* (3.2.7) *such that the estimate*

$$\|w;\, V^2_\gamma(\Omega_j)\| \le c\|F;\, V^0_\gamma(\Omega_j)\|, \tag{3.2.9}$$

holds with a constant c *independent of* F. *If* $F \in C^\infty_c(\overline{\Omega}_j)$, *then* w *is smooth on* $\overline{\Omega}_j$ *and admits the representation*

$$w(\xi_j,\eta_j) = \begin{cases} \alpha_j \rho_j^{-\pi/\omega}\Phi(\pi - \varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j < 0, \\ \beta_j \rho_j^{-\pi/\omega}\Phi(\varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j > 0, \end{cases} \tag{3.2.10}$$

as $\rho_j \to \infty$; here (ρ_j, φ_j) are polar coordinates in Ω_j with center at O_j, and Φ is the same as in Proposition 3.2.1. *The constants α_j and β_j are found with the formulas*

$$\alpha_j = -(F, w_j^l)_\Omega, \qquad \beta_j = -(F, w_j^r)_\Omega,$$

where w_j^l and w_j^r are the unique solutions to (3.2.7) *satisfying*

$$w_j^l = \begin{cases} \left(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}\right)\Phi(\pi - \varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j < 0; \\ \beta\rho_j^{-\pi/\omega}\Phi(\varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j > 0; \end{cases} \tag{3.2.11}$$

$$w_j^r = \begin{cases} \beta\rho_j^{-\pi/\omega}\Phi(\pi - \varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j < 0; \\ \left(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}\right)\Phi(\varphi_j) + O\big(\rho_j^{-3\pi/\omega}\big), & \xi_j > 0; \end{cases} \tag{3.2.12}$$

as $\rho_j \to \infty$; the coefficients α and β depend only on the geometry of Ω and have to be calculated.

3.3 Special solutions to homogeneous first kind limit problems

In each of the domains G_j, $j = 1, 2, 3$, we introduce special solutions to the homogeneous problems (3.2.1). These solutions are necessary for construction of the wave function asymptotics in the next section. It follows from Propositions 3.2.1 and 3.2.2 that the bounded solutions to the homogeneous problems (3.2.1) are trivial (except the eigenfunctions of the problem in the resonator). Therefore, we consider only solutions unbounded in the neighborhood of O_j.

Let us analyze the problem

$$\Delta u + k^2 u = 0 \quad \text{in} \quad K, \qquad u = 0 \quad \text{on} \quad \partial K. \tag{3.3.1}$$

The function

$$v(r, \varphi) = \widetilde{N}_{\pi/\omega}(kr)\Phi(\varphi) \tag{3.3.2}$$

satisfies (3.3.1); here $\widetilde{N}_{\pi/\omega}$ is the Neumann function multiplied by such a constant that

$$\widetilde{N}_{\pi/\omega}(kr) = r^{-\pi/\omega} + o(r^{-\pi/\omega}),$$

and Φ is the same as in Proposition 3.2.1. Let $t \mapsto \Theta(t)$ be a cut-off function on $\mathbb{R}$, equal to 1 for $t < \delta/2$ and to 0 for $t > \delta$, δ being a small positive number. Introduce the solution

$$\mathbf{v}_1(x, y) = \Theta(r_1)v(r_1, \varphi_1) + \widetilde{v}_1(x, y) \tag{3.3.3}$$

to the homogeneous problem (3.2.1) in G_1, where $\widetilde{v}_1$ satisfies (3.2.1) with

$$f = -[\Delta, \Theta]v,$$

the existence of $\widetilde{v}_1$ is provided by Proposition 3.2.2. Therefore,

$$\mathbf{v}_1(x,y)=\begin{cases}\big(\widetilde{N}_{\pi/\omega}(kr_1)+a\widetilde{J}_{\pi/\omega}(kr_1)\big)\Phi(\pi-\varphi_1)+O(r_1^{3\pi/\omega}), & r_1\to 0,\\ AU_1^-(x,y)+O(e^{\delta x}), & x\to-\infty,\end{cases} \tag{3.3.4}$$

where $\widetilde{J}_{\pi/\omega}$ is the same as in Propositions 3.2.1 and 3.2.2, and the constant $A\neq 0$ depends only on the geometry of G_1 and has to be calculated.

Define the solution $\mathbf{v}_3$ to the problem (3.2.1) in G_3 by $\mathbf{v}_3(x,y)=\mathbf{v}_1(d-x,y)$, where $d=\operatorname{dist}(O_1,O_2)$. Then

$$\mathbf{v}_3(x,y)=\begin{cases}\big(\widetilde{N}_{\pi/\omega}(kr_2)+a\widetilde{J}_{\pi/\omega}(kr_2)\big)\Phi(\varphi_2)+O(r_2^{3\pi/\omega}), & r_2\to 0,\\ Ae^{-i\nu_1 d}U_2^-(x,y)+O(e^{-\delta x}), & x\to+\infty,\end{cases} \tag{3.3.5}$$

Lemma 3.3.1. *There holds the equality* $|A|^2=\operatorname{Im}a$.

Proof. Let $(u,v)_Q$ denote the integral $\int_Q u(x)\overline{v(x)}\,dx$ and let $G_{N,\delta}$ stand for the truncated domain $G_1\cap\{x>-N\}\cap\{r_1>\delta\}$. By the Green formula,

$$\begin{aligned}0&=(\Delta\mathbf{v}_1+k^2\mathbf{v}_1,\mathbf{v}_1)_{G_{N,\delta}}-(\mathbf{v}_1,\Delta\mathbf{v}_1+k^2\mathbf{v}_1)_{G_{N,\delta}}\\&=(\partial\mathbf{v}_1/\partial n,\mathbf{v}_1)_{\partial G_{N,\delta}}-(\mathbf{v}_1,\partial\mathbf{v}_1/\partial n)_{\partial G_{N,\delta}}=2i\operatorname{Im}(\partial\mathbf{v}_1/\partial n,\mathbf{v}_1)_E,\end{aligned}$$

where $E=(\partial G_{N,\delta}\cap\{x=-N\})\cup(\partial G_{N,\delta}\cap\{r_1=\delta\})$. Taking into account (3.3.4) as $x\to+\infty$ and (3.1.5), we have

$$\begin{aligned}\operatorname{Im}(\partial\mathbf{v}_1/\partial n,\mathbf{v}_1)_{\partial G_{N,\delta}\cap\{x=-N\}}&=-\operatorname{Im}\int_{-l/2}^{l/2}A\frac{\partial U_1^-}{\partial x}(x,y)\overline{AU_1^-}(x,y)\Big|_{x=-N}dy+o(1)\\&=|A|^2\nu_1\int_{-l/2}^{l/2}|\Psi_1(y)|^2dy+o(1)=|A|^2+o(1).\end{aligned}$$

Using (3.3.4) as $r_1\to 0$ and the definition of Φ (see Proposition 3.2.1), we obtain

$$\begin{aligned}\operatorname{Im}(\partial\mathbf{v}_1/\partial n,\mathbf{v}_1)_{\partial G_{N,\delta}\cap\{r_1=\delta\}}&=\operatorname{Im}\int_{\pi-\omega/2}^{\pi+\omega/2}\Big[-\frac{\partial}{\partial r_1}\big(\widetilde{N}_{\pi/\omega}(kr_1)+a\widetilde{J}_{\pi/\omega}(kr_1)\big)\Big]\\&\quad\times\big(\widetilde{N}_{\pi/\omega}(kr_1)+\bar{a}\widetilde{J}_{\pi/\omega}(kr_1)\big)|\Phi(\pi-\varphi_1)|^2r_1\Big|_{r_1=\delta}d\varphi_1+o(1)\\&=-(\operatorname{Im}a)\frac{2\pi}{\omega}\int_{\pi-\omega/2}^{\pi+\omega/2}|\Phi(\pi-\varphi_1)|^2d\varphi_1+o(1)=-\operatorname{Im}a+o(1).\end{aligned}$$

Thus $|A|^2-\operatorname{Im}a+o(1)=0$ as $N\to\infty$ and $\delta\to 0$. □

Let $k_{0,\pm}^2$ be a simple eigenvalue of (3.2.2) in G_2 and let $v_0^\pm$ be a corresponding eigenfunction normalized by $\int_{G_2}|v_0^\pm|^2dx=1$. By Proposition 3.2.1

$$v_0^\pm(x)\sim\begin{cases}b_1^\pm\widetilde{J}_{\pi/\omega}(k_{0,\pm}r_1)\Phi(\varphi_1), & r_1\to 0,\\ b_2^\pm\widetilde{J}_{\pi/\omega}(k_{0,\pm}r_2)\Phi(\pi-\varphi_2), & r_2\to 0.\end{cases} \tag{3.3.6}$$

We assume that $b_j^\pm\neq 0$. For $H=0$ it is true, e.g. for the eigenfunction corresponding to the least eigenvalue of the resonator. For nonzero H this condition may not hold because of the Aharonov–Bohm effect. We do not describe the phenomenon here. For k^2 in a punctured neighborhood of $k^2_{0,\pm}$ separated from the other eigenvalues, we introduce solutions $v^{\pm}_{0j}$ to the homogeneous problem (3.2.2) by

$$v^{\pm}_{0j}(x,y) = \Theta(r_j)v(r_j,\varphi_j) + \widetilde{v}^{\pm}_{0j}(x,y), \qquad j = 1,2, \tag{3.3.7}$$

where v is defined by (3.3.2), and $\widetilde{v}^{\pm}_{0j}$ is the bounded solution to the problem (3.2.2) with

$$f_j(x,y) = -[\Delta, \Theta(r_j)]v(r_j,\varphi_j).$$

Lemma 3.3.2. *In a neighborhood $V \subset \mathbb{C}$ of $k^2_{0,\pm}$ containing no eigenvalues of the problem* (3.2.2) *in G_2 except $k^2_{0,\pm}$, the equalities*

$$\widetilde{v}^{\pm}_{0j} = -\overline{b^{\pm}_j}(k^2 - k^2_{0,\pm})^{-1}v^{\pm}_0 + \widehat{v}^{\pm}_{0j}$$

hold with $b^{\pm}_j$ in (3.3.6) *and functions $\widehat{v}^{\pm}_{0j}$ analytic in $k^2 \in V$.*

Proof. First check the equality $(v^{\pm}_{0j}, v^{\pm}_0)_{G_2} = -\overline{b^{\pm}_j}/(k^2 - k^2_{0,\pm})$, where $v^{\pm}_{0j}$ are defined by (3.3.7). We have

$$(\Delta v^{\pm}_{0j} + k^2 v^{\pm}_{0j}, v^{\pm}_0)_{G_\delta} - (v^{\pm}_{0j}, \Delta v^{\pm}_0 + k^2 v^{\pm}_0)_{G_\delta} = -(k^2 - k^2_{0,\pm})(v^{\pm}_{0j}, v^{\pm}_0)_{G_\delta};$$

the domain G_δ is obtained from G_2 by excluding discs with radius δ and centers O_1 and O_2. Using the Green formula, as in Lemma 3.3.1, we get the equality

$$-(k^2 - k^2_{0,\pm})(v^{\pm}_{0j}, v^{\pm}_0)_{G_\delta} = \overline{b^{\pm}_j} + o(1).$$

It remains to let δ tend to zero.

Since $k^2_{0,\pm}$ is a simple eigenvalue, we have

$$\widetilde{v}^{\pm}_{0j} = \frac{B^{\pm}_j(k^2)}{k^2 - k^2_{0,\pm}} v^{\pm}_0 + \widehat{v}^{\pm}_{0j}, \tag{3.3.8}$$

where $B^{\pm}_j(k^2)$ does not depend on (x,y), and $\widehat{v}^{\pm}_{0j}$ are some functions analytic with respect to k^2 near the point $k^2 = k^2_{0,\pm}$. Multiplying (3.3.7) by $v^{\pm}_0$ and taking into account (3.3.8), the obtained formula for $(v^{\pm}_{0j}, v^{\pm}_0)_{G_2}$, and the condition $(v^{\pm}_0, v^{\pm}_0)_{G_2} = 1$, we get the equality $B^{\pm}_j(k^2) = -\overline{b^{\pm}_j} + (k^2 - k^2_{0,\pm})\widetilde{B}^{\pm}_j(k^2)$, where $\widetilde{B}^{\pm}_j$ are some analytic functions. Together with (3.3.8) that leads to the required statement. $\square$

In view of Lemma 3.3.2 the expressions $\mathbf{v}^{\pm}_{21} = (k^2 - k^2_{0,\pm})v^{\pm}_{01}$ and $\mathbf{v}^{\pm}_{22} = \overline{b^{\pm}_2}v_{01} - \overline{b^{\pm}_1}v^{\pm}_{02}$ may be extended to functions continuous at $k^2_{0,\pm}$ with respect to k^2. According to Proposition 3.2.1,

$$\mathbf{v}^{\pm}_{21}(x,y) \sim \begin{cases} \big((k^2 - k^2_{0,\pm})\widetilde{N}_{\pi/\omega}(kr_1) + c^{\pm}_1(k)\widetilde{J}_{\pi/\omega}(kr_1)\big)\Phi(\varphi_1), & r_1 \to 0, \\ c^{\pm}_2(k)\widetilde{J}_{\pi/\omega}(kr_2)\Phi(\pi - \varphi_2), & r_2 \to 0, \end{cases} \tag{3.3.9}$$

$$\mathbf{v}^{\pm}_{22}(x,y) \sim \begin{cases} \big(\overline{b^{\pm}_2}\widetilde{N}_{\pi/\omega}(kr_1) + d^{\pm}_1(k)\widetilde{J}_{\pi/\omega}(kr_1)\big)\Phi(\varphi_1), & r_1 \to 0, \\ \big(-\overline{b^{\pm}_1}\widetilde{N}_{\pi/\omega}(kr_2) + d^{\pm}_2(k)\widetilde{J}_{\pi/\omega}(kr_2)\big)\Phi(\pi - \varphi_2), & r_2 \to 0. \end{cases} \tag{3.3.10}$$

The proof of Lemma 3.3.2 shows that $c^{\pm}_j(k_{0,\pm}) = -\overline{b^{\pm}_1}b^{\pm}_j$.

3.4 Asymptotic formulas

This section is devoted to the derivation of the asymptotic formulas. In Section 3.4.1, we present a formula for the wave function (see (3.4.1)), explain its structure, and describe the solutions of the first kind limit problems involved in the formula. The construction of formula (3.4.1) is completed in Section 3.4.2, where the solutions to the second kind limit problems are given and the coefficients in the expressions for the solutions of the first kind limit problems are calculated. In Section 3.4.3, we analyze the expression for $\widetilde{s}_{12}$ obtained in 3.4.2, and derive formal asymptotics for the characteristics of resonant tunneling. Notice, that the remainders in the formulas (3.4.20)–(3.4.22) arose in the intermediate stage of considerations while simplifying the principal part of the asymptotics; they are not the remainders in the final asymptotic formulas. The "final" remainders are estimated in the next Section 3.5, see Theorem 3.5.3. First we derive the integral estimate (3.5.13) of the remainder in (3.4.1), which proves to be sufficient to obtain more simplified estimates of the remainders in the formulas for the resonant tunneling characteristics. The formula (3.4.1) and the estimate (3.5.13) are auxiliary and are analyzed only to that extent which is necessary for deriving the asymptotic expressions for the characteristics of resonant tunneling. For brevity, in this section we omit "$\pm$" in the notations bearing in mind one of the equations (3.1.1) and not specifying, which is considered.

3.4.1 Asymptotics of the wave function

In the waveguide $G(\varepsilon)$, we consider the scattering of the wave $U = e^{i\nu_1 x}\Psi_1(y)$, incoming from $-\infty$ (see (3.1.5)). The corresponding wave function admits the representation

$$\begin{aligned} u(x,y;\varepsilon) = {} & \chi_{1,\varepsilon}(x,y)v_1(x,y;\varepsilon) \\ & + \Theta(r_1)w_1(\varepsilon^{-1}x_1,\varepsilon^{-1}y_1;\varepsilon) + \chi_{2,\varepsilon}(x,y)v_2(x,y;\varepsilon) \\ & + \Theta(r_2)w_2(\varepsilon^{-1}x_2,\varepsilon^{-1}y_2;\varepsilon) + \chi_{3,\varepsilon}(x,y)v_3(x,y;\varepsilon) + R(x,y;\varepsilon). \end{aligned} \tag{3.4.1}$$

Let us explain the notation and the structure of this formula. When composing the formula, we first describe the behavior of the wave function u outside of the narrows, where the solutions v_j to the homogeneous problems (3.2.1) in G_j serve as approximations to u. The function v_j is a linear combination of the special solutions introduced in the previous section; v_1 and v_3 are subject to the same radiation conditions as u:

$$\begin{aligned} v_1(x,y;\varepsilon) &= \frac{1}{A}\overline{\mathbf{v}}_1(x,y) + \frac{\widetilde{s}_{11}(\varepsilon)}{A}\mathbf{v}_1(x,y) \\ &\sim U_1^+(x,y) + \widetilde{s}_{11}(\varepsilon)U_1^-(x,y), \quad x \to -\infty; \end{aligned} \tag{3.4.2}$$

$$v_2(x,y;\varepsilon) = C_1(\varepsilon)\mathbf{v}_{21}(x,y) + C_2(\varepsilon)\mathbf{v}_{22}(x,y); \tag{3.4.3}$$

$$v_3(x,y;\varepsilon) = \frac{\widetilde{s}_{12}(\varepsilon)}{Ae^{-i\nu_1 d}}\mathbf{v}_3(x,y) \sim \widetilde{s}_{12}(\varepsilon)U_2^-(x,y), \quad x \to +\infty; \tag{3.4.4}$$

the approximations $\widetilde{s}_{11}(\varepsilon)$, $\widetilde{s}_{12}(\varepsilon)$ to the scattering matrix entries $s_{11}(\varepsilon)$, $s_{12}(\varepsilon)$ and the coefficients $C_1(\varepsilon)$, $C_2(\varepsilon)$ are yet unknown. By $\chi_{j,\varepsilon}$ we denote the cut-off functions defined by

$$\begin{aligned}
\chi_{1,\varepsilon}(x,y) &= (1-\Theta(r_1/\varepsilon))\,\mathbf{1}_{G_1}(x,y),\\
\chi_{2,\varepsilon}(x,y) &= (1-\Theta(r_1/\varepsilon)-\Theta(r_2/\varepsilon))\,\mathbf{1}_{G_2}(x,y),\\
\chi_{3,\varepsilon}(x,y) &= (1-\Theta(r_2/\varepsilon))\,\mathbf{1}_{G_3}(x,y),
\end{aligned}$$

where $r_j = \sqrt{x_j^2+y_j^2}$, and (x_j,y_j) are the coordinates of a point (x,y) in the system obtained by shifting the origin to the point O_j; $\mathbf{1}_{G_j}$ is the indicator of G_j (equal to 1 in G_j and to 0 outside G_j); $\Theta(\rho)$ is the same cut-off function as in (3.3.3) (equal to 1 for $0 \leqslant \rho \leqslant \delta/2$ and to 0 for $\rho \geqslant \delta$, δ being a fixed positive number). Thus, $\chi_{j,\varepsilon}$ are defined on the whole waveguide $G(\varepsilon)$ as well as the functions $\chi_{j,\varepsilon}v_3$ in (3.4.1).

