Chapter 2
Transport in Locally Perturbed Tubes

Our next aim is to discuss the systems of the previous chapter from the viewpoint of particle transport. For simplicity we are going to pay most attention to the two-dimensional case where Ω is a Dirichlet strip in the plane. The perturbations of the ideal straight waveguide which we shall consider here are again of a local nature; this allows us to work in the scattering-theory setting where the time evolution is compared to an appropriate free asymptotic dynamics.

2.1 Existence and Completeness

The natural comparison operator is that of a straight tube, $H_0 = -\Delta_D^{\Omega_0}$. In the usual scattering theory for Schrödinger operators we most often compare pairs of operators acting on the same Hilbert space. For waveguides this happens, e.g., if the perturbation is a potential or a measure in the kinetic term which we have discussed in Sect. 1.4. In that case the existence and asymptotic completeness of the ***wave operators*** defined as usual by

$$\Omega_{\pm}(H, H_0) := \operatorname*{s-lim}_{t\to\pm\infty} \mathrm{e}^{iHt}\mathrm{e}^{-iH_0t} P_{\mathrm{ac}}(H_0)$$

is easily established (Problems 3 and 4). This is not the case for perturbations of a geometric nature, however, such a comparison is still possible if we can replace the Hamiltonian by a unitarily equivalent operator on $L^2(\Omega_0)$.

A prime example of this is given by smoothly bent planar strips where we can use the straightening transformation and pass from $-\Delta_D^{\Omega}$ to the operator H given by formula (1.7). The scattering problem is then well defined under suitable regularity and asymptotic straightness requirements on the strip Ω.

Theorem 2.1 *Let assumptions (i), (ii)$_2$, and (iii)$_2$ of Sect. 1.1 be valid and* $a\|\gamma\|_\infty < 1$. *Furthermore, suppose that the functions* $\gamma, \dot\gamma^2, \ddot\gamma$ *are* $\mathcal{O}(|s|^{-1-\delta})$ *for*

P. Exner and H. Kovařík, *Quantum Waveguides*,
Theoretical and Mathematical Physics, DOI 10.1007/978-3-319-18576-7_2

some $\delta > 0$ as $|s| \to \infty$. Then the wave operators $\Omega_\pm(H, H_0)$ exist, are complete, and the singularly continuous spectrum of H is empty.

Proof Using the notation of Sect. 1.6 we can write the difference of the two operators as $-\partial_s(b-1)\partial_s + V = B^*A$, where the operator $A : L^2(\Omega_0) \to L^2(\Omega_0) \otimes \mathbb{C}^2$ acts as $\binom{A_0}{-iA_1\partial_s}$ with $A_0 := |V|^{1/2}$, $A_1 := |b-1|^{1/2}$, and B is the analogous operator with the coefficients replaced by $V^{1/2} := |V|^{1/2}\mathrm{sgn}\, V$ and $(b-1)^{1/2}$, respectively. This factorization allows us to employ the smooth-perturbation method similarly as it is done in the case of one-dimensional Schrödinger operators (see the notes).

Putting $\varrho(s) := (1+s^2)^{-(1+\varepsilon)/4}$ for a fixed $\varepsilon \in (0, \delta]$, we infer from the curvature decay assumptions that $\max\{\|A_l\varrho^{-1}\|_\infty, \|B_l\varrho^{-1}\|_\infty\} < \infty$ holds for $l = 0, 1$. The free resolvent $R_0(z) := (H_0-z)^{-1}$ then satisfies the estimate

$$\|A_l(-i\partial_s)^l R_0(z)\| \le \|A_l\varrho^{-1}\|_\infty \sup_j \left\| \varrho(s)(-i\partial_s)^l(-\partial_s^2 + \nu_j - z)^{-1} \right\|$$

for $l = 0, 1$, where $\nu_j = \kappa_1^2 j^2$ are the transverse eigenvalues, and the analogous inequalities hold with B_l. The last factor can be estimated by the product of L^2 norms of the functions g and $p \mapsto p^l(p^2 + \nu_j - z)^{-1}$, cf. Theorem 11.20 of [RS]. Using the first resolvent identity we conclude that the operator-norm limit of $I - A[BR_0(\lambda \pm i\eta)]^*$ as $\eta \to 0$ exists away from the thresholds, i.e. for any $\lambda \ne \nu_j$. In a similar way we derive the inequality