Being substituted to (3.1.1), the sum $\sum_{j=1}^{3}\chi_{j,\varepsilon}v_j$ gives a discrepancy in the right-hand side of the Helmholtz equation supported near the narrows. We compensate the principal part of the discrepancy by means of the second kind limit problems. Namely, the discrepancy supported near O_j is rewritten into coordinates $(\xi_j,\eta_j) = (\varepsilon^{-1}x_j, \varepsilon^{-1}y_j)$ in the domain Ω_j and is taken as a right-hand side for the Laplace equation. The solution w_j of the corresponding problem (3.2.7) is rewritten into coordinates (x_j,y_j) and multiplied by a cut-off function. As a result, there arise the terms $\Theta(r_j)w_j(\varepsilon^{-1}x_j,\varepsilon^{-1}y_j;\varepsilon)$ in (3.4.1).

Proposition 3.2.3 provides the existence of solutions w_j decaying at infinity as $O(\rho_j^{-\pi/\omega})$ (see (3.2.10)). But those solutions will not lead us to the goal, because substitution of (3.4.1) into (3.1.1) gives a discrepancy of high order which has to be compensated again. Therefore we require the rate $w_j = O(\rho_j^{-3\pi/\omega})$ as $\rho_j \to \infty$. By Proposition 3.2.3, such a solution exists if the right-hand side of the problem (3.2.7) satisfies the additional conditions

$$(F,w_j^l)_{\Omega_j} = 0, \qquad (F,w_j^r)_{\Omega_j} = 0.$$

These conditions (two in each narrow) uniquely determine the coefficients $\widetilde{s}_{11}(\varepsilon)$, $\widetilde{s}_{12}(\varepsilon)$, $C_1(\varepsilon)$, and $C_2(\varepsilon)$. The remainder $R(x,y;\varepsilon)$ is small in comparison with the principal part of (3.4.1) as $\varepsilon \to 0$.

3.4.2 Formulas for $\widetilde{s}_{11}$, $\widetilde{s}_{12}$, C_1, and C_2

Now let us specify the right-hand sides F_j of the problems (3.2.7) and find $\widetilde{s}_{11}(\varepsilon)$, $\widetilde{s}_{12}(\varepsilon)$, $C_1(\varepsilon)$, and $C_2(\varepsilon)$. Substituting $\chi_{1,\varepsilon}v_1$ into (3.1.1), we get the discrepancy

$$(\Delta+k^2)\chi_{1,\varepsilon}v_1 = [\Delta,\chi_{\varepsilon,1}]v_1 + \chi_{\varepsilon,1}(\Delta+k^2)v_1 = [\Delta, 1-\Theta(\varepsilon^{-1}r_1)]v_1,$$

which is nonzero only near O_1, where v_1 can be replaced by asymptotics; the boundary condition (3.1.2) is fulfilled. According to (3.4.2) and (3.3.4),

$$v_1(x,y;\varepsilon) = \big(a_1^-(\varepsilon)\widetilde{N}_{\pi/\omega}(kr_1) + a_1^+(\varepsilon)\widetilde{J}_{\pi/\omega}(kr_1)\big)\Phi(\pi-\varphi_1) + O(r_1^{3\pi/\omega}), \quad r_1 \to 0,$$

where

$$a_1^-(\varepsilon) = \frac{1}{\overline{A}} + \frac{\widetilde{s}_{11}(\varepsilon)}{A}, \quad a_1^+ = \frac{\overline{a}}{\overline{A}} + \frac{\widetilde{s}_{11}(\varepsilon)a}{A}. \tag{3.4.5}$$

Choose in each summand the leading term and take $\rho_1 = r_1/\varepsilon$, then

$$\begin{aligned}(\Delta + k^2)\chi_{\varepsilon,1}v_1 &\sim [\Delta, 1-\Theta(\varepsilon^{-1}r_1)] \left(a_1^- r_1^{-\pi/\omega} + a_1^+ r_1^{\pi/\omega}\right)\Phi(\pi-\varphi_1)\\ &= \varepsilon^{-2}[\Delta_{(\rho_1,\varphi_1)}, 1-\Theta(\rho_1)]\left(a_1^-\varepsilon^{-\pi/\omega}\rho_1^{-\pi/\omega} + a_1^+\varepsilon^{\pi/\omega}\rho_1^{\pi/\omega}\right)\Phi(\pi-\varphi_1).\end{aligned} \tag{3.4.6}$$

In the same way, by using (3.4.3) and (3.3.9)–(3.3.10), we write down the leading term of the discrepancy from $\chi_{\varepsilon,2}v_2$ supported near O_1:

$$(\Delta + k^2)\chi_{\varepsilon,1}v_1 \sim \varepsilon^{-2}[\Delta_{(\rho_1,\varphi_1)}, 1-\Theta(\rho_1)]\left(b_1^-\varepsilon^{-\pi/\omega}\rho_1^{-\pi/\omega} + b_1^+\varepsilon^{\pi/\omega}\rho_1^{\pi/\omega}\right)\Phi(\varphi_1), \tag{3.4.7}$$

where

$$b_1^- = C_1(\varepsilon)(k^2-k_0^2) + C_2(\varepsilon)\overline{b}_2, \qquad b_1^+ = C_1(\varepsilon)c_1 + C_2(\varepsilon)d_1. \tag{3.4.8}$$

As right-hand side F_1 of the problem (3.2.7) in Ω_1, we take the function

$$\begin{aligned}F_1(\xi_1,\eta_1) = &-[\Delta,\zeta^-]\left(a_1^-\varepsilon^{-\pi/\omega}\rho_1^{-\pi/\omega} + a_1^+\varepsilon^{\pi/\omega}\rho_1^{\pi/\omega}\right)\Phi(\pi-\varphi_1)\\ &-[\Delta,\zeta^+]\left(b_1^-\varepsilon^{-\pi/\omega}\rho_1^{-\pi/\omega} + b_1^+\varepsilon^{\pi/\omega}\rho_1^{\pi/\omega}\right)\Phi(\varphi_1),\end{aligned} \tag{3.4.9}$$

where ζ^+ (resp. ζ^-) stands for the function $1-\Theta$, first restricted to the domain $\xi_1 > 0$ (resp. $\xi_1 < 0$) and then extended by zero onto the whole domain Ω_1. Let w_1 be the corresponding solution, then the term $\Theta(r_1)w_1(\varepsilon^{-1}x_1, \varepsilon^{-1}y_1;\varepsilon)$ in (3.4.1), being substituted in (3.1.1), compensates the discrepancies (3.4.6)–(3.4.7).

In the same way, using (3.4.3)–(3.4.4), (3.3.9)–(3.3.10), and (3.3.5), we find the right-hand side of the problem (3.2.7) with $j = 2$:

$$\begin{aligned}F_2(\xi_2,\eta_2) = &-[\Delta,\zeta^-]\left(a_2^-\varepsilon^{-\pi/\omega}\rho_2^{-\pi/\omega} + a_2^+\varepsilon^{\pi/\omega}\rho_2^{\pi/\omega}\right)\Phi(\pi-\varphi_2)\\ &-[\Delta,\zeta^+]\left(b_2^-\varepsilon^{-\pi/\omega}\rho_2^{-\pi/\omega} + b_2^+\varepsilon^{\pi/\omega}\rho_2^{\pi/\omega}\right)\Phi(\varphi_2);\end{aligned}$$

$$\begin{aligned}a_2^-(\varepsilon) &= -C_2(\varepsilon)\overline{b}_1, & a_2^+(\varepsilon) &= C_1(\varepsilon)c_2 + C_2(\varepsilon)d_2,\\ b_2^-(\varepsilon) &= \frac{\widetilde{s}_{12}(\varepsilon)}{Ae^{-i\nu_1 d}}, & b_2^+(\varepsilon) &= \frac{a\widetilde{s}_{12}(\varepsilon)}{Ae^{-i\nu_1 d}}.\end{aligned} \tag{3.4.10}$$

Lemma 3.4.1. *If the solution w_j to the problem (3.2.7) with right-hand side*

$$\begin{aligned}F_j(\xi_j,\eta_j) = &-[\Delta,\zeta^-]\left(a_j^-\varepsilon^{-\pi/\omega}\rho_j^{-\pi/\omega} + a_j^+\varepsilon^{\pi/\omega}\rho_j^{\pi/\omega}\right)\Phi(\pi-\varphi_j)\\ &-[\Delta,\zeta^+]\left(b_j^-\varepsilon^{-\pi/\omega}\rho_j^{-\pi/\omega} + b_j^+\varepsilon^{\pi/\omega}\rho_j^{\pi/\omega}\right)\Phi(\varphi_j), \qquad j=1,2,\end{aligned}$$

is $O(\rho_j^{-3\pi/\omega})$ as $\rho_j \to \infty$, then the relations

$$\begin{aligned}a_j^-\varepsilon^{-\pi/\omega} - \alpha a_j^+\varepsilon^{\pi/\omega} - \beta b_j^+\varepsilon^{\pi/\omega} &= 0,\\ b_j^-\varepsilon^{-\pi/\omega} - \alpha b_j^+\varepsilon^{\pi/\omega} - \beta a_j^+\varepsilon^{\pi/\omega} &= 0,\end{aligned} \tag{3.4.11}$$

hold with α and β in (3.2.11) – (3.2.12).

Proof. In view of Proposition 3.2.3 we have $w_j = O(\rho_j^{-3\pi/\omega})$ as $\rho_j \to \infty$ if and only if the right-hand side of the problem (3.2.7) satisfies the conditions

$$(F_j, w_j^l)_{\Omega_j} = 0, \qquad (F_j, w_j^r)_{\Omega_j} = 0, \tag{3.4.12}$$

where w_j^l and w_j^r are solutions to the homogeneous problem (3.2.7) for which the expansions in (3.2.11)–(3.2.12) hold. Introduce the functions $f_\pm$ on Ω_j by

$$f_\pm(\rho_j, \varphi_j) = \rho_j^{\pm\pi/\omega}\Phi(\varphi_j).$$

To derive (3.4.11) from (3.4.12), it suffices to check that

$$\begin{aligned}
([\Delta, \zeta^-]f_-, w_j^l)_{\Omega_j} &= ([\Delta, \zeta^+]f_-, w_j^r)_{\Omega_j} = -1,\\
([\Delta, \zeta^-]f_+, w_j^l)_{\Omega_j} &= ([\Delta, \zeta^+]f_+, w_j^r)_{\Omega_j} = \alpha,\\
([\Delta, \zeta^+]f_-, w_j^l)_{\Omega_j} &= ([\Delta, \zeta^-]f_-, w_j^r)_{\Omega_j} = 0,\\
([\Delta, \zeta^+]f_+, w_j^l)_{\Omega_j} &= ([\Delta, \zeta^-]f_+, w_j^r)_{\Omega_j} = \beta.
\end{aligned}$$

Let us prove the first equality, the rest ones are treated in a similar way. Since $[\Delta, \zeta^+]f_-$ is compactly supported, in the calculation of $([\Delta, \zeta^-]f_-, w_j^l)_{\Omega_j}$ one may replace Ω_j by $\Omega_j^R = \Omega_j \cap \{\rho_j < R\}$ with sufficiently large R. Let

$$E := \partial\Omega_j^R \cap \{\rho_j = R\} \cap \{\xi_j > 0\}.$$

By the Green formula,

$$\begin{aligned}
([\Delta, \zeta^-]f_-, w_j^l)_{\Omega_j} &= (\Delta\zeta^- f_-, w_j^l)_{\Omega_j^R} - (\zeta^- f_-, \Delta w_j^l)_{\Omega_j^R}\\
&= (\partial f_-/\partial n, w_j^l)_E - (f_-, \partial w_j^l/\partial n)_E.
\end{aligned}$$

Taking account of (3.2.11) for $\xi_j < 0$ and the definition of Φ in Proposition 3.2.1, we arrive at

$$\begin{aligned}
([\Delta, \zeta^-]f_-, w_j^l)_{\Omega_j} &= \mathcal{S}(R)\int_{\pi-\omega/2}^{\pi+\omega/2} \Phi(\pi - \varphi_j)^2 d\varphi_j + o(1)\\
&= -\frac{2\pi}{\omega}\int_{\pi-\omega/2}^{\pi+\omega/2} \Phi(\pi - \varphi_j)^2 d\varphi_j + o(1) = -1 + o(1),
\end{aligned}$$

where $\mathcal{S}(R)$ stands for the expression

$$\left[\frac{\partial\rho_j^{-\pi/\omega}}{\partial\rho_j}(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}) - \rho_j^{-\pi/\omega}\frac{\partial}{\partial\rho_j}(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega})\right]\rho_j\Bigg|_{\rho_j=R}$$

It remains to let $R \to \infty$. □

Remark 3.4.2. *The solutions w_j mentioned in Lemma 3.4.1 can be represented as linear combinations of functions independent of ε. We write down the corresponding expression* *which will be of use in the next section. Let w_j^l and w_j^r be the solutions of the problem (3.2.7) specified by conditions (3.2.11) – (3.2.12), and let ζ^+ and ζ^- be the same cut-off functions as in (3.4.9). Put*

$$\mathbf{w}_j^l = w_j^l - \zeta^- \left(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}\right)\Phi(\pi - \varphi_j) - \zeta^+\beta\rho_j^{-\pi/\omega}\Phi(\varphi_j),$$
$$\mathbf{w}_j^r = w_j^r - \zeta^-\beta\rho_j^{-\pi/\omega}\Phi(\pi - \varphi_j) - \zeta^+ \left(\rho_j^{\pi/\omega} + \alpha\rho_j^{-\pi/\omega}\right)\Phi(\varphi_j).$$

A direct verification shows that

$$\begin{aligned} w_j &= a_j^+\varepsilon^{\pi/\omega}\mathbf{w}_j^l + \frac{1}{\beta}\left(a_j^-\varepsilon^{-\pi/\omega} - \alpha a_j^+\varepsilon^{\pi/\omega}\right)\mathbf{w}_j^r \\ &= \frac{1}{\beta}\left(b_j^-\varepsilon^{-\pi/\omega} - \alpha b_j^+\varepsilon^{\pi/\omega}\right)\mathbf{w}_j^l + b_j^+\varepsilon^{\pi/\omega}\mathbf{w}_j^r. \end{aligned} \tag{3.4.13}$$

Using (3.4.5) and (3.4.8), we transform (3.4.11) with $j = 1$ to the expressions

$$\begin{aligned} \gamma(\varepsilon)\widetilde{s}_{11}(\varepsilon) + \overline{\gamma(\varepsilon)} &= C_1(\varepsilon)c_1 + C_2(\varepsilon)d_1, \\ \delta(\varepsilon)\widetilde{s}_{11}(\varepsilon) + \overline{\delta(\varepsilon)} &= C_1(\varepsilon)(k^2 - k_0^2) + C_2(\varepsilon)\overline{b}_2, \end{aligned} \tag{3.4.14}$$

where

$$\gamma(\varepsilon) = \frac{1}{A\beta}\left(\varepsilon^{-2\pi/\omega} - a\alpha\right), \qquad \delta(\varepsilon) = \frac{1}{A\beta}\left(\alpha + a(\beta^2 - \alpha^2)\varepsilon^{2\pi/\omega}\right). \tag{3.4.15}$$

For $j = 2$, taking (3.4.10) into account, reduce (3.4.11) to the equalities

$$\gamma(\varepsilon)\widetilde{s}_{12}(\varepsilon) = (C_1(\varepsilon)c_2 + C_2(\varepsilon)d_2)e^{-i\nu_1 d}, \quad \delta(\varepsilon)\widetilde{s}_{12}(\varepsilon) = -C_2(\varepsilon)\overline{b}_1 e^{-i\nu_1 d}. \tag{3.4.16}$$

From (3.4.14) and (3.4.16), by means of Lemma 3.3.1, we find $C_1(\varepsilon)$, $C_2(\varepsilon)$, $\widetilde{s}_{11}(\varepsilon)$, and $\widetilde{s}_{12}(\varepsilon)$:

$$C_1(\varepsilon) = (\overline{b}_1 c_2)^{-1}\left(\gamma(\varepsilon)\overline{b}_1 + \delta(\varepsilon)d_2\right)\widetilde{s}_{12}(\varepsilon)e^{i\nu_1 d}, \quad C_2(\varepsilon) = -\overline{b}_1^{-1}\delta(\varepsilon)\widetilde{s}_{12}(\varepsilon)e^{i\nu_1 d}, \tag{3.4.17}$$

$$\begin{aligned} \widetilde{s}_{11}(\varepsilon) =& (2i\overline{b}_1 c_2)^{-1}\big((k^2 - k_0^2)\overline{b}_1|\gamma(\varepsilon)|^2 + ((k^2 - k_0^2)d_2 - \overline{b}_2 c_2)\overline{\gamma(\varepsilon)}\delta(\varepsilon) \\ & - \overline{b}_1 c_1\gamma(\varepsilon)\overline{\delta(\varepsilon)} - (c_1 d_2 - c_2 d_1)|\delta(\varepsilon)|^2\big)\widetilde{s}_{12}(\varepsilon)e^{i\nu_1 d}, \end{aligned} \tag{3.4.18}$$

$$\begin{aligned} \widetilde{s}_{12}(\varepsilon) =& 2i\overline{b}_1 c_2 e^{-i\nu_1 d}\big(-(k^2 - k_0^2)\overline{b}_1\gamma(\varepsilon)^2 - ((k^2 - k_0^2)d_2 - \overline{b}_1 c_1 - \overline{b}_2 c_2)\gamma(\varepsilon)\delta(\varepsilon) \\ & + (c_1 d_2 - c_2 d_1)\delta(\varepsilon)^2\big)^{-1}. \end{aligned} \tag{3.4.19}$$

3.4.3 The formulas for the characteristics of resonant tunneling

The solutions of the first kind limit problems involved in (3.4.1) are defined for the complex k^2 as well. The obtained expression (3.4.19) for $\widetilde{s}_{12}$ has a pole k_p^2 in the lower complex half-plane. To find k_p^2 we equate $2i\overline{b}_1 c_2 e^{-i\nu_1 d}/\widetilde{s}_{12}$ to zero and solve the equation for $k_2 - k_0^2$:

$$k^2 - k_0^2 = \left((\overline{b}_1 c_1 + \overline{b}_2 c_2)\gamma(\varepsilon)\delta(\varepsilon) + (c_1 d_2 - c_2 d_1)\delta(\varepsilon)^2\right)\left(\overline{b}_1\gamma(\varepsilon)^2 + d_2\gamma(\varepsilon)\delta(\varepsilon)\right)^{-1}.$$

Since the right-hand side of the last equation behaves like $O(\varepsilon^{2\pi/\omega})$ as $\varepsilon \to 0$, it may be solved by the method of successive approximations. Considering the formulas (3.4.15), $c_j(k_0) = -\overline{b}_1 b_j$, Lemma 3.3.1, and dropping the lower order terms, we get

$$\begin{aligned} k_p^2 &= k_r^2 - ik_i^2, \\ k_r^2 &= k_0^2 - \alpha(|b_1|^2 + |b_2|^2)\varepsilon^{2\pi/\omega} + O(\varepsilon^{4\pi/\omega}), \\ k_i^2 &= \beta^2(|b_1|^2 + |b_2|^2)|A(k_0^2)|^2\varepsilon^{4\pi/\omega} + O(\varepsilon^{6\pi/\omega}). \end{aligned} \tag{3.4.20}$$

For small $k^2 - k_p^2$ the formula (3.4.19) takes the form

$$\widetilde{s}_{12}(k,\varepsilon) = -\varepsilon^{4\pi/\omega}\frac{2i\beta^2 A(k)^2 c_2(k)e^{-i\nu_1 d}}{k^2 - k_p^2}\left(1 + O(|k^2 - k_p^2| + \varepsilon^{2\pi/\omega})\right).$$

Let $k^2 - k_0^2 = O(\varepsilon^{2\pi/\omega})$, then

$$\begin{aligned} |k^2 - k_p^2| &= O(\varepsilon^{2\pi/\omega}), & A(k) &= A(k_0^2) + O(\varepsilon^{2\pi/\omega}), \\ c_2(k^2) &= -\overline{b}_1 b_2 + O(\varepsilon^{2\pi/\omega}), & \nu_1(k) &= \nu_1(k_0^2) + O(\varepsilon^{2\pi/\omega}), \end{aligned}$$

and

$$\begin{aligned} \widetilde{s}_{12}(k,\varepsilon) &= \varepsilon^{4\pi/\omega}\frac{2i\beta^2\overline{b}_1 b_2 A(k_0)^2 e^{-i\nu_1(k_0)d}}{k^2 - k_p^2}\left(1 + O(\varepsilon^{2\pi/\omega})\right) \\ &= \frac{\dfrac{\overline{b}_1}{|b_1|}\dfrac{b_2}{|b_2|}\left(\dfrac{A(k_0)}{|A(k_0)|}\right)^2 e^{-i\nu_1(k_0)d}}{\dfrac{1}{2}\left(\dfrac{|b_1|}{|b_2|} + \dfrac{|b_2|}{|b_1|}\right) - iP\dfrac{k^2 - k_r^2}{\varepsilon^{4\pi/\omega}}}\left(1 + O(\varepsilon^{2\pi/\omega})\right), \end{aligned}$$

where $P = (2|b_1||b_2|\beta^2|A(k_0)|^2)^{-1}$. Thereby,

$$\widetilde{T}(k,\varepsilon) = |\widetilde{s}_{12}|^2 = \frac{1}{\dfrac{1}{4}\left(\dfrac{|b_1|}{|b_2|} + \dfrac{|b_2|}{|b_1|}\right)^2 + P^2\left(\dfrac{k^2 - k_r^2}{\varepsilon^{4\pi/\omega}}\right)^2}(1 + O(\varepsilon^{2\pi/\omega})). \tag{3.4.21}$$

The obtained approximation $\widetilde{T}$ to the transition coefficient has a peak at $k^2 = k_r^2$ whose width at its half-height is

$$\widetilde{\Upsilon}(\varepsilon) = \left(\frac{|b_1|}{|b_2|} + \frac{|b_2|}{|b_1|}\right)P^{-1}\varepsilon^{4\pi/\omega}, \tag{3.4.22}$$

which determines the resonator Q-factor (quality factor) equal to $k_r^2/\widetilde{\Upsilon}(\varepsilon)$.

3.5 Justification of the asymptotics

As in the previous section, here we omit "$\pm$" in the notations and do not specify which equation of (3.1.1) is considered. We return to the full notations in Theorem 3.5.3.

Introduce functional spaces for the problem

$$(-i\nabla + \mathbf{A})^2 u \pm Hu = k^2 u \quad \text{in } G(\varepsilon), \qquad u = 0 \quad \text{on } \partial G(\varepsilon). \tag{3.5.1}$$

Recall, that the functions $\mathbf{A}$ and H are compactly supported, and besides, they are nonzero only in the resonator at some distance from the narrows. Let Θ be the same function as in (3.3.3), and let the cut-off functions η_j, $j = 1, 2, 3$, be nonzero in G_j and satisfy the relation $\eta_1(x, y) + \Theta(r_1) + \eta_2(x, y) + \Theta(r_2) + \eta_3(x, y) = 1$ in $G(\varepsilon)$. For $\gamma \in \mathbb{R}$, $\delta > 0$, and $l = 0, 1, \dots$ the space $V^l_{\gamma,\delta}(G(\varepsilon))$ is the completion in the norm

$$\|u; V^l_{\gamma,\delta}(G(\varepsilon))\| = \left(\int_{G(\varepsilon)} \mathcal{S}(u)\, dx\, dy \right)^{1/2} \tag{3.5.2}$$

of the set of smooth functions compactly supported on $\overline{G(\varepsilon)}$; here

$$\mathcal{S}(u) := \sum_{|\alpha|=0}^{l} \left(\sum_{j=1}^{2} \Theta^2(r_j)\ (r_j^2 + \varepsilon_j^2)^{\gamma - l + |\alpha|} + \eta_1^2 e^{2\delta|x|} + \eta_2 + \eta_3^2 e^{2\delta|x|} \right) |\partial^\alpha u|^2.$$

We denote by $V^{0,\perp}_{\gamma,\delta}$ the space of functions f analytic in k^2 which take values in $V^0_{\gamma,\delta}(G(\varepsilon))$ and satisfy at $k^2 = k_0^2$ the condition $(\chi_{2,\varepsilon^\sigma} f, v_0)_{G_2} = 0$ with a small positive σ.

Proposition 3.5.1. *Let k_r^2 be a resonance, $k_r^2 \to k_0^2$ as $\varepsilon \to 0$, and let*

$$|k^2 - k_r^2| = O(\varepsilon^{2\pi/\omega}).$$

Assume, that γ satisfies the condition $\pi/\omega - 2 < \gamma - 1 < \pi/\omega$, $f \in V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$, and u is the solution of the problem (3.5.1) *which admits the representation*

$$u = \widetilde{u} + \eta_1 A_1^- U_1^- + \eta_3 A_2^- U_2^-;$$

here $A_j^- = const$, $\widetilde{u} \in V^2_{\gamma,\delta}(G(\varepsilon))$ for small $\delta > 0$. Then

$$\|\widetilde{u}; V^2_{\gamma,\delta}(G(\varepsilon))\| + |A_1^-| + |A_2^-| \le c\|f; V^0_{\gamma,\delta}(G(\varepsilon))\|, \tag{3.5.3}$$

where c is a constant independent of f and ε.

Proof. Step A. First we construct an auxiliary function u_p. As it was mentioned before, $\widetilde{s}_{12}$ has a pole $k_p^2 = k_r^2 - ik_i^2$ (see (3.4.20)). Multiply the solutions to the limit problems, involved in (3.4.1), by $A(k) b_2 \beta \varepsilon^{2\pi/\omega} / s_{12}(\varepsilon, k) e^{i\nu_1 d}$, put $k = k_p$, and denote the resulting functions by adding the subscript p. Then

$$\begin{aligned} v_{1p}(x,y;\varepsilon) &= \varepsilon^{2\pi/\omega}(b_1\beta + O(\varepsilon^{2\pi/\omega}))\mathbf{v}_1(x,y;k_p), \\ v_{3p}(x,y;\varepsilon) &= \varepsilon^{2\pi/\omega} b_2\beta\mathbf{v}_1(x,y;k_p); \end{aligned} \tag{3.5.4}$$

$$\begin{aligned} v_{2p}(x,y;\varepsilon) = &\left(-\frac{1}{\overline{b}_1} + O(\varepsilon^{2\pi/\omega})\right)\mathbf{v}_{21}(x,y;k_p) \\ &+ \varepsilon^{2\pi/\omega}\left(-\alpha\frac{b_2}{\overline{b}_1} + O(\varepsilon^{2\pi/\omega})\right)\mathbf{v}_{22}(x,y;k_p), \end{aligned}$$

$$\begin{aligned} w_{1p}(\xi_1,\eta_1;\varepsilon) = b_1\varepsilon^{\pi/\omega}\Big(&\varepsilon^{2\pi/\omega}\left(a(k_p)\beta + O(\varepsilon^{2\pi/\omega})\right)\mathbf{w}_1^l(\xi_1,\eta_1) \\ &+ \left(1 + O(\varepsilon^{2\pi/\omega})\right)\mathbf{w}_1^r(\xi_1,\eta_1)\Big), \end{aligned} \tag{3.5.5}$$

$$\begin{aligned} w_{2p}(\xi_2,\eta_2;\varepsilon) = b_2\varepsilon^{\pi/\omega}\Big(&\left(1 + O(\varepsilon^{2\pi/\omega})\right)\mathbf{w}_1^l(\xi_2,\eta_2) \\ &+ a(k_p)\beta\varepsilon^{2\pi/\omega}\mathbf{w}_1^r(\xi_2,\eta_2)\Big); \end{aligned} \tag{3.5.6}$$

the dependence of k_p on ε is not shown. We set

$$\begin{aligned} u_p(x,y;\varepsilon) = \Xi(x,y)\Big(&\chi_{1,\varepsilon}(x,y)v_{1p}(x,y;\varepsilon) + \Theta(\varepsilon^{-2\sigma}r_1)w_{1p}(\varepsilon^{-1}x_1,\varepsilon^{-1}y_1;\varepsilon) \\ &+ \chi_{2,\varepsilon}(x,y)v_{2p}(x,y;\varepsilon) + \Theta(\varepsilon^{-2\sigma}r_2)w_{2p}(\varepsilon^{-1}x_2,\varepsilon^{-1}y_2;k,\varepsilon) \\ &+ \chi_{3,\varepsilon}(x,y)v_{2p}(x,y;k,\varepsilon)\Big), \end{aligned} \tag{3.5.7}$$

where Ξ is a cut-off function in $G(\varepsilon)$ that is equal to 1 on $G(\varepsilon)\cap\{|x|<R\}$ and to 0 on $G(\varepsilon)\cap\{|x|>R+1\}$ for a large $R>0$. The principal part of the norm of u_p is given by $\chi_{2,\varepsilon}v_{2p}$. Considering the definitions of v_{2p} and $\mathbf{v}_{21}$ (see Section 3.2) and Lemma 3.3.2, we get $\|\chi_{2,\varepsilon}v_{2p}\| = \|v_0\| + o(1)$.

Step B. Let us show that

$$\|((-i\nabla + \mathbf{A})^2 \pm H - k_p^2)u_p; V^0_{\gamma,\delta}(G(\varepsilon))\| \le c\varepsilon^{\pi/\omega+\kappa}, \tag{3.5.8}$$

where

$$\kappa = \min\{\pi/\omega,\ 3\pi/\omega - \sigma_1,\ \gamma+1\}, \quad \sigma_1 = 2\sigma(3\pi/\omega - \gamma + 1).$$

If $\pi/\omega < \gamma+1$ and σ is sufficiently small so that $2\pi/\omega > \sigma_1$, then $\kappa = \pi/\omega$.

In view of (3.5.7),

$$
\begin{aligned}
&((-i\nabla+\mathbf{A})^2 \pm H - k_p^2)u_p(x,y;\varepsilon)\\
&= [\Delta,\chi_{1,\varepsilon}]\Big(v_1(x,y;\varepsilon) - b_1\beta\varepsilon^{2\pi/\omega}(r_1^{-\pi/\omega}+a(k_p)r_1^{\pi/\omega})\Phi(\pi-\varphi_1)\Big)\\
&+ [\Delta,\Theta]w_{1p}(\varepsilon^{-1}x_1,\varepsilon^{-1}y_1;\varepsilon) - k^2\Theta(\varepsilon^{-2\sigma}r_1)w_{1p}(\varepsilon^{-1}x_1,\varepsilon^{-1}y_1;\varepsilon)\\
&+ [\Delta,\chi_{2,\varepsilon}]\Big(v_2(x,y;\varepsilon) - \Theta(r_1)\big(b_{1p}^-(\varepsilon)r_1^{-\pi/\omega}+b_{1p}^+(\varepsilon)r_1^{\pi/\omega}\big)\Phi(\pi-\varphi_1)\\
&\qquad\qquad - \Theta(r_2)\big(a_{2p}^-(\varepsilon)r_2^{-\pi/\omega}+a_{2p}^+(\varepsilon)r_2^{\pi/\omega}\big)\Phi(\varphi_2)\Big)\\
&+ [\Delta,\Theta]w_{2p}(\varepsilon^{-1}x_2,\varepsilon^{-1}y_2;\varepsilon) - k^2\Theta(\varepsilon^{-2\sigma}r_2)w_{2p}(\varepsilon^{-1}x_2,\varepsilon^{-1}y_2;\varepsilon)\\
&+ [\Delta,\chi_{3,\varepsilon}]\Big(v_3(x,y;\varepsilon) - b_2\beta\varepsilon^{2\pi/\omega}(r_2^{-\pi/\omega}+a(k_p)r_2^{\pi/\omega})\Phi(\varphi_2)\Big)\\
&\qquad\qquad + [\Delta,\Xi]v_1(x,y;\varepsilon) + [\Delta,\Xi]v_3(x,y;\varepsilon),
\end{aligned}
$$

where

$$
b_{1p}^- = O(\varepsilon^{2\pi/\omega}),\ b_{1p}^+ = b_1 + O(\varepsilon^{2\pi/\omega}),\ a_{2p}^- = O(\varepsilon^{2\pi/\omega}),\ a_{2p}^+ = b_2 + O(\varepsilon^{2\pi/\omega}).
$$

Taking into account the asymptotics of $\mathbf{v}_1$ as $r_1 \to 0$ and passing to the variables $(\xi_1,\eta_1) = (\varepsilon^{-1}x_1,\varepsilon^{-1}y_1)$, we obtain

$$
\begin{aligned}
&\Big\|(x,y)\mapsto [\Delta,\chi_{1,\varepsilon}]\Big(\mathbf{v}_1(x,y) - (r_1^{-\pi/\omega}+a(k_p)r_1^{\pi/\omega})\Phi(\pi-\varphi_1)\Big)\Big\|^2\\
&\qquad \le c\int_{G(\varepsilon)}(r_1^2+\varepsilon^2)^\gamma\Big|[\Delta,\chi_{1,\varepsilon}]r_1^{-\pi/\omega+2}\Phi(\pi-\varphi_1)\Big|^2 dxdy \le c\varepsilon^{2(\gamma-\pi/\omega+1)},
\end{aligned}
$$

where $\|\cdot\|$ stands for $\|\cdot\,; V^0_{\gamma,\delta}(G(\varepsilon))\|$. This and (3.5.4) imply the estimate

$$
\Big\|(x,y)\mapsto [\Delta,\chi_{1,\varepsilon}]\Big(v_1(x,y) - (r_1^{-\pi/\omega}+a(k_p)r_1^{\pi/\omega})\Phi(\pi-\varphi_1)\Big)\Big\| \le c\varepsilon^{\gamma+\pi/\omega+1}.
$$

In the same way,

$$
\begin{aligned}
&\Big\|(x,y)\mapsto [\Delta,\chi_{2,\varepsilon}]\Big(v_2(x,y) - \Theta(r_1)\big(b_{1p}^-(\varepsilon)r_1^{-\pi/\omega}+b_{1p}^+(\varepsilon)r_1^{\pi/\omega}\big)\Phi(\pi-\varphi_1)\\
&\qquad\qquad - \Theta(r_2)\big(a_{2p}^-(\varepsilon)r_2^{-\pi/\omega}+a_{2p}^+(\varepsilon)r_2^{\pi/\omega}\big)\Phi(\varphi_2)\Big)\Big\| \le c\varepsilon^{\gamma+\pi/\omega+1},\\
&\Big\|(x,y)\mapsto [\Delta,\chi_{3,\varepsilon}]\Big(v_3(x,y) - (r_2^{-\pi/\omega}+a(k_p)r_2^{\pi/\omega})\Phi(\varphi_2)\Big)\Big\| \le c\varepsilon^{\gamma+\pi/\omega+1}.
\end{aligned}
$$

It is evident, that

$$
\|[\Delta,\Xi]v_l\| \le c\varepsilon^{2\pi/\omega}, \quad l=1,3.
$$

Further, since $\mathbf{w}_j^l$ behaves like $O(\rho_j^{-3\pi/\omega})$ at infinity, we have

$$
\begin{aligned}
&\int_{G(\varepsilon)}(r_j^2+\varepsilon^2)^\gamma\Big|[\Delta,\Theta]\mathbf{w}_j^l(\varepsilon^{-1}x_j,\varepsilon^{-1}y_j)\Big|^2 dx_jdy_j\\
&\qquad \le c\int_{K_j}(r_j^2+\varepsilon^2)^\gamma\Big|[\Delta,\Theta](\varepsilon^{-1}r_j)^{-3\pi/\omega}\Phi_2(\varphi_j)\Big|^2 dx_jdy_j \le c\varepsilon^{2(3\pi/\omega-\sigma_1)},
\end{aligned}
$$

where $\sigma_1 = 2\sigma(3\pi/\omega - \gamma + 1)$. A similar inequality holds with $\mathbf{w}_j^l$ replaced by $\mathbf{w}_j^r$. Considering (3.5.5)–(3.5.6), we get the estimate

$$\left\|[\Delta, \Theta]w_{jp}\right\| \le c\varepsilon^{4\pi/\omega - \sigma_1}.$$

Finally, using (3.5.5)–(3.5.6) once more, taking into account the estimate

$$\begin{aligned} &\int_{G(\varepsilon)} (r_j^2 + \varepsilon^2)^\gamma \left|\Theta(\varepsilon^{-2\sigma} r_j)\mathbf{w}_j^l(\varepsilon^{-1}x_j, \varepsilon^{-1}y_j)\right|^2 dx_j dy_j \\ = \;& \varepsilon^{2\gamma+2} \int_\Omega (\rho_j^2 + 1)^\gamma \left|\Theta(\varepsilon^{1-2\sigma}\rho_j)\mathbf{w}_j^l(\xi_j, \eta_j)\right|^2 d\xi_j d\eta_j \le c\varepsilon^{2\gamma+2} \end{aligned}$$

and a similar estimate for $\mathbf{w}_j^r$, we derive

$$\left\|(x,y) \mapsto \Theta(\varepsilon^{-2\sigma} r_j) w_{jp}(\varepsilon^{-1}x_j, \varepsilon^{-1}y_j)\right\| \le c\varepsilon^{\pi/\omega + \gamma + 1}.$$

Combining the obtained estimates, we arrive at (3.5.8).