$$\|AR_0(\lambda \pm i\eta)\|^2 + \|BR_0(\lambda \pm i\eta)\|^2 \le c\eta^{-1}$$

with some $c > 0$ for λ in any compact interval I which does not contain any of the points ν_j (Problem 1). Moreover, since $A_l, B_l \in L^2$ by assumption, one can check that the operator $AR_0(z)[BR_0(z')]^*$ is trace class as a product of two Hilbert-Schmidt operators, and thus compact for any non-real z, z'. The rest of the argument proceeds as in the potential scattering case, cf. Theorem 10.5.1 of [Sch], since only a finite number of transverse modes is involved in expressions containing the spectral projection $E_{H_0}(I)$. We arrive thus at the condition

$$\int_{\mathbb{R}} \sup_{-a<u<a} \left\{ |V(s,u)|^2 + |b(s,u)-1|^2 \right\} \varrho(s)^\alpha < \infty\,,$$

which is satisfied for any $\alpha > 0$ in view of the decay assumptions we made. ∎

Remark 2.1.1 In a similar way one can prove asymptotic completeness for scattering in a three-dimensional smoothly bent tube (Problem 2), as well as for tubes perturbed by a potential or a kinetic-term weight (Problems 3 and 4).

An alternative way to prove, under slightly modified assumptions, that a bent and asymptotically straight tube has no singularly continuous spectrum is to employ ***Mourre's method*** of positive commutator. Let us sketch its main ideas briefly with our purpose in mind; for more information we refer to the literature indicated in the notes. The method is based on a suitable choice of a ***conjugate operator***: one looks for an operator A, self-adjoint on $L^2(\Omega_0)$, such that for a given interval $I \subset \sigma(H)$ there is an operator K, compact in $L^2(\Omega_0)$, and a positive constant c such that

$$E_H(I)\,[H,\, iA]\,E_H(I) \,\geq\, c\,E_H(I) + K\,, \tag{2.1}$$

where $E_H(I)$ denotes the spectral projection of H onto the interval I and the commutator $[iA,\, H]$ is understood as a bounded operator from $H_0^1(\Omega_0)$ to its dual $(H_0^1(\Omega_0))^*$. Inequality (2.1) is referred to as ***Mourre's estimate***; if it holds with $K = 0$ we say it is strictly valid. This estimate has, under certain conditions, consequences for the structure of the spectrum of H in the interval I. These conditions can be expressed in terms of the regularity of the map

$$\mathbb{R} \ni t \mapsto \mathrm{e}^{itA}(H-i)^{-1}\mathrm{e}^{-itA} \tag{2.2}$$

from $\mathbb{R}$ to $\mathcal{B}(L^2(\Omega_0))$. We say that $H \in C^1(A)$ if the above map is of class C^1 in the strong operator topology; if, moreover, the derivative of (2.2) is Hölder continuous of order $\alpha > 0$, we write $H \in C^{1+\alpha}(A)$. Using these notions one is able to state the following result:

Theorem 2.2 *Suppose that* e^{itA} *leaves the form domain of* H *invariant and that* $H \in C^{1+\alpha}(A)$ *for some* $\alpha > 0$. *If (2.1) holds true on an interval* $I \subset \sigma(H)$, *then the singularly continuous spectrum of* H *on* I *is empty and the interval* I *contains at most finitely many eigenvalues of* H, *each of them being of a finite multiplicity. If, in addition, (2.1) holds with* $K = 0$, *then the spectrum of* H *on* I *is purely absolutely continuous.*

To apply *Theorem* 2.2 to our problem, consider an open interval separated from the transverse thresholds, $I \subset \sigma(H) \setminus T$ with $T = \{\nu_j\}_{j\in\mathbb{N}}$, and choose

$$A = -\frac{i}{2}(s\,\partial_s + \partial_s s)$$

defined initially, say, on $C_0^\infty(\Omega_0)$ and extended to a closed operator on $L^2(\Omega_0)$. It is not difficult to check that

$$(\mathrm{e}^{itA}f)(u,s) = \mathrm{e}^{t/2}f(u,\mathrm{e}^t s) \quad \text{for} \;\; t \in \mathbb{R} \;\; \text{and} \;\; f \in L^2(\Omega_0)\,,$$