Step C. This part contains somewhat modified arguments from the proof of Theorem 5.5.1 in [6]. Rewrite the right-hand side of the problem (3.5.1) in the form:

$$\begin{aligned} f(x,y) = \;& f_1(x,y;\varepsilon) + f_2(x,y;\varepsilon) + f_3(x,y;\varepsilon) \\ & + \varepsilon^{-\gamma-1} F_1(\varepsilon^{-1}x_1, \varepsilon^{-1}y_1; \varepsilon_1) + \varepsilon^{-\gamma-1} F_2(\varepsilon^{-1}x_2, \varepsilon^{-1}y_2; \varepsilon), \end{aligned} \tag{3.5.9}$$

where

$$\begin{aligned} f_l(x,y;\varepsilon) &= \chi_{l,\varepsilon^\sigma}(x,y) f(x,y), \\ F_j(\xi_j, \eta_j; \varepsilon) &= \varepsilon^{\gamma+1}\Theta(\varepsilon^{1-\sigma}\rho_j) f(x_{O_j} + \varepsilon\xi_j, y_{O_j} + \varepsilon\eta_j); \end{aligned}$$

(x,y) are arbitrary Cartesian coordinates; (x_{O_j}, y_{O_j}) stand for the coordinates of O_j in the system (x,y); x_j, y_j have been introduced in Section 3.4. From the definition of the norms it follows that

$$\|f_1; V^0_{\gamma,\delta}(G_1)\| + \|f_2; V^0_\gamma(G_2)\| + \|f_3; V^0_{\gamma,\delta}(G_3)\| + \|F_j; V^0_\gamma(\Omega_j)\| \le \|f; V^0_{\gamma,\delta}(G(\varepsilon))\|. \tag{3.5.10}$$

Consider solutions v_l and w_j to the limit problems

$$\begin{aligned} -(-i\nabla + \mathbf{A})^2 v \pm Hv + k^2 v = f_2 \quad & \text{in } G_2, \quad v = 0 \quad \text{on } \partial G_2, \\ \Delta v + k^2 v = f_l \quad & \text{in } G_l, \quad v = 0 \quad \text{on } \partial G_l, \quad l = 1,3, \\ \Delta w = F_j \quad & \text{in } \Omega_j, \quad w = 0 \quad \text{on } \partial\Omega_j, \end{aligned}$$

respectively; moreover, v_l with $l = 1,3$ satisfy the intrinsic radiation conditions at infinity, and v_2 satisfies the condition $(v_2, v_0)_{G_2} = 0$. According to Propositions 3.2.1, 3.2.2, and 3.2.3, the problems in G_l and Ω_j are uniquely solvable and

$$\begin{aligned} \|v_2; V^2_\gamma(G_2)\| &\le c_2\|f_2; V^0_\gamma(G_2)\|, \\ \|v_l; V^2_{\gamma,\delta,-}(G_l)\| &\le c_l\|f_l; V^0_{\gamma,\delta}(G_l)\|, \; l = 1,3 \\ \|w_j; V^2_\gamma(\Omega_j)\| &\le C_j\|F_j; V^0_\gamma(\Omega_j)\|, \; j = 1,2, \end{aligned} \tag{3.5.11}$$

where c_l and C_j are independent of ε. We set

$$U(x,y;\varepsilon) = \chi_{1,\varepsilon}(x,y)v_1(x,y;\varepsilon) + \varepsilon^{-\gamma+1}\Theta(r_1)w_1(\varepsilon^{-1}x_1,\varepsilon^{-1}y_1;\varepsilon)$$
$$+\chi_{2,\varepsilon}(x,y)v_2(x,y;\varepsilon) + \varepsilon^{-\gamma+1}\Theta(r_2)w_2(\varepsilon^{-1}x_2,\varepsilon^{-1}y_2;\varepsilon) + \chi_{3,\varepsilon}(x,y)v_3(x,y;\varepsilon).$$

The estimates (3.5.10) and (3.5.11) lead to

$$\|U; V^2_{\gamma,\delta,-}(G(\varepsilon))\| \le c\|f; V^0_{\gamma,\delta}(G(\varepsilon))\| \tag{3.5.12}$$

with c independent of ε. Denote the mapping $f \mapsto U$ by R_ε. Arguing as in the proof of Theorem 5.5.1 in [6], we obtain $(-(-i\nabla + \mathbf{A})^2 \pm H + k^2)R_\varepsilon = I + S_\varepsilon$, where S_ε is an operator in $V^0_{\gamma,\delta}(G(\varepsilon))$ of small norm.

Step D. Recall that the operator S_ε is defined on the subspace $V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$. We need the image of the operator S_ε to be included in $V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$, too. To this end, replace the mapping R_ε by $\widetilde{R}_\varepsilon : f \mapsto U(f) + a(f)u_p$, where u_p has been constructed in Step **A**, $a(f)$ is a constant. Then $(-(-i\nabla + \mathbf{A})^2 \pm H + k^2)\widetilde{R}_\varepsilon = I + \widetilde{S}_\varepsilon$ with

$$\widetilde{S}_\varepsilon = S_\varepsilon + a(\cdot)(-(-i\nabla + \mathbf{A})^2 \pm H + k^2)u_p.$$

The condition $(\chi_{2,\varepsilon^\sigma}\widetilde{S}_\varepsilon f, v_0)_{G_2} = 0$ as $k = k_0$ gives

$$a(f) = -\frac{(\chi_{2,\varepsilon^\sigma}S_\varepsilon f, v_0)_{G_2}}{(\chi_{2,\varepsilon^\sigma}(-(-i\nabla + \mathbf{A})^2 \pm H + k_0^2)u_p, v_0)_{G_2}}.$$

Prove that $\|\widetilde{S}_\varepsilon\| \le c\|S_\varepsilon\|$, where c is independent of ε, k. We have

$$\|\widetilde{S}_\varepsilon f\| \le \|S_\varepsilon f\| + |a(f)|\,\|(-(-i\nabla + \mathbf{A})^2 \pm H + k^2)u_p\|.$$

The estimate (3.5.8) (with $\gamma > \pi/\omega - 2$ and $2\pi/\omega > \sigma_1$), the formula for k_p, and the condition $k^2 - k_0^2 = O(\varepsilon^{2\pi/\omega})$ imply the inequality

$$\|(-(-i\nabla + \mathbf{A})^2 \pm H + k^2)u_p; V^0_{\gamma,\delta}\|$$
$$\le |k^2 - k_p^2|\,\|u_p; V^0_{\gamma,\delta}\| + \|(-(-i\nabla + \mathbf{A})^2 \pm H + k_p^2)u_p; V^0_{\gamma,\delta}\| \le c\varepsilon^{2\pi/\omega}.$$

Since the supports of the functions $(-(-i\nabla + \mathbf{A})^2 \pm H + k_p^2)u_p$ and $\chi_{2,\varepsilon^\sigma}$ do not intersect, we have

$$|(\chi_{2,\varepsilon^\sigma}(-(-i\nabla + \mathbf{A})^2 \pm H + k_0^2)u_p, v_0)_{G_2}| = |(k_0^2 - k_p^2)(u_p, v_0)_{G_2}| \ge c\varepsilon^{2\pi/\omega}.$$

Further, $\gamma - 1 < \pi/\omega$, so

$$|(\chi_{2,\varepsilon^\sigma}S_\varepsilon f, v_0)_{G_2}| \le \|S_\varepsilon f; V^0_{\gamma,\delta}(G(\varepsilon))\|\,\|v_0; V^0_{-\gamma}(G_2)\| \le c\|S_\varepsilon f; V^0_{\gamma,\delta}(G(\varepsilon))\|.$$

Hence,

$$|a(f)| \le c\varepsilon^{-2\pi/\omega}\|S_\varepsilon f; V^0_{\gamma,\delta}(G(\varepsilon))\|$$

and $\|\widetilde{S}_\varepsilon f\| \leq c\|S_\varepsilon f\|$. Thus, the operator $I + \widetilde{S}_\varepsilon$ in $V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$ is invertible, which is also true for the operator of the problem (3.5.1):

$$A_\varepsilon : u \mapsto -(-i\nabla + \mathbf{A})^2 u \pm Hu + k^2 u : \mathring{V}^{2,\perp}_{\gamma,\delta,-}(G(\varepsilon)) \mapsto V^{0,\perp}_{\gamma,\delta}(G(\varepsilon));$$

here $\mathring{V}^{2,\perp}_{\gamma,\delta,-}(G(\varepsilon))$ denotes the space of elements in $V^{2}_{\gamma,\delta,-}(G(\varepsilon))$ that vanish on $\partial G(\varepsilon)$ and are sent by the operator $-(-i\nabla + \mathbf{A})^2 \pm H + k^2$ into $V^{0,\perp}_{\gamma,\delta}$. The inverse operator $A_\varepsilon^{-1} = \widetilde{R}_\varepsilon(I + \widetilde{S}_\varepsilon)^{-1}$ is bounded uniformly with respect to ε, k. Therefore, the inequality (3.5.3) holds with c independent of ε, k. □

We consider a solution u_1 to the homogeneous problem (3.1.1) defined by

$$u_1(x,y) = \begin{cases} U_1^+(x,y) + s_{11}\, U_1^-(x,y) + O(\exp(\delta x)), & x \to -\infty, \\ s_{12}\, U_2^-(x,y) + O(\exp(-\delta x)), & x \to +\infty. \end{cases}$$

Let s_{11} and s_{12} be the elements of the scattering matrix determined by this solution. Denote by $\widetilde{u}_{1,\sigma}$ the function defined by (3.4.1) with $\Theta(r_j)$ replaced by $\Theta(\varepsilon_j^{-2\sigma} r_j)$ and with removed R; $\widetilde{s}_{11}$, $\widetilde{s}_{12}$ are the same as in (3.4.18) – (3.4.19).

Theorem 3.5.2. *Let the conjectures in Proposition* 3.5.1 *be fulfilled. Then the inequality*

$$|s_{11} - \widetilde{s}_{11}| + |s_{12} - \widetilde{s}_{12}| \leq c|\widetilde{s}_{12}|\varepsilon^{2-\delta}$$

holds with constant c independent of ε and k, δ being an arbitrarily small positive number.

Proof. The difference $R = u_1 - \widetilde{u}_{1,\sigma}$ is in the space $V^2_{\gamma,\delta,-}(G(\varepsilon))$ and

$$f_1 := (-(-i\nabla + \mathbf{A})^2 \pm H + k^2)(u_1 - \widetilde{u}_{1,\sigma})$$

is in $V^{0,\perp}_{\gamma,\delta}(G(\varepsilon))$. By Proposition 3.5.1,

$$\|R; V^2_{\gamma,\delta,-}(G(\varepsilon))\| \leq c\, \|f_1; V^0_{\gamma,\delta}(G(\varepsilon))\|. \tag{3.5.13}$$

Let us show that

$$\|f_1; V^0_{\gamma,\delta}(G(\varepsilon))\| \leq c|\widetilde{s}_{12}|(\varepsilon^{\gamma-\pi/\omega+1} + \varepsilon^{2\pi/\omega-\sigma_1}), \tag{3.5.14}$$

where $\sigma_1 = 2\sigma(3\pi/\omega - \gamma + 1)$. The required estimate is a consequence of the last two inequalities with $\gamma = \pi/\omega + 1 - \delta$ and $\sigma_1 = \delta$.

Arguing as in Step B of the proof of the previous statement, we obtain the estimate

$$\begin{aligned} \|f_1; V^0_{\gamma,\delta}(G(\varepsilon))\| &\leq c(\varepsilon^{\gamma+1} + \varepsilon^{3\pi/\omega-\sigma_1}) \\ &\times \max_{j=1,2}(|a_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |a_j^+(\varepsilon)|\varepsilon^{\pi/\omega} + |b_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |b_j^+(\varepsilon)|\varepsilon^{\pi/\omega}). \end{aligned}$$

From (3.4.11) it follows that

$$(|a_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |a_j^+(\varepsilon)|\varepsilon^{\pi/\omega}) \leq c(|b_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |b_j^+(\varepsilon)|\varepsilon^{\pi/\omega}).$$

Using the formulas (3.4.8) and (3.4.10) for $b_j^\pm$ and relations (3.4.17) and (3.4.15), we get

$$|b_j^-(\varepsilon)|\varepsilon^{-\pi/\omega} + |b_j^+(\varepsilon)|\varepsilon^{\pi/\omega} \leq c\varepsilon^{-\pi/\omega}|\widetilde{s}_{12}(\varepsilon)|.$$

Comparing the obtained estimates, we arrive at (3.5.14). □

Now we return to the detailed notations introduced in the first three sections. Theorem 3.5.2 and formulas (3.4.21)–(3.4.22) lead to the next statement.

Theorem 3.5.3. *For $|k^2 - k^2_{r,\pm}| = O(\varepsilon^{2\pi/\omega})$ the asymptotic expansions*

$$T^{\pm}(k,\varepsilon) = \frac{1}{\dfrac{1}{4}\left(\dfrac{|b_1^{\pm}|}{|b_2^{\pm}|} + \dfrac{|b_2^{\pm}|}{|b_1^{\pm}|}\right)^2 + P_{\pm}^2\left(\dfrac{k^2 - k^2_{r,\pm}}{\varepsilon^{4\pi/\omega}}\right)^2}(1 + O(\varepsilon^{2-\delta})),$$

$$k^2_{r,\pm} = k^2_{0,\pm} - \alpha(|b_1^{\pm}|^2 + |b_2^{\pm}|^2)\varepsilon^{2\pi/\omega} + O\big(\varepsilon^{2\pi/\omega+2-\delta}\big),$$

$$\Upsilon^{\pm}(\varepsilon) = \left(\frac{|b_1^{\pm}|}{|b_2^{\pm}|} + \frac{|b_2^{\pm}|}{|b_1^{\pm}|}\right) P_{\pm}^{-1}\varepsilon^{4\pi/\omega}\big(1 + O(\varepsilon^{2-\delta})\big),$$

hold, where $\Upsilon^{\pm}(\varepsilon)$ is the width of the resonant peak at its half-height,

$$P_{\pm} = (2|b_1^{\pm}||b_2^{\pm}|\beta^2|A(k_0)|^2)^{-1},$$

and δ is an arbitrarily small positive number.

3.6 Comparison of asymptotic and numerical approaches

The principal parts of the asymptotic formulas in Theorem 3.5.3 contain the constants $b_j^{\pm}$, $|A|$, α, β. To find them one has to solve numerically several boundary value problems. In this section, we state the problems and describe a way to solve them. We also outline a method for computing the waveguide scattering matrix S taken from the paper [15]. Then we compare the asymptotics having calculated constants and the numerically found scattering matrix.

3.6.1 Problems and methods for numerical analysis

Calculation of b_j

To find b_j, we solve the spectral problem

$$\begin{aligned} (-i\nabla + \mathbf{A}(x,y))^2 v(x,y) \pm H(\rho)v(x,y) &= k^2 v(x,y) \quad \text{in} \quad G_2, \\ v(x,y) &= 0 \quad \text{on} \quad \partial G_2, \end{aligned} \tag{3.6.1}$$

by FEM (for the details see Appendix 1). Let V_0 be an eigenfunction corresponding to k_0^2 and normalized by

$$\int_{G_2} |V_0(x,y)|^2\, dxdy = 1.$$

We have

$$V_0(x,y) \sim \begin{cases} b_1^{\pm} r_1^{\pi/\omega}\Phi(\varphi_1) & \text{as} \quad r_1 \to 0, \\ b_2^{\pm} r_2^{\pi/\omega}\Phi(\pi - \varphi_2) & \text{as} \quad r_2 \to 0, \end{cases} \tag{3.6.2}$$

where (ρ_j, φ_j) are polar coordinates centered in $\mathbf{r}_j$, and $\Phi(\theta) = \pi^{-1/2}\cos(\pi\theta/\omega)$. Then $b_1^{\pm}$ and $b_2^{\pm}$ in (3.6.2) can be defined by

$$b_1^{\pm} = \epsilon^{-\pi/\omega}\frac{V_0(\epsilon,0)}{\Phi(0)} = \sqrt{\pi}\epsilon^{-\pi/\omega}V_0(\epsilon,0), \qquad b_2^{\pm} = \sqrt{\pi}\epsilon^{-\pi/\omega}V_0(d-\epsilon,0),$$

where ϵ is a small positive number.

Calculation of $|A|$

To calculate $|A|$ we must solve numerically the problem

$$\begin{aligned} -\Delta v(x,y) &= k^2 v(x,y) \quad \text{in} \quad G_1, \\ v(x,y) &= 0 \quad \text{on} \quad \partial G_1, \end{aligned} \tag{3.6.3}$$

with conditions

$$\begin{aligned} v(x,y) &\sim 2i\overline{A}\rho^{\pi/\omega}\Phi(\pi-\varphi) && \text{as} \quad \rho \to 0, \\ v(x,y) &= \left(e^{-i\nu_1 x} + \frac{\overline{A}}{A}e^{i\nu_1 x}\right)\Psi_1(y) + O(e^{-\gamma|x|}) && \text{as} \quad x \to -\infty, \end{aligned} \tag{3.6.4}$$

where (ρ, φ) are polar coordinates centered in $\mathbf{r}_1$. Denote the truncated domain

$$G_1 \cap \{(x,y) : x > -D\}$$

by G_1^D and the artificial part of the boundary $\partial G_1^D \cap \{(x,y) : x = -D\}$ by Γ^D.

Consider the following problem

$$\begin{aligned} \Delta v^D(x,y) + k^2 v^D(x,y) &= 0 && \text{in} \quad G_1^D, \\ v^D(x,y) &= 0 && \text{on} \quad \partial G_1^D \backslash \Gamma^D, \\ (\partial_n + i\nu_1)\, v^D(x,y) &= f(x,y) && \text{on} \quad \Gamma^D. \end{aligned} \tag{3.6.5}$$

If $\nu_1 \in \mathbb{R}\backslash 0$ and $f \in L_2(\Gamma^D)$, the problem has a unique solution v^D, and v^D satisfies the inequality

$$\|v^D\|_{G_1^D} \leqslant C_1\|f\|_{\Gamma^D},$$

where $\|v^D\|_{G_1^D} := \|v^D\|_{L_2(G_1^D)}$; similar notation is used for the norms and the inner products below.

Let v be a solution to the problem (3.6.3), (3.6.4), and let V be a solution to the problem (3.6.5) with $f = 2i\nu_1 e^{i\nu_1 D}\Psi_1(y)$. Then $u = v - V$ satisfies (3.6.5) with $f = O(e^{-\gamma D})$. Hence, $\|v - V\|_{G_1^D} \leqslant C_0 e^{-\gamma D}$.

We find V with FEM (for the details see Appendix 2) and put

$$A = i\sqrt{\pi}\epsilon^{-\pi/\omega}\overline{V}(-\epsilon,0)/2.$$

Calculation of α and β

To calculate α and β, we consider the boundary value problem

$$\begin{aligned} -\Delta w(\xi,\eta) &= 0 \quad \text{in} \quad \Omega, \\ w(\xi,\eta) &= 0 \quad \text{on} \quad \partial\Omega, \end{aligned} \tag{3.6.6}$$

with the following conditions at infinity

$$w(\xi,\eta) = \begin{cases} (\rho^{\pi/\omega} + \alpha\rho^{-\pi/\omega})\Phi(\varphi) + O(\rho^{-3\pi/\omega}) & \text{as} \quad \rho \to \infty,\ \xi > 0, \\ \beta\rho^{-\pi/\omega}\Phi(\pi - \varphi) + O(\rho^{-3\pi/\omega}) & \text{as} \quad \rho \to \infty,\ \xi < 0, \end{cases} \tag{3.6.7}$$

where (ρ, φ) are polar coordinates centered in $\mathbf{r}_1$. Introduce the notations

$$\begin{aligned} \Omega^D &= \Omega \cap \{(\rho,\varphi) : \rho < D\}, \\ \Gamma^D &= \partial\Omega^D \cap \{(\rho,\varphi) : \rho = D\}. \end{aligned}$$

Consider the problem

$$\begin{aligned} \Delta w^D(\xi,\eta) &= 0 & \text{in} & \quad \Omega^D, \\ w^D(\xi,\eta) &= 0 & \text{on} & \quad \partial\Omega^D \backslash \Gamma^D, \\ (\partial_n + \zeta)\, w^D(\xi,\eta) &= g(\xi,\eta) & \text{on} & \quad \Gamma^D. \end{aligned} \tag{3.6.8}$$

If w^D is a solution and $\zeta > 0$, then

$$\|w^D\|_{\Gamma^D} \leqslant \zeta^{-1}\|g\|_{\Gamma^D}. \tag{3.6.9}$$

Denote the left-hand part of Γ^D by Γ^D_- and the right-hand part of Γ^D by Γ^D_+. Let W satisfy (3.6.8) with

$$\zeta = \pi/\omega D, \quad g|_{\Gamma^D_-} = 0, \quad g|_{\Gamma^D_+} = (2\pi/\omega)D^{(\pi/\omega)-1}\Phi(\varphi).$$

Since the conditions (3.6.7) can be differentiated, $w - W$ satisfies (3.6.8) with

$$g = O(D^{-(3\pi/\omega)-1}).$$

According to (3.6.9),

$$\|w - W\|_{\Gamma^D} \leqslant c\frac{\omega D}{\pi}D^{-(3\pi/\omega)-1} = c'D^{-3\pi/\omega}$$

as $D \to +\infty$. We find W with FEM (for the details see Appendix 2) and take

$$\beta = \frac{W(-D,0)}{\Phi(0)}D^{\pi/\omega} = \sqrt{\pi}W(-D,0)D^{\pi/\omega}.$$

Obviously, $\|(w - D^{\pi/\omega}\Phi(\varphi)) - (W - D^{\pi/\omega}\Phi(\varphi))\|_{\Gamma^D} \leqslant c'D^{-3\pi/\omega}$, therefore we put

$$\alpha = \frac{W(D,0) - D^{\pi/\omega}\Phi(0)}{\Phi(0)}D^{\pi/\omega} = \sqrt{\pi}W(D,0)D^{\pi/\omega} - D^{2\pi/\omega}.$$

Now the coefficients in the asymptotic formulas have been calculated, so we can use the asymptotics for a quantitative description of the polarization process. However, the formulas are designed for sufficiently small narrows' diameters. Thus, it remains to estimate the range of ε where asymptotics works. To this end we calculate the scattering matrix employing the method suggested in [7]. Here we present the needed description of the method. Introduce

$$\begin{aligned} G(\varepsilon, D) &= G(\varepsilon) \cap \{(x,y) : -D < x < d + D\}, \\ \Gamma_1^D &= \partial G(\varepsilon, D) \cap \{(x,y) : x = -D\}, \\ \Gamma_2^D &= \partial G(\varepsilon, D) \cap \{(x,y) : x = d + D\} \end{aligned}$$

for large D. As an approximation to the row (s_{11}, s_{12}) of the scattering matrix $S(k)$ we take the minimizer of a quadratic functional. To construct such a functional we consider the problem

$$\begin{aligned} (-i\nabla + \mathbf{A})^2 \mathcal{X}_\pm^D \pm H \mathcal{X}_\pm^D = k^2 \mathcal{X}_\pm^D \quad &\text{in} \quad G(\varepsilon, D), \\ \mathcal{X}_\pm^D = 0 \quad &\text{on} \quad \partial G(\varepsilon, D) \setminus (\Gamma_1^D \cup \Gamma_2^D), \end{aligned} \tag{3.6.10}$$

$$\begin{aligned} (\partial_n + i\zeta)\mathcal{X}_\pm^D &= i(-\nu_1 + \zeta)e^{-i\nu_1 D}\Psi_1(y) + a_1\, i(\nu_1 + \zeta)e^{i\nu_1 D}\Psi_1(y) \text{ on } \Gamma_1^D, \\ (\partial_n + i\zeta)\mathcal{X}_\pm^D &= a_2\, i(\nu_1 + \zeta)e^{i\nu_1(d+D)}\Psi_1(y) \quad \text{on } \Gamma_2^D, \end{aligned} \tag{3.6.11}$$

where $\zeta \in \mathbb{R} \setminus \{0\}$ is an arbitrary fixed number, and a_1, a_2 are complex numbers. As approximation to the row (s_{11}, s_{12}) we take the minimizer $a^0(D) = (a_1^0(D), a_2^0(D))$ of the functional

$$J^D(a_1, a_2) = \left\| \mathcal{X}_\pm^D - e^{-i\nu_1 D}\Psi_1 - a_1 e^{i\nu_1 D}\Psi_1 \right\|^2_{\Gamma_1^D} + \left\| \mathcal{X}_\pm^D - a_2\, e^{i\nu_1(d+D)}\Psi_1 \right\|^2_{\Gamma_2^D}, \tag{3.6.12}$$

where $\mathcal{X}_\pm^D$ is a solution to problem (3.6.10). From the results of the paper [7] it follows that $a_j^0(D,k) \to s_{1j}(k)$ with exponential rate as $D \to \infty$. More precisely, there exist positive constants Λ and C such that

$$|a_j^0(D,k) - s_{1j}(k)| \leqslant Ce^{-\Lambda D}, \qquad j = 1, 2,$$

for all $k^2 \in [\mu_1, \mu_2]$ and sufficiently large D; the interval $[\mu_1, \mu_2]$ of continuous spectrum of the problem (3.1.1) lies between the first and the second thresholds and does not contain the thresholds. (Note, that application of the method is not hindered by possible presence on the interval $[\mu_1, \mu_2]$ of eigenvalues of the problem (3.1.1) corresponding to eigenfunctions exponentially decaying at infinity.) To express $\mathcal{X}_\pm^D$ by means of a_1, a_2, we consider the problems

$$\begin{aligned} (-i\nabla + \mathbf{A})v_{\pm,1}^\pm \pm H v_{\pm,1}^\pm = k^2 v_{\pm,1}^\pm \quad &\text{in} \quad G(\varepsilon, D), \\ v_{\pm,1}^\pm = 0 \quad &\text{on} \quad \partial G(\varepsilon, D) \setminus (\Gamma_1^D \cup \Gamma_2^D), \\ (\partial_n + i\zeta)v_{\pm,1}^\pm = i(\mp\nu_1 + \zeta)e^{\mp i\nu_1 D}\Psi_1 \quad &\text{on} \quad \Gamma_1^D, \\ (\partial_n + i\zeta)v_{\pm,1}^\pm = 0 \quad &\text{on} \quad \Gamma_2^D \end{aligned} \tag{3.6.13}$$

and

$$\begin{aligned} (-i\nabla + \mathbf{A})v^{\pm}_{\pm,2} \pm H v^{\pm}_{\pm,2} &= k^2 v^{\pm}_{\pm,2} && \text{in} \quad G(\varepsilon, D), \\ v^{\pm}_{\pm,2} &= 0 && \text{on} \quad \partial G(\varepsilon, D) \setminus (\Gamma_1^D \cup \Gamma_2^D), \\ (\partial_n + i\zeta)v^{\pm}_{\pm,2} &= 0 && \text{on} \quad \Gamma_1^D, \\ (\partial_n + i\zeta)v^{\pm}_{\pm,2} &= i(\mp\nu_1 + \zeta)e^{\mp i\nu_1(d+D)}\Psi_1 && \text{on} \quad \Gamma_2^D. \end{aligned} \tag{3.6.14}$$

In $v^{\pm}_{\pm,j}$ the upper and lower $\pm$ correspond to $\mp$ in the condition on $\Gamma_1^D \cup \Gamma_2^D$ and to the sign in the Pauli equation, respectively. Let us express $\mathcal{X}^D_{\pm,m}$ by means of the solutions $v^{\pm}_{\pm,j}$ to problems (3.6.13) and (3.6.14). We have

$$\mathcal{X}^D_{\pm} = v^{+}_{\pm} + a_1 v^{-}_{\pm,1} + a_2 v^{-}_{\pm,2}.$$

The functional (3.6.12) can be rewritten in the form

$$J^D(a,k) = \langle a\mathcal{E}^D(k), a\rangle + 2\,\mathrm{Re}\left(\langle \mathcal{F}_1^D(k), a\rangle\right) + \mathcal{G}_1^D(k),$$

where $\langle\cdot,\cdot\rangle$ is the inner product on $\mathbb{C}^2$, and $\mathcal{E}^D$ stands for the 2×2–matrix with entries

$$\begin{aligned} \mathcal{E}^D_{11} &= \left((v^{-}_{\pm,1} - e^{i\nu_1 D}\Psi_1), (v^{-}_{\pm,1} - e^{i\nu_1 D}\Psi_1)\right)_{\Gamma_1^D} + \left(v^{-}_{\pm,1}, v^{-}_{\pm,1}\right)_{\Gamma_2^D}, \\ \mathcal{E}^D_{1,2} &= \left((v^{-}_{\pm,1} - e^{i\nu_1 D}\Psi_1), v^{-}_{\pm,2}\right)_{\Gamma_1^D} + \left(v^{-}_{\pm,1}, (v^{-}_{\pm,2} - e^{i\nu_1(d+D)}\Psi_1)\right)_{\Gamma_2^D}, \\ \mathcal{E}^D_{2,1} &= \left(v^{-}_{\pm,2}, (v^{-}_{\pm,1} - e^{i\nu_1 D}\Psi_1)\right)_{\Gamma_1^D} + \left((v^{-}_{\pm,2} - e^{i\nu_1(d+D)}\Psi_1), v^{-}_{\pm,1}\right)_{\Gamma_2^D}, \\ \mathcal{E}^D_{2,2} &= \left(v^{-}_{\pm,2}, v^{-}_{\pm,2}\right)_{\Gamma_1^D} + \left((v^{-}_{\pm,2} - e^{i\nu_1(d+D)}\Psi_1), (v^{-}_{\pm,2} - e^{i\nu_1(d+D)}\Psi_1)\right)_{\Gamma_2^D}; \end{aligned}$$

$\mathcal{F}_1^D(k)$ is the row $(\mathcal{F}_{11}^D(k), \mathcal{F}_{12}^D(k))$ and $\mathcal{G}_1^D(k)$ is the number defined by

$$\begin{aligned} \mathcal{F}^D_{11} &= \left((v^{+}_{\pm,1} - e^{-i\nu_1 D}\Psi_1), (v^{-}_{\pm,1} - e^{i\nu_1 D}\Psi_1)\right)_{\Gamma_1^D} + \left(v^{+}_{\pm,1}, v^{-}_{\pm,1}\right)_{\Gamma_2^D}, \\ \mathcal{F}^D_{12} &= \left((v^{+}_{\pm,1} - e^{-i\nu_1 D}\Psi_1), v^{-}_{\pm,2})\right)_{\Gamma_1^D} + \left(v^{+}_{\pm,1}, (v^{-}_{\pm,2} - e^{i\nu_1(d+D)}\Psi_1)\right)_{\Gamma_2^D}, \\ \mathcal{G}^D_{1} &= \left((v^{+}_{\pm,1} - e^{-i\nu_1 D}\Psi_1), (v^{+}_{\pm,1} - e^{-i\nu_1 D}\Psi_1)\right)_{\Gamma_1^D} + \left(v^{+}_{\pm,1}, v^{+}_{\pm,1}\right)_{\Gamma_2^D}, \end{aligned}$$

The minimizer $a^0 = (a_1^0(D,k), a_2^0(D,k))$ satisfies $a^0\mathcal{E}^D + \mathcal{F}_1^D = 0$. The solution to this equation serves as an approximation to the first row of the scattering matrix. In the same way one can show that the approximation to the scattering matrix is the solution $S^D(k)$ to the matrix equation of the form $S^D\mathcal{E}^D + \mathcal{F}^D = 0$. If one chooses $\zeta = -\nu_1$, then $v^{-}_{\pm,1} = v^{-}_{\pm,2} = 0$, $\mathcal{E}^D = (1/\nu_1)\mathrm{Id}$, and $S^D = -\nu_1\mathcal{F}^D$.

3.6.2 Comparison of asymptotic and numerical results

Let us compare the asymptotics $k^2_{res,a}(\varepsilon)$ of resonant energy $k^2_{res}(\varepsilon)$ and the approximate value $k^2_{res,n}(\varepsilon)$ obtained by the numerical method.

The 'numerical' and 'asymptotic' resonant energies are shown in Figure 10. The discrepancy between the curves depends on the magnetic field H_0 and the narrows' opening ω. Numerical resonance is calculated by the iteration process, the asymptotic resonant energy taken for initial value.

The shapes of "asymptotic" and "numerical" resonant peaks are almost the same (see Figure 11). The difference between the peaks is quantitatively depicted in Figure 12 (note the logarithmic scale on the axes). Moreover, it turns out that the ratio of the width $\Delta_n(h, \varepsilon)$ of numerical peak at height h to the width $\Delta_a(h, \varepsilon)$ of asymptotic peak is independent of h. The ratio as function of ε is displayed in Figure 13.

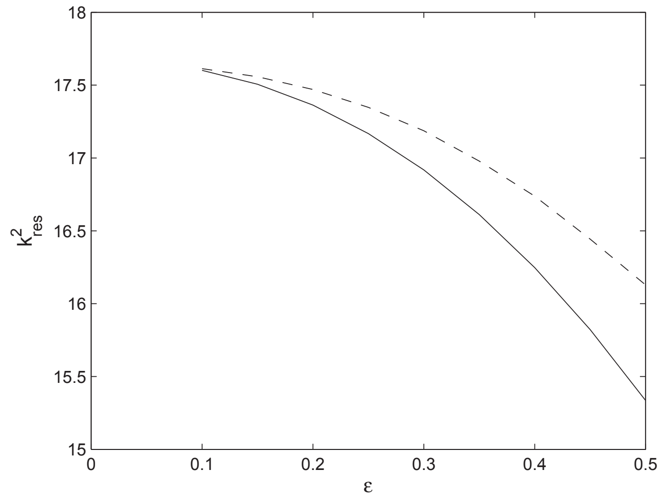


FIGURE 10 Asymptotic description $k^2_{res,a}(\varepsilon)$ (solid curve) and numerical description $k^2_{res,n}(\varepsilon)$ (dashed curve) for resonant energy $k^2_{res}(\varepsilon)$.

The obtained data show that asymptotic and numerical methods give equivalent results at the band of the narrows' diameters $0.1 < \varepsilon < 0.5$ (see Figures 10 and 12). The numerical method becomes ill-conditioned as $\varepsilon < 0.1$, while the asymptotics remains reliable. The explanation is the same as in the previous chapter. On the other hand, the asymptotics gives way to the numerical method as the diameter increases.