i.e. that A generates the group of dilations in the longitudinal variable. This implies, in particular, that e^{itA} leaves $H_0^1(\Omega_0)$ invariant. Moreover, a direct computation shows that

$$[H, iA] = -2\partial_s(1+u\gamma(s))^{-2}\,\partial_s - 2\partial_s\, s\,\frac{\dot\gamma(s)}{(1+u\gamma(s))^3}\,\partial_s - s\,\partial_s V(u,s), \tag{2.3}$$

where $V(u,s)$ is the effective potential (1.8). Under suitable decay assumptions on the curvature one can check that the difference $(H-i)^{-1}-(H_0-i)^{-1}$ is compact on $L^2(\Omega_0)$ which yields the inequality

$$E_H(I)\,[H,iA]\,E_H(I) = -2\partial_s^2\,E_H(I)+K \tag{2.4}$$

with a compact K. In view of our assumption about I, it is not difficult to see that the operator $-\partial_s^2\,E_H(I)$ is strictly positive, hence if one can show that $H\in C^{1+\alpha}(A)$ holds for some $\alpha>0$, *Theorem* 2.2 could be applied. It turns out that the needed regularity of the map (2.2) can be demonstrated under appropriate decay assumptions on the curvature γ and its derivatives.

Theorem 2.3 *Let assumptions (i), (ii)$_3$ of Sect. 1.1 hold. Furthermore, suppose that $\gamma(s),\ddot\gamma(s)\to 0$ holds as $|s|\to\infty$ and that $\dot\gamma(s),\dddot\gamma(s)$ are $\mathcal{O}(|s|^{-1-\delta})$ for some $\delta>0$ as $|s|\to\infty$. Then (a) $\sigma_{\mathrm{ess}}(H)=[\nu_1,\infty)$, (b) $\sigma_{\mathrm{sc}}(H)=\emptyset$, (c) $\sigma_{\mathrm{p}}(H)\cup T$ is countable and closed, and (d) $\sigma_{\mathrm{p}}(H)\setminus T$ consists at most of eigenvalues of finite multiplicity which can accumulate only at points of T.*

2.2 The On-Shell S-Matrix: An Example

Full information about scattering requires, of course, more than just checking that the problem is well posed. The central question is to find the ***on-shell scattering operator*** $S(k)$ which describes scattering at a given energy k^2. In general it is not unusual that the space on which $S(k)$ acts depends on energy. In case of waveguide scattering this dependence has a characteristic form: the on-shell space dimension is

$$\sum_{j=1}^{n_a} N_j(k)\,, \tag{2.5}$$

where n_a is the number of tubes leaving the scattering region, for example $n_a=2$ if Ω is a single locally deformed strip, and $N_j(k)$ is the number of propagating modes in the j-th outgoing tube which obviously coincides with the number of transverse eigenvalues satisfying the inequality $\nu_n^{(j)}\le k^2$, thus $N_j(k)=[k\kappa_{1,j}^{-1}]$ holds if the outgoing channel is an asymptotically straight Dirichlet strip.

Since we consider situations where n_a is finite, the operator $S(k)$ can be regarded as a matrix of the dimension given by (2.5) the elements of which are the reflection and transmission amplitudes understood in the general sense, i.e. taking into account that the particle may leave the scattering region in a state whose transverse component differs from the one with which it entered.

Finding these amplitudes is a difficult task. A class of systems for which it can be accomplished numerically is represented by those Ω which decompose into a union of regions where the corresponding Schrödinger equation can be solved by separation of variables; the global scattering solution is then constructed using mode matching similar to that used in Sects. 1.2 and 1.5. We shall illustrate this method on the example of a pair of window-coupled waveguides having generally different widths d_1, d_2 which we have introduced in Sect. 1.5.1.