The difference between the asymptotic and numerical values is more significant for larger ε because the asymptotics becomes unreliable. However, as the numerical method shows, for $\varepsilon \geq 0.5$ the resonant peak turns out to be so wide that the resonant tunneling phenomenon dies out by itself.

Numerical simulations show sharp decrease of $T(k^2_{res})$ at certain values H_{cr} of the magnetic field (see Figure 14). The phenomenon is connected with the Aharonov–Bohm effect and is caused by the phase shift and mutual interference of electron waves bypassing the magnetic field along curves 1 and 2 (see Figure 8). At $H = H_{cr}$ the waves cancel each other out.

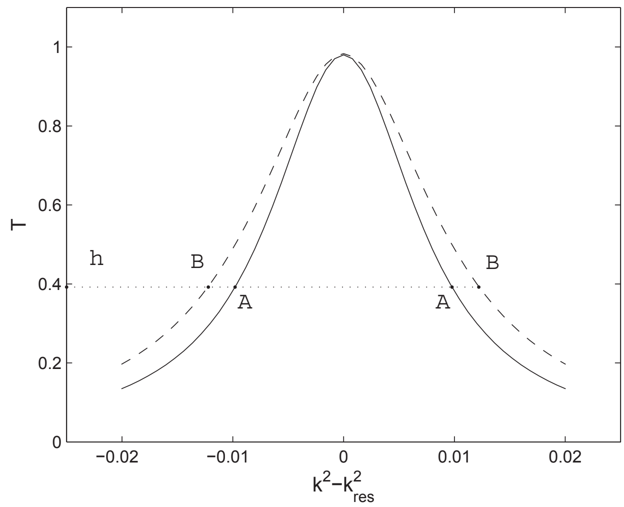


FIGURE 11 Transition coefficient for $\varepsilon = 0.2$, asymptotic description $T_a(k^2 - k^2_{res,a})$ (solid curve) and numerical description $T_n(k^2 - k^2_{res,n})$ (dashed curve). The width of resonant peak at height h: asymptotic $\Delta_a(h, \varepsilon) = AA$; numerical $\Delta_n(h, \varepsilon) = BB$.

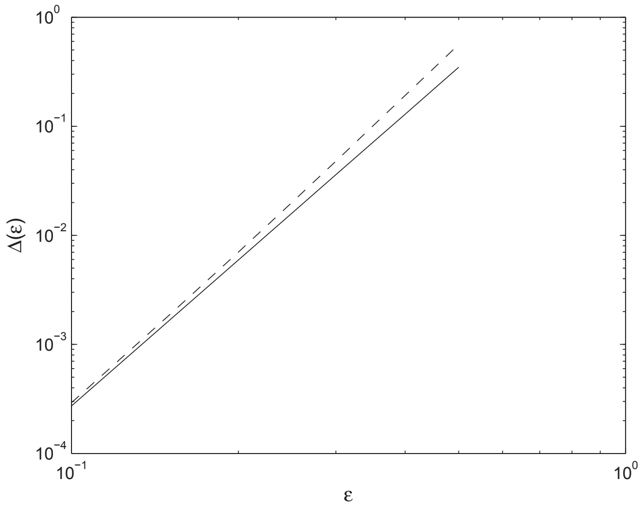


FIGURE 12 The width $\Delta(\varepsilon)$ of resonant peak at half-height of the peak (dashed line for numerical description, solid line for asymptotic description).

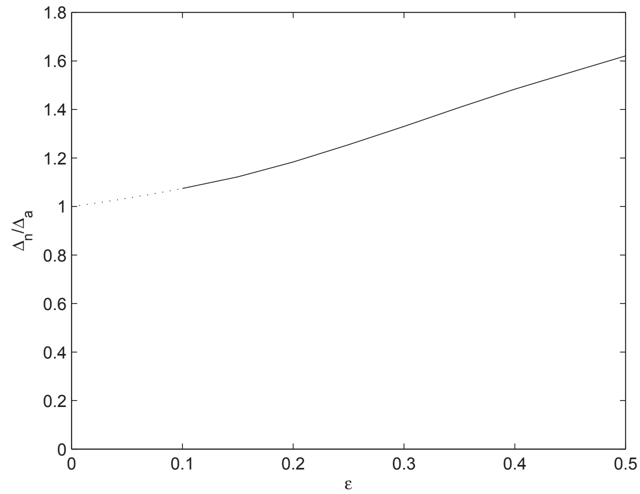


FIGURE 13 Ratio $\Delta_n(h, \varepsilon)/\Delta_a(h, \varepsilon)$ as function in ε. The ratio is independent of h within the accuracy of the analysis.

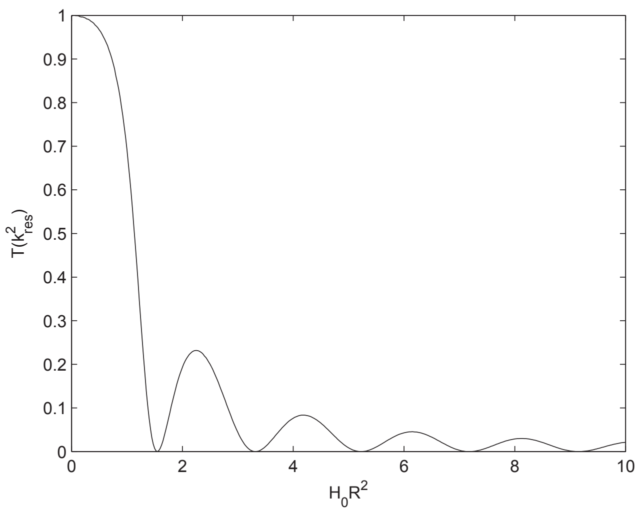


FIGURE 14 The transition coefficient at resonance for $R = 0.2$.

4 MULTICHANNEL SCATTERING

We consider an infinite two-dimensional waveguide that far from the coordinate origin coincides with a strip. The waveguide has two narrows which play the role of effective potential barriers for the longitudinal electron motion and, thereby, form a resonator between them. We analyze the resonator scattering characteristics. The results show that the eigenvalues of the resonator and the resonant energies of the waveguide are effectively approximated by a simple formula.

Also, as the obtained data show, to avoid dealing with transmission between transversal states and to get sharp resonant peaks, the devices based on the phenomenon must be designed with such parameters (geometry, voltage, etc.) that ensure the electron energy being below the third threshold.

4.1 Preliminaries

The total energy E of an electron moving in a cylindrical quantum waveguide can be represented in the form

$$E = E_{\perp} + E_{||}, \tag{4.1.1}$$

where $E_{\perp}$ is the transversal and $E_{||}$ is the longitudinal components.

The values of $E_{\perp}$ are quantized and depend on the form of the waveguide cross-section. For instance, if the waveguide cross-section is a disk of radius R, then the n-th level of $E_{\perp}$ satisfies

$$E_{\perp}(n) = \frac{\hbar^2}{2m_t^* R^2}\mu_n^2, \tag{4.1.2}$$

μ_n being the n-th root of the Bessel function J_0, $J_0(\mu_n) = 0$, and m_t^* the transversal effective electron mass (see, e.g. [16]). The effective mass of an electron takes into account the average effect of the grating periodic potential on the electron motion. For the anisotropic gratings the effective mass depends on the motion direction. In the simplest two-dimensional case, where the waveguide is a strip of width D, we have

$$E_\perp(n) = \frac{\hbar^2\pi^2}{2m_t^* D^2} n^2. \tag{4.1.3}$$

The spectrum of $E_{||}$ is continuous,

$$E_{||} = \frac{\hbar^2 k_{||}^2}{2m_l^*}. \tag{4.1.4}$$

Here $k_{||}$ is an electron wave number, m_l^* is the effective electron mass along the waveguide axis. In the dimensionless form for the strip

$$\widetilde{E}_\perp(n) = \frac{\pi^2}{\widetilde{D}^2} n^2, \qquad \widetilde{E}_{||} = \frac{m_t^*}{m_l^*}\widetilde{k}_{||}^2, \tag{4.1.5}$$

where $\widetilde{E}_\perp = E_\perp/E_0$ and $\widetilde{E}_{||} = E_{||}/E_0$ are the transverse and longitudinal dimensionless energies, $\widetilde{D} = D/D_0$ is the dimensionless waveguide width, $\widetilde{k}_{||} = k_{||}D_0$ is the dimensionless wave number, $E_0 = \hbar^2/(2m_t^* D_0^2)$ is the unit of energy, D_0 is the unit of length.

In what follows we analyze in the dimensionless form a waveguide coinsiding with a strip, where $m_l^* = m_t^*$, and omit $\sim$ in the notations. Then

$$E = E_\perp + E_{||}, \qquad E_\perp(n) = \frac{\pi^2}{D^2} n^2, \qquad E_{||} = k_{||}^2, \tag{4.1.6}$$

Assume that inside a waveguide the electron potential energy vanishes while outside it is equal to infinity (i.e. sufficiently large). Then the wave function of an electron going along the x-axis (from $-\infty$ to $+\infty$) can be written in the form

$$\psi(x, \vec{x}_\perp, t) = e^{-i\sqrt{E}t} \sum_{n=1}^{n_{max}} a_n \chi_n(\vec{x}_\perp) e^{i\sqrt{E_{||}}x}. \tag{4.1.7}$$

Here $\vec{x}_\perp$ is a vector in the cross-sectional plane; $\chi_n(\vec{x}_\perp)$ are solutions to the equation

$$\Delta\chi_n + E_\perp(n)\chi_n = 0,$$

satisfying the condition $\chi_n = 0$ on the cross-section boundary. The number n_{max} is found from the condition that $E_{||}$ be non-negative.

The summands in (4.1.7) are called modes, and $E_\perp(n)$ is called n-th energy threshold. If the electron energy satisfies $E_\perp(1) < E < E_\perp(2)$, then only one mode (a wave with transversal number $n = 1$) can propagate in the waveguide. The value of $E_\perp(n)$ depends on the shape and the area of the cross-section (it increases as the cross-section area decreases). In the simplest two-dimensional case (a strip of width D), we have $E_\perp(n) = \pi^2 n^2/D^2$ and $\chi_n(y) = \cos(\pi n y/D)$.

Note that an electron with the same total energy can be in distinct trasnversal states. For example, in the waveguide of width $D = 1$, an electron with energy

$E = 300$ can be in the five distinct states:

$$\begin{aligned} n = 1: &\quad E_\perp(1) = 9.87, &\quad E_{||} = 290.13, \\ n = 2: &\quad E_\perp(2) = 39.5, &\quad E_{||} = 260.5, \\ n = 3: &\quad E_\perp(3) = 88.8, &\quad E_{||} = 211.2, \\ n = 4: &\quad E_\perp(4) = 157.9, &\quad E_{||} = 142.1, \\ n = 5: &\quad E_\perp(5) = 246.7, &\quad E_{||} = 53.3. \end{aligned} \tag{4.1.8}$$

An electron with $E = 100$ can have the three distinct states:

$$\begin{aligned} n = 1: &\quad E_\perp(1) = 9.87, &\quad E_{||} = 90.13, \\ n = 2: &\quad E_\perp(2) = 39.5, &\quad E_{||} = 60.5, \\ n = 3: &\quad E_\perp(3) = 88.8, &\quad E_{||} = 11.2, \end{aligned} \tag{4.1.9}$$

The representation $E = E_\perp + E_{||}$ is valid only for the cylindrical waveguides. However, if a waveguide cross-section slowly changes, then (4.1.6) are approximately satisfied (with D changed for $D(x)$). For the quallitative analysis, we assume such relation to be fulfilled.

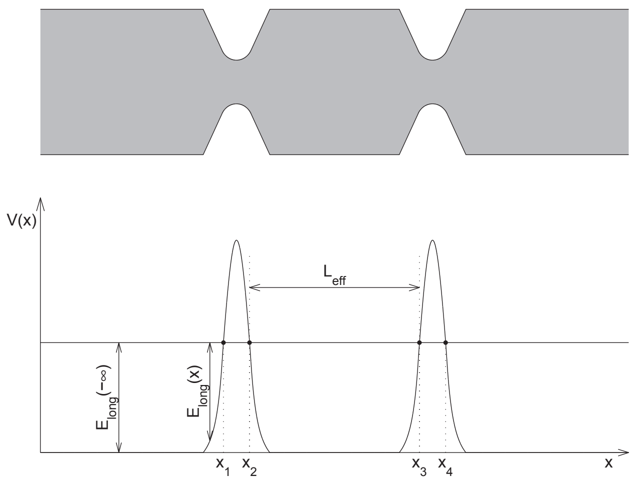


FIGURE 15 The potential corresponding to the 2D waveguide.

Let us consider an electron moving from $-\infty$ to $+\infty$ along a waveguide with $D(-\infty) = 1$. If the waveguide width decreases along the x-axis, then $E_\perp(n, x)$ increases. Since the total energy E remains constant, $E_{||}$ decreases. This can be interpreted as arising a potential barrier depending on x,

$$V_n(x) = \pi^2 n^2 \left(\frac{1}{D^2(x)} - 1 \right). \tag{4.1.10}$$

A point x_1 such that $E_{||}(x_1) = 0$ is called a turning point (Figure 15). The coordinate of such a point is determined by $E = \pi^2 n^2 / D^2(x_1)$. At x_1, an electron with energy E is reflected while the electron wave function exponentially decaying for $x > x_1$ (under the barrier). Let us emphasize that the barrier depends on the transversal quantum number n. At a certain point x_{min} the waveguide width becomes minimal, $D(x_{min}) = D_{min}$. The electrons with total energy

$$E > \pi^2 n^2 / D_{min}^2 = E_{cr,n}$$

go over the barrier. The barrier height (the maximal $V_n(x)$) is equal to

$$V_n = \pi^2 n^2 (D_{min}^{-2} - 1).$$

If E slightly exceeds $E_{cr,n}$ then there is some probability of over-barrier reflection.

The electrons with $E < \pi^2 n^2 / D_{min}^2$ are reflected with probability close to 1. If the resonator becomes wider behind the narrow, then $V_n(x)$ decreases and at a point x_2 (also called a turning point) the electron appears over the barrier; there exists a small probability for tunneling through the potential barrier. The tunneling probability is proportional to

$$\exp\left[-\alpha \int_{x_1}^{x_2} \sqrt{V_n(x) - E_{||}} dx\right].$$

The larger the integral in the expression, the less the width of the resonant peak.

In our calculations we have assumed $D_{min} = 0.3$, so the barrier heights (depending on n) are $V_1 = 99.8$, $V_2 = 399.1$, $V_3 = 898.1$, and $V_4 = 1597$. The critical values of the total electron energy are $E_{cr,1} = 109.7$, $E_{cr,2} = 438.6$, $E_{cr,3} = 987$ and $E_{cr,4} = 1755$.

If there are two narrows in a waveguide, then the domain between the narrows plays the role of a quantum resonator. If an electron went under the barrier corresponding to the first narrow and entered the resonator, it would be reflected at the point x_3 by the barrier created by the second narrow (see Figure 15). If

$$k_{||}(x_4 - x_3) = k_{||} L_{eff} \approx \pi m, \quad m = 1, 2, \ldots \tag{4.1.11}$$

then there arise conditions for strengthening waves moving in the resonator in opposite direction (the so-called constructive interference). In such a process, the probability sharply inreases for the electron to pass through the resonator. If the narrows are identical, the probability turns out to be 1 for certain values of the energy (the resonant energies). The full resonant electron energy satisfies

$$E_{res} = \pi^2 n^2 + \frac{\pi^2 m^2}{L_{eff}^2}. \tag{4.1.12}$$

For the narrows considered in this work, $L_{eff} \approx L$, where L is the resonator length, i.e. the distance between the x_{min}-coordinates of the two barriers.

For electrons with the same full energy having distinct transversal quantum numbers, the resonant conditions can be distinct. For example, for the resoantor with length $L = 1.5$, an electron with energy $E = 49.3$ and transversal quantum number $n = 1$ passes through the resonator with probability close to 1 (this energy is resonant for $n = 1$, $m = 3$). However, an electron with the same full energy and transversal quantum number $n = 2$ has a negligible transition probability (the resonant conditions are not fulfilled). An electron with $E = 43.9$ will pass through the resonator for $n = 2$, $m = 1$ will not pass for $n = 1$.

Due to scattering by an effective potential, when entering the resonator, an electron can change its transversal state (keeping the full energy). For the waveguide with axial symmetry, only such changes are possible that keep the transversal state evenness.

Even in the case that the original electron state is not resonant, for the new state with changed transversal quantum number the resonant condition can be fulfilled. Leaving the resonator, such an electron can recover its original state. As a result, the transition probability sharply increases for formally non-resonant energy values.

The aforementioned resonator systems can serve as a base for building various amplifiers, in particular, transistors. Their operation has been analyzed under the assumption that the electron energy lies between the first and the second thresholds. However, this condition is not always fulfilled. With modern technologies the waveguide diameter cannot apparently be made less than 15–20 periods of crystal lattice, i.e. 5–8 nm, and the operation voltage (and consequently, the energy of electrons in the channel) less than 0.1–0.2 eV. The energy corresponding to the first threshold (in the dimensional units) is $E_1 = \pi^2\hbar^2/2m^*D^2$. Only if the effective mass of the electron is not greater than $0.01m_e$, the mentioned assumption is fulfilled. If the effective mass m^* of an electron in the conductor is close to the free electron mass m_e, the current is affected by electrons with n_{max} up to 4–5. For wider waveguides the number of channels is even greater.

In elastic scattering of the incident wave by the waveguide narrows, transitions between transversal states are possible with particle's total energy being invariant. This process of multichannel scattering can cause significant decrease of tunneling probability at resonance and operation problems in the devices created on the basis of the effect of resonant tunneling.

The frequency characteristics of the quantum resonance devices are determined by the time τ_R during which the electron resides in the resonator. The parameter also determines the Coulomb extrusion of incident electrons by the space charge of electrons in the resonator (Coulomb blockade). To find τ_R we have to consider the process of scattering of wave packet moving in the quantum waveguide towards the resonator.

Even in one-dimensional case the scattering of wave packets on one potential barrier leads to unexpected results [17, 18]. For instance, in the scattering of a spatially narrow wave packet, the appearance of a transmitted packet of small amplitude is possible before the packet fully transits through the barrier (the Hartman paradox, see [19]). This is conditioned by the influence of the wave packet components with large energies for which the probability of tunneling is high.

Naturally, in the two-dimensional case the process of transition of a wave packet through a narrow and, a fortiori, through a quantum resonator has even more complicated character. It is explained by the fact, that the components of the wave packet with large energies can change the transversal part of the energy during the scattering (i.e. switch from one scattering channel to another). Determination of the transition amplitudes with respect to parameters of the resonator (the narrows diameter and shape, the resonator length, etc.) is necessary for calculation of time characteristics of the devices based on resonant tunneling.

4.2 The eigenfunctions of the 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 (Figure 16). Therefore we expose the calculated values of k_{ev}^2 and figures of the corresponding eigenfunctions in Table 1.

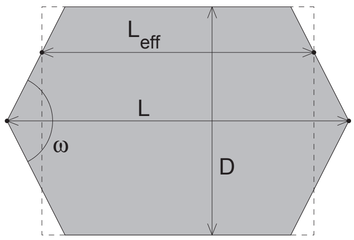


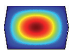
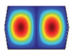
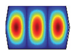
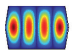
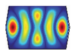
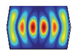
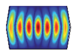
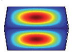
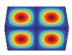
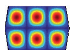
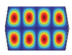
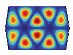
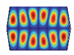
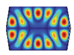
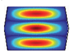
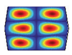
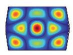
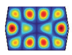
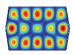
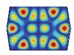
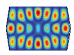
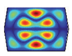
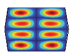
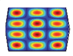
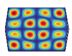
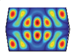
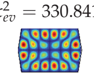
FIGURE 16 The resonator.

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

$$k_{ev}^2 = \pi^2 n^2 + \pi^2 m^2 / L^2, \qquad (4.2.1)$$

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 (4.2.1) with L replaced by L_{eff} (this L_{eff} is slightly less than L_{eff} in the previous section). 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 $n > 1$.

TABLE 1 The closed resonator eigenvalues and eigenfunctions

n \ m	1	2	3	4	5	6	7
1	$k_{ev}^2 = 14.5765$ 	$k_{ev}^2 = 28.6845$ 	$k_{ev}^2 = 52.1479$ 	$k_{ev}^2 = 84.8217$ 	$k_{ev}^2 = 125.6741$ 	$k_{ev}^2 = 180.1483$ 	$k_{ev}^2 = 240.3497$ 
2	$k_{ev}^2 = 44.3978$ 	$k_{ev}^2 = 59.1481$ 	$k_{ev}^2 = 83.7015$ 	$k_{ev}^2 = 117.9935$ 	$k_{ev}^2 = 161.2690$ 	$k_{ev}^2 = 214.9305$ 	$k_{ev}^2 = 273.2698$ 
3	$k_{ev}^2 = 93.7270$ 	$k_{ev}^2 = 108.5681$ 	$k_{ev}^2 = 134.3437$ 	$k_{ev}^2 = 165.5023$ 	$k_{ev}^2 = 209.7926$ 	$k_{ev}^2 = 261.8551$ 	$k_{ev}^2 = 326.4400$ 
4	$k_{ev}^2 = 163.4579$ 	$k_{ev}^2 = 177.5804$ 	$k_{ev}^2 = 202.4174$ 	$k_{ev}^2 = 237.7302$ 	$k_{ev}^2 = 287.1038$ 	$k_{ev}^2 = 330.8411$ 	$k_{ev}^2 > 370$

The disparity between the calculated eigenvalues and approximations by formula (4.2.1) 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).

4.3 The method for computing the scattering matrix

Here we give a description of the scattering matrix calculation method used in the computations (see [7]). We consider only the scattering of waves incident on the resonator from $-\infty$, i.e. we consider solutions of the form

$$u_n(x,y) = U_n^{in}(x,y) + \sum_{j=1}^{2n_{max}} s_{nj} U_j^{out}(x,y) + O(e^{\delta|x|}), \quad |x| \to \infty,$$

where

$$\begin{aligned} U_n^{in}(x,y) &:= \mathbf{1}_{left} e^{i\sqrt{E_{||}(n)}x} \chi_n(y), & n &= 1,2,\dots,n_{max}, \\ U_j^{out}(x,y) &:= \mathbf{1}_{left} e^{-i\sqrt{E_{||}(j)}x} \chi_j(y), & j &= 1,2,\dots,n_{max}, \\ U_j^{out}(x,y) &:= \mathbf{1}_{right} e^{i\sqrt{E_{||}(j-n_{max})}x} \chi_{j-n_{max}}(y), & j &= n_{max}+1, n_{max}+2, \dots, 2n_{max}, \end{aligned}$$

$E_{||}(j) = E - E_{\perp}(j)$ and $\mathbf{1}_{left}$, $\mathbf{1}_{right}$ are the indicators of the left and the right outlets of the waveguide. The matrix $s = \{s_{nj}\}$, $n = 1,2,\dots,n_{max}$, $j = 1,2,\dots,2n_{max}$, is the upper half of the waveguide scattering matrix. Denote the domain occupied by the waveguide by G. Introduce the notations:

$$\begin{aligned} G^R &:= G \cap \{(x,y) : -R < x < L+R\}, \\ \Gamma^R &:= \partial G^R \cap \{(x,y) : |x - L/2| = L/2 + R\}. \end{aligned}$$

Here R is a sufficiently large positive constant (see Figure 17).

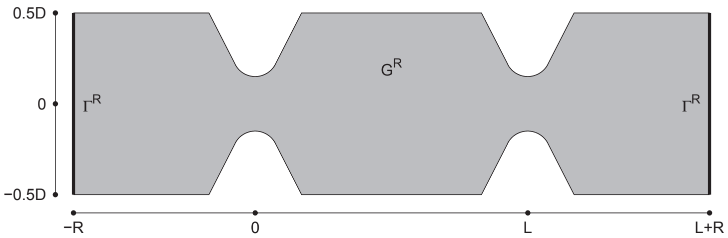


FIGURE 17 The truncated domain G^R.

As an approximation for the n-th row of the scattering matrix we take the minimizer $a_n^0 = (a_{n1}^0, a_{n2}^0, \dots, a_{n,2n_{max}}^0)$ of the functional

$$J_n^R = \|\mathcal{X}_n^R - U_n^{in} - \sum_{j=1}^{2n_{max}} a_{nj} U_j^{out}\|^2_{L_2(\Gamma^R)}.$$

Here $\mathcal{X}_n^R$ is a solution to the problem

$$\begin{aligned} (\Delta + E)\mathcal{X}_n^R &= 0 && \text{in } G^R, \\ \mathcal{X}_n^R &= 0 && \text{on } \partial G^R \setminus \Gamma^R, \\ (\partial_\nu + i\zeta)\mathcal{X}_n^R &= (\partial_\nu + i\zeta)\Big(U_n^{in} + \sum_{j=1}^{2n_{max}} a_{nj} U_j^{out}\Big) && \text{on } \Gamma^R, \end{aligned}$$

where $\zeta \in \mathbb{R} \setminus \{0\}$ is an arbitrary fixed number, ν being the outward normal. From the results of the paper [7] it follows that $a_{nj}^0(R,k) \to s_{nj}(k)$ with exponential rate as $R \to \infty$. More precisely, there exist positive constants Λ and C such that

$$|a_{nj}^0(R,k) - s_{nj}(k)| \leqslant C \exp(-\Lambda R), \quad j = 1, 2, \dots, 2n_{max},$$

for all $k^2 \in [\mu_1, \mu_2]$ and sufficiently large R; the interval $[\mu_1, \mu_2]$ of continuous spectrum of the problem lies between two consequent thresholds and does not contain the thresholds. (Note, that application of the method is not hindered by possible presence on the interval $[\mu_1, \mu_2]$ of eigenvalues of the problem).

We can put $\mathcal{X}_n^R = v_n^{in} + \sum_{j=1}^{2n_{max}} a_{nj} v_j^{out}$, where v_n^{in}, v_n^{out} are solutions to the problems

$$\begin{aligned} (\Delta + E)v_n^{in} &= 0 && \text{in } G^R, \\ v_n^{in} &= 0 && \text{on } \partial G^R \setminus \Gamma^R, \\ (\partial_\nu + i\zeta)v_n^{in} &= (\partial_\nu + i\zeta)U_n^{in} && \text{on } \Gamma^R \end{aligned}$$

and

$$\begin{aligned} (\Delta + E)v_j^{out} &= 0 && \text{in } G^R, \\ v_j^{out} &= 0 && \text{on } \partial G^R \setminus \Gamma^R, \\ (\partial_\nu + i\zeta)v_j^{out} &= (\partial_\nu + i\zeta)U_j^{out} && \text{on } \Gamma^R, \qquad j = 1, 2, \dots, 2n_{max}. \end{aligned}$$

Now we can rewrite the functional J_n^R in the form

$$J_n^R = \langle a_n \mathcal{E}^R, a_n \rangle + 2\mathrm{Re}\, \langle \mathcal{F}_n^R, a_n \rangle + \mathcal{G}_n^R,$$

where $\langle \cdot, \cdot \rangle$ is the inner product on $\mathbb{C}^{2n_{max}}$, by $\mathcal{E}^R$ we denote the matrix with entries

$$\mathcal{E}_{pq}^R = \Big(v_p^{out} - U_p^{out}, v_q^{out} - U_q^{out}\Big)_{L_2(\Gamma^R)}, \quad p, q = 1, 2, \dots, 2n_{max},$$

the row $\mathcal{F}_n^R$ consists of the elements

$$\mathcal{F}_{nq}^R = \Big(v_n^{in} - U_n^{in}, v_q^{out} - U_q^{out}\Big)_{L_2(\Gamma^R)}, \quad q = 1, 2, \dots, 2n_{max},$$

and the number $\mathcal{G}_n^R$ is defined by

$$\mathcal{G}_n^R = \left\| v_n^{in} - U_n^{in} \right\|_{L_2(\Gamma^R)}^2.$$

The minimizer of J_n^R satisfies $a_n \mathcal{E}^R + \mathcal{F}_n^R = 0$. We take the solution of this equation for an approximation to n-th row of the scattering matrix.

4.4 Discussion

A transversal quantum number is an adiabatic invariant. Therefore, for smooth variations of the waveguide cross-section, the change of a transversal quantum number will be unlikely. However, with sharp variation of the cross-section diameter (at distances comparable to the electron wavelength) the probability of a change of transversal state becomes high.

If the resonator is symmetric about x-axis, then only scattering with preserved evenness is possible (the incident and scattered waves have the same evenness). It is explained by the fact, that the matrix element $\langle \psi_{in}|V|\psi_{out}\rangle$ of transition between channels vanishes for wave functions of different evenness because of the symmetry of the potential V providing the transition. Let us explain the fact in more detail. The original problem reads

$$\begin{aligned} \Delta u_n + k^2 u_n &= 0 \quad \text{in} \quad G, \\ u_n &= 0 \quad \text{on} \quad \partial G, \end{aligned} \tag{4.4.1}$$

$$u_n = U_n^{in} + \sum_{j=1}^{2n_{max}} s_{nj} U_j^{out} + O(e^{-\delta|x|}) \quad \text{as} \quad |x| \to \infty.$$

Let $v_n(x,y) = u_n(x,-y)$ and $n \leq n_{max}$ (we consider only the upper half of the scattering matrix). The function v_n satisfies

$$\begin{aligned} \Delta v_n + k^2 v_n &= 0 \quad \text{in} \quad G, \\ v_n &= 0 \quad \text{on} \quad \partial G, \end{aligned} \tag{4.4.2}$$

and

$$v_n = (-1)^{n+1} U_n^{in} + \sum_{j=1}^{n_{max}} s_{nj} (-1)^{j+1} U_j^{out} + \sum_{j=n_{max}+1}^{2n_{max}} s_{nj} (-1)^{j-n_{max}+1} U_j^{out} + O(e^{-\delta|x|})$$

as $|x| \to \infty$. Let n be even. Then $w_n = (u_n + v_n)/2$ satisfies

$$\begin{aligned} \Delta w_n + k^2 w_n &= 0 \quad \text{in} \quad G, \\ w_n &= 0 \quad \text{on} \quad \partial G, \end{aligned} \tag{4.4.3}$$

and

$$w_n = \sum_{j=1}^{n_{max}} s_{nj} U_j^{out} + \sum_{j=n_{max}+1}^{2n_{max}} s_{nj} U_j^{out} + O(e^{-\delta|x|}) \quad \text{as} \quad |x| \to \infty,$$

where the sums do not contain the terms with even j and $j - n_{max}$, respectively. The solution of the problem is $w_n = 0$ and, consequently, s_{nj} with odd j (for $j \leq n_{max}$) and $j - n_{max}$ (for $j > n_{max}$) are zero.

If n is odd, then we consider $w_n = (u_n - v_n)/2$ and conclude that s_{nj} with even j (for $j \leq n_{max}$) and $j - n_{max}$ (for $j > n_{max}$) are zero.

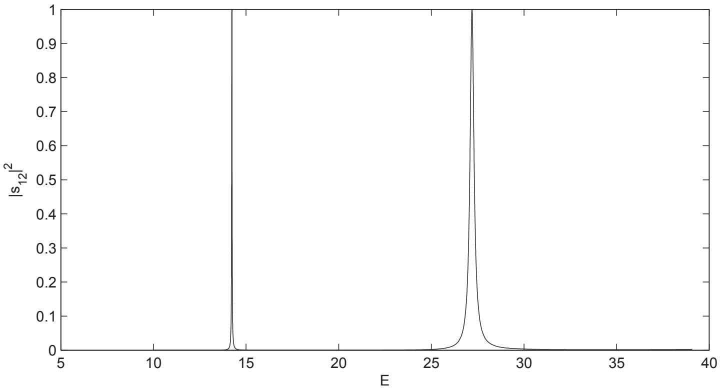


FIGURE 18 Transition probability for the wave U_1^{in} ($n_{max} = 1$, the transversal quantum number $n = 1$ for the scattered wave).

For example, if the electron energy is between the second and the third thresholds ($4\pi^2 < E < 9\pi^2$), we have $s_{12} = s_{14} = 0$. It means that there are no transitions between the transversal states.

The energies $E \approx 14.58$ and $E \approx 28.68$ are resonant and correspond to $n = 1$ and $m = 1, 2$ (Figure 18). For $4\pi^2 < E < 9\pi^2$ (the electron energy between the second and the third thresholds) there are no changes of the transversal states due to the evenness invariance. For the incident wave with $n = 1$, the resonant tunneling occurs at $E \approx 48$ and $E \approx 76$ (Figure 19), which correspond to the closed resonator eigenvalues $E \approx 52.15$ and $E \approx 84.8$ with $n = 1$, $m = 3, 4$. The shift of the resonant energies to the left is caused by small increase of the distance between the turning points in the open resonator.

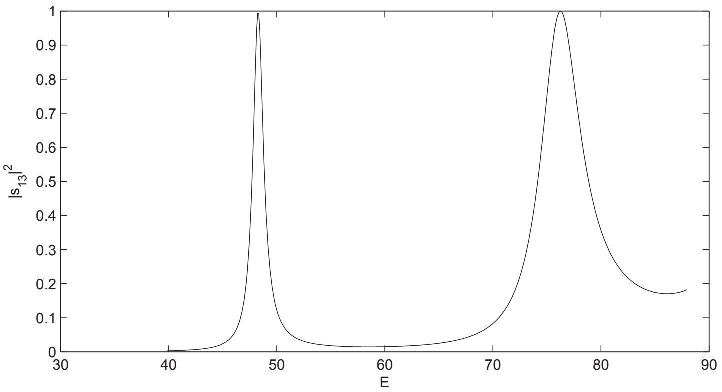


FIGURE 19 Transition probability for the wave U_1^{in} ($n_{max} = 2$, the transversal quantum number $n = 1$ for the scattered wave).

For incident wave U_2^{in}, resonant tunneling occurs at energies $E \approx 44.4, 59.1$, and 83.7 (Figure 20), which correspond to $n = 2$, $m = 1, 2, 3$. The width of the resonant peaks for this case is significantly less than that for the wave U_1^{in}.

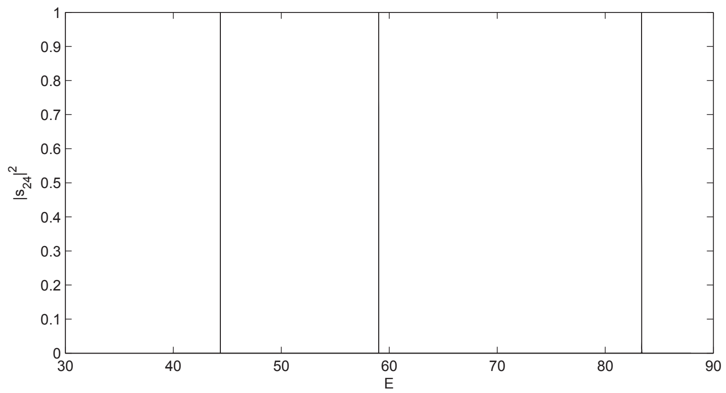


FIGURE 20 Transition probability for the wave U_2^{in} ($n_{max} = 2$, the transversal quantum number $n = 2$ for the scattered wave).

The explanation is that the height of the potential barrier is much greater for the wave U_2^{in}. This also explains the smaller distance between the resonant peaks and the corresponding eigenvalues of the closed resonator.

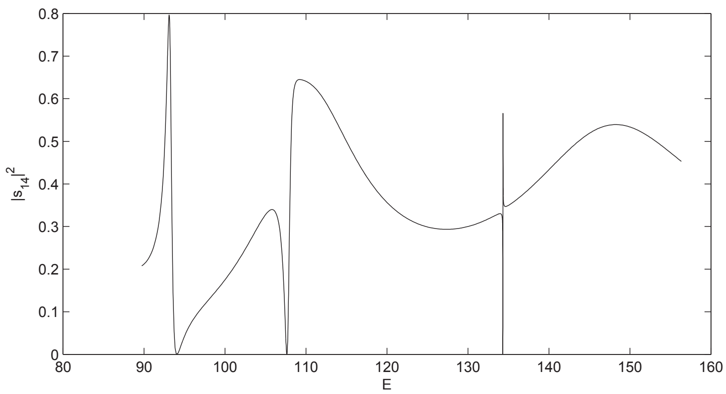


FIGURE 21 Transition probability for the wave U_1^{in} ($n_{max} = 3$, the transversal quantum number $n = 1$ for the scattered wave).

For a waveguide symmetric about x-axis, transition between channels becomes possible only when $9\pi^2 < E < 16\pi^2$, i.e. when the electron energy is between the third and the fourth thresholds. Since for the wave U_1^{in} the longitudinal energy $E_{||}$ is large (it is above the barrier height for $E > E_{cr,1} = 109,7$), the probability of electron transition without change of a transversal quantum number is fairly high (Figure 21). The probability of electron transition with a change of transversal state $(n = 1) \to (n = 3)$ is high as well (Figure 22). Both $|s_{14}|^2$ and $|s_{16}|^2$ have sharp resonance at $E \approx 93$, which corresponds to the eigenenergy of the closed resonator with $n = 3$, $m = 1$. For $|s_{16}|^2$ the peak is natural, since for the longitudinal component the conditions of resonance hold. But for $|s_{14}|^2$ the resonance is caused by transition $(n = 1) \to (n = 3)$ at the entrance into the

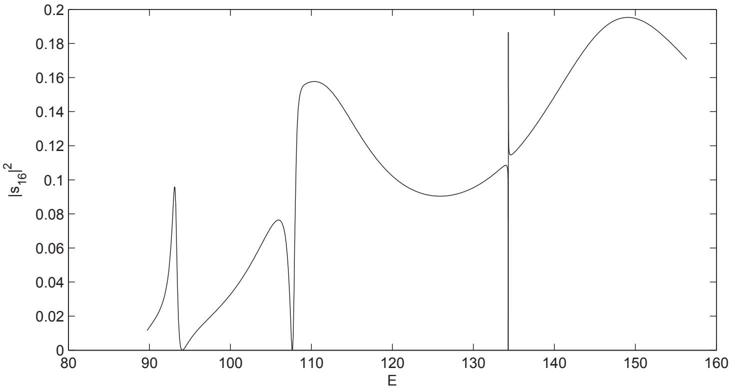


FIGURE 22 Transition probability for the wave U_1^{in} ($n_{max} = 3$, the transversal quantum number $n = 3$ for the scattered wave).

resonator, resonant magnification of the wave amplitude, and subsequent transition to the initial state $(n = 3) \to (n = 1)$. Similarly behaves the wave U_3^{in}, with strong direct $(n = 3) \to (n = 1)$ and reverse $(n = 1) \to (n = 3)$ transitions with a change of the transversal quantum number and the resonance at $E \approx 93$.

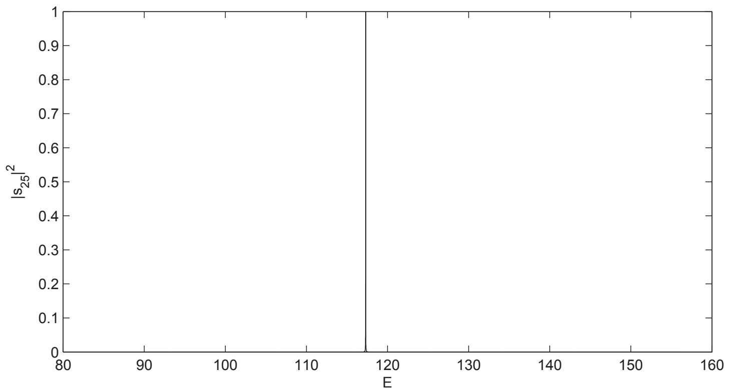


FIGURE 23 Transition probability for the wave U_2^{in} ($n_{max} = 3$, the transversal quantum number $n = 2$ for the scattered wave).

For incident electrons with $n = 2$ no change of transversal state is possible and there is a sharp resonance of unit height at $E \approx 117$ (Figure 23). For an incident electron with energy $16\pi^2 < E < 25\pi^2$ the situation is even more complicated, since transitions with change of transversal quantum number become possible for $n = 2$, too. We do not analyze the obtained results here, because qualitatively the effects are similar to those for $9\pi^2 < E < 16\pi^2$.

The wave U_3^{in} with energy greater than $E_{cr,1}$ approaches the narrows and partially goes in the state with $n = 1$, so the probability to pass through the resonator is large even for non-resonant energies (due to passing over the barrier), see Figure 26. The crititcal energy $E_{cr,3}$ for the original mode is greater than

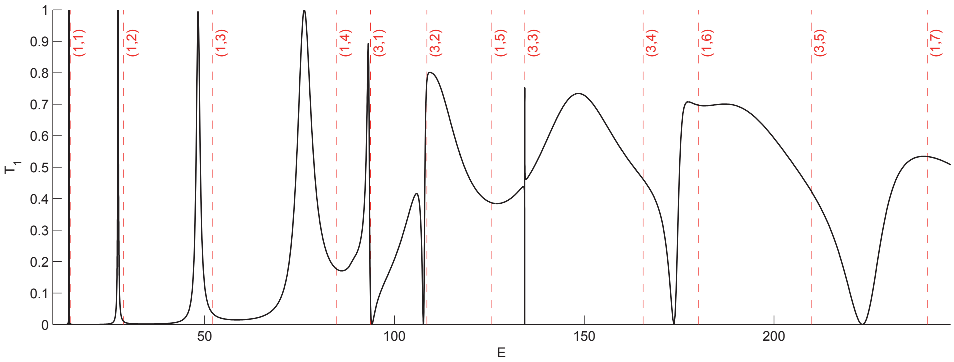


FIGURE 24 Total transition probability for U_1^{in}.

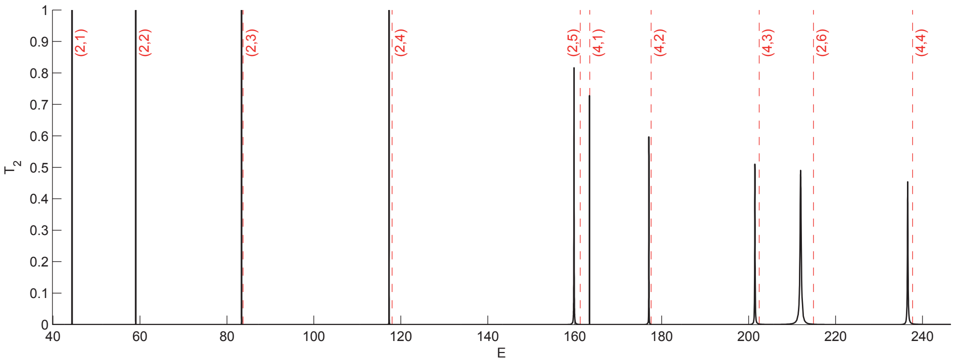


FIGURE 25 Total transition probability for U_2^{in}.

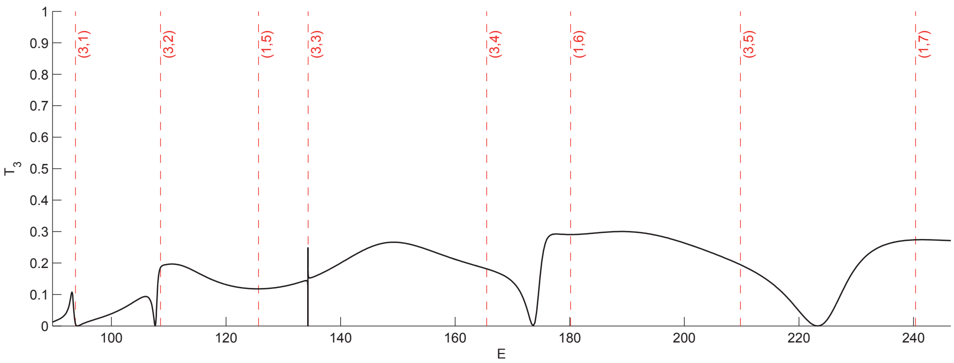


FIGURE 26 Total transition probability for U_3^{in}.

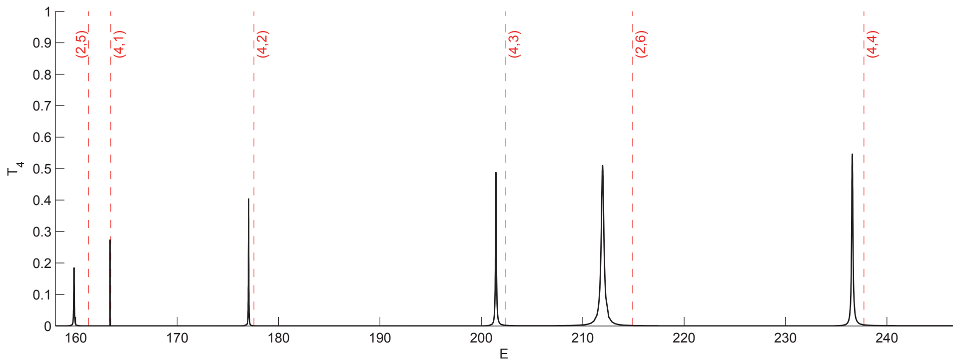


FIGURE 27 Total transition probability for U_4^{in}.

the electron energy and the transition probability without changing the state has peaks at the energies which are resonant for the state with $n = 3$. The sharp oscilations at energies close to the eigenvalues of the resonator for $n = 3$ (see Figure 26) is apparently the manifestation of the interference of the modes with $n = 1$ and $n = 3$ at the exit of the resonator. An electron with $n = 1$ whose energy exceeds the third threshold partially goes in the state with $n = 3$, having resonances at the same energies as an electron in the state with $n = 3$.

Figures 24–27 show the graphs of T_1–T_4 as functions in E; here T_n stands for total transition probability of U_n^{in}. The numbers (n, m) are the transversal and longitudinal quantum numbers of the respective eigenvalues of the closed resonator. Similarly to U_3^{in}, the wave U_4^{in} partially changes its transversal state (goes in the state with $n = 2$) and has resonances corresponding to the states $n = 4$ and $n = 2$. However, the forth threshold is less than $E_{cr,2}$ and, a fortiori, than $E_{cr,4}$ (the barriers are very high), so the free path through the resonator is impossible for $n = 2$ and $n = 4$. Therefore, the peaks in Figures 25, 27 are very narrow regardless the interference of the modes with $n = 2$ and $n = 4$ (causing the slight asymmetry of the peaks).

The peaks in Figure 27 corresponding to the resonant energies for $n = 2$ ($E \approx 160$ and $E \approx 212$) are wider than the nearest peaks with $n = 4$ because the barrier height for the state with $n = 2$ is notably lower than $n = 4$.

Evidently, the sharp resonances with transition probability T close to unit exist only below the third threshold. Therefore, in designing electronic devices based on the resonant tunneling in quantum waveguides of variable cross-section, the parameters of the system (the cross-section area, the waveguide material, the operation voltage) should be chosen so that the energy of an electron in the system would not exceed the third threshold.

YHTEENVETO (FINNISH SUMMARY)

Väitöskirjassa tutkitaan elektronisirontaa kvanttiaaltojohtimissa, joiden poikkileikkaus ei pysy vakiona.

Elektronit liikkuvat äärettömän pituisessa kaksiulotteisessa aaltojohtimessa. Johtimessa on kaksi kapeikkoa, jotka toimivat kuten potentiaalivallit. Kapeikkojen välisestä aaltojohtimen osasta muodostuu resonaattori, jolloin sillä alueella tapahtuu elektronin tunneloitumista. Ilmiön ominaisuuksia voidaan muuttaa lisäämällä resonaattoriin magneettikenttä. Tällöin elektronivirta voidaan polarisoida siten, että sen elektroneilla on samansuuntainen spin.

Kapeikkojen läpimitta määritetään parametriksi, minkä avulla johdetaan asymptoottiset kaavat tunneloitumisen ominaisuuksille. Kaavojen sisältämät tuntemattomat vakiot määrätään ratkaisemalla useita reuna-arvotehtäviä rajoittamattomissa alueissa. Vastaavasti sirontamatriisi lasketaan numeerisesti, minkä jälkeen asymptoottisia ja numeerisia tuloksia verrataan toisiinsa.

Resonaattorin toiminnan analysoinnissa oletetaan, että elektronien energia on ensimmäisen ja toisen kynnysarvon välillä. Tätä ehtoa ei välttämättä pystytä aina täyttämään tämän päivän teknologialla. Väitöskirjassa analysoidaan monikanavasironnan ominaisuuksia myös tilanteessa, jossa elektronien energia ylittää toisen kynnysarvon.

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APPENDIX 1 THE SPECTRAL PROBLEM IN G_2

Let us rewrite the problem in the weak form

$$(\nabla v, \nabla u) - 2i(\mathbf{A}\nabla v, u) + (|A|^2 v, u) \pm (Hv, u) - k^2(v, u) = 0, \qquad \text{(A1.1)}$$

where $u \in \mathrm{H}_0^1(G_2) := \{v : v \in \mathrm{H}^1(G_2),\ v = 0 \text{ on } \partial G_2\}$ and the inner products mean those in $L_2(G_2)$.

Let P_N be N-dimensional space of piecewise polynomial functions equal to 0 on ∂G_2, and let $\{\eta_p\}_{p=1}^N$ be a basis in P_N. The space P_N is defined by dividing the geometry into small elements and choosing the basis functions η_p. In the calculations we used triangular mesh (for triangulation the 'advancing front' method is used) and second order Lagrange elements.

We replace both the sought-for function v and the test function u by functions $\mathcal{V}, \mathcal{U} \in P_N$. Then using the representation

$$\mathcal{V} = \sum_{p=1}^{N} \mathcal{V}_p \eta_p$$

and writing the equation (A1.1) for $\mathcal{U} = \eta_q$, $q = 1, 2, \ldots, N$, we get the generalized eigenvalue problem

$$\mathcal{A}\vec{\mathcal{V}} = k^2 \mathcal{B}\vec{\mathcal{V}}, \qquad \text{(A1.2)}$$

where $\mathcal{A}$ and $\mathcal{B}$ are matrices with entries

$$\begin{aligned} \mathcal{A}_{pq} &= (\nabla\eta_p, \nabla\eta_q) - 2i(\mathbf{A}\nabla\eta_p, \eta_q) + (|A|^2\eta_p, \eta_q) \pm (H\eta_p, \eta_q), \\ \mathcal{B}_{pq} &= (\eta_p, \eta_q), \end{aligned}$$

and $\vec{\mathcal{V}} = (\mathcal{V}_1, \mathcal{V}_2, \ldots, \mathcal{V}_N)$. The eigenvalue problem (A1.2) is solved by the Arnoldi method (see, e.g. [20]). This description includes the case of a resonator without magnetic field (Chapter 2), which is specified by setting $H = 0$. The calculations have been carried out in the environments MATLAB and COMSOL, where one can also find elementary introductions to the used methods and techniques.

APPENDIX 2 THE PROBLEMS IN $G(\varepsilon)$, G_1, Ω

Consider the problem

$$\begin{aligned}(-i\nabla + \mathbf{A})^2 v \pm Hv &= k^2 v \quad \text{in} \quad X,\\ v &= 0 \qquad \text{on} \quad Y_1,\\ (\partial_n + i\zeta)v &= f \qquad \text{on} \quad Y_2,\end{aligned} \tag{A2.1}$$

where $Y_1 + Y_2 = \partial X$. Let us rewrite the problem in the integral form

$$(\nabla v, \nabla u)_X - 2i(\mathbf{A}\nabla v, u)_X + (|A|^2 v, u)_X \pm (Hv, u)_X - k^2(v,u)_X + i\zeta(v,u)_{Y_2} = (f,u)_{Y_2}, \tag{A2.2}$$

where $u \in \mathrm{H}^1_0(X) := \{v: \ v \in \mathrm{H}^1(X), \ v = 0 \text{ on } Y_1\}$ and the inner products mean that in L_2.

As in Appendix 1, we choose a sequence of spaces $P_N \subset \mathrm{H}^1_0(X)$ of piecewise polynomial functions and replace v and u by $\mathcal{V}, \mathcal{U} \in P_N$. Then we expand $\mathcal{V}$ in the basis $\{\eta_p\}$:

$$\mathcal{V} = \sum_{p=1}^{N} \mathcal{V}_p \eta_p$$

and writing the equation (A1.1) for $\mathcal{U} = \eta_q$, $q = 1, 2, \ldots, N$, we get the equation

$$\mathcal{A}\vec{\mathcal{V}} = \mathcal{B}, \tag{A2.3}$$

where $\mathcal{A}$ is a matrix and $\mathcal{B}$ is a column with elements

$$\begin{aligned}\mathcal{A}_{pq} =& (\nabla\eta_p, \nabla\eta_q)_X - 2i(\mathbf{A}\nabla\eta_p, \eta_q)_X\\ &+ (|A|^2\eta_p, \eta_q)_X \pm (H\eta_p, \eta_q)_X - k^2(\eta_p,\eta_q)_X + i\zeta(\eta_p,\eta_q)_{Y_2},\\ \mathcal{B}_q =& (f, \eta_q)_{Y_2},\end{aligned}$$

and $\vec{\mathcal{V}} = (\mathcal{V}_1, \mathcal{V}_2, \ldots, \mathcal{V}_N)$. The system (A2.3) is solved by incomplete LU-factorization (LU-factorization for sparse SLAE). The environments MATLAB and COMSOL have been used in the computations.

This description includes several cases. To solve the problems for scattering matrix in the presence of magnetic field (Chapter 3), we set

$$X = G(\varepsilon), \ Y_2 = \Gamma_1^D \cup \Gamma_2^D.$$

Additional setting $H = 0$ corresponds to the problem without magnetic field. The problems for multichannel scattering matrix (Chapter 4) correspond to $X = G^R, \ Y_2 = \Gamma^R$. Assuming $X = G_1^D, \ Y_2 = \Gamma^D$, we get the problem in G_1 in Chapters 2 and 3. Finally, the problem in Ω in Chapters 2 and 3 are solved by setting $X = \Omega^D, \ Y_2 = \Gamma^D$.

We use 'advancing front' method for triangulation and second order Lagrange elements as basis functions. We do not carry out any analysis of theoretical aspects of FEM, like convergence, accuracy, etc. For the issues we refer to the wide literature devoted to the theory of FEM, e.g. see [21, 22, 23].