For definiteness let us suppose that the incident wave is in the upper channel, being of the form $\chi_j^{(+)}(y)\,\exp(-ik_j^{(+)}x)$, where $k_j^{(\pm)} := \kappa_1\sqrt{k^2 - j^2\varrho^{-(1\mp1)}}$ are used as symbols for channel momenta. We denote by $r_{jj'}^{(\pm)}$, $t_{jj'}^{(\pm)}$, respectively, the corresponding reflection and transmission amplitudes to the j'-th transverse mode in the upper and lower guide. Due to the mirror symmetry with respect to the line $x = 0$, we can again consider separately the two parities, writing

$$r_{jj'}^{(\pm)} = \frac{1}{2}\left(\rho_{jj'}^{(s,\pm)} + \rho_{jj'}^{(a,\pm)}\right), \quad t_{jj'}^{(\pm)} = \frac{1}{2}\left(\rho_{jj'}^{(s,\pm)} - \rho_{jj'}^{(a,\pm)}\right), \tag{2.6}$$

where $\rho_{jj'}^{(\sigma,\pm)}$, $\sigma = s, a$, are the appropriate reflection amplitudes. In the even case, which corresponds to the Neumann condition at $x = 0$, we seek solutions using for $0 < x \le a$ and $x \ge a,\ y \in \mathcal{C}_+$, respectively, the following Ansatz,

$$\psi(x,y) := \begin{cases} \sum_{\ell=1}^{\infty} a_\ell \frac{\cos(ip_\ell x)}{\cos(ip_\ell a)}\,\eta_\ell(y) \\ \sum_{j'=1}^{\infty}\left(\delta_{jj'}\,\mathrm{e}^{-ik_j^{(+)}(x-a)} + \rho_{jj'}^{(+)}\mathrm{e}^{ik_{j'}^{(+)}(x-a)}\right)\chi_{j'}^{(+)}(y) \\ \sum_{j'=1}^{\infty} \rho_{jj'}^{(-)}\mathrm{e}^{ik_{j'}^{(-)}(x-a)}\ \chi_{j'}^{(-)}(y) \end{cases} \tag{2.7}$$

where p_j is the same as in (1.37). The exterior part can also be written as

$$\psi(x,y) = \sum_{m'=1}^{\infty}\left(\delta_{mm'}\,\mathrm{e}^{-ik_m(x-a)} + \rho_{mm'}\mathrm{e}^{ik_{m'}(x-a)}\right)\xi_{m'}(y)\,,$$

where ξ_m are elements of the ordered basis corresponding to (1.36),

$$\rho_{mm'} := \begin{cases} \rho_{jj'}^{(+)} \ \ldots\ \theta_m = j\,,\ \theta_{m'} = j' \\ \rho_{jj'}^{(-)} \ \ldots\ \theta_m = j\,,\ \theta_{m'} = j'\varrho^{-1} \end{cases}$$

and $k_m := k_j^{(\pm)}$ for $\theta_m = j\,,\ j\varrho^{-1}$, respectively. Matching the functions (2.7) smoothly at $x = a$ we arrive at the equation

$$\sum_{m'=1}^{\infty}\left(ik_\ell + p_{m'}\tan(ip_{m'}a)\right)(\xi_\ell, \eta_{m'})\,a_{m'} = 2ik_\ell\delta_{m\ell}\,, \tag{2.8}$$

where the index m corresponds to the incident wave and the overlap integrals $(\xi_\ell, \eta_{m'})$ are the same as in (1.38); in the odd case corresponding to the Dirichlet condition at $x = 0$ one has to replace $\tan$ by $-\cot$. The reflection amplitudes are then given by

$$\rho_{m\ell}^{(\pm)} = -\delta_{m\ell} + \sum_{m'=1}^{\infty} a_{m'}^{(\pm)}(\xi_\ell, \eta_{m'})\,;$$

they determine the original quantities via (2.6). In a similar way one finds the reflection and transmission amplitudes in the case when the incident wave is in the lower channel and by that the full on-shell S-matrix; convergence of the truncating approximations is checked as in *Proposition* 1.2.3.

Often it is not the S-matrix itself but a quantity derived from it which is of primary physical interest. When perturbed waveguides are used to model systems of quantum wires coupled to macroscopic reservoirs we are concerned with ***conductance*** (or its inverse quantity, resistance) between a given pair of leads, which is given by the ***Landauer-Büttiker formula***. Suppose, for instance, that we deal with the incoming current in the upper right guide and the outgoing one in the lower left, then the conductance (measured in the standard units e^2/h) is given by

$$G_{l+,r-}(k) = \sum_{j=1}^{N_+(k)} \sum_{j'=1}^{N_-(k)} \frac{k_{j'}^{(-)}}{k_j^{(+)}}\, |t_{jj'}^{(-)}(k)|^2, \tag{2.9}$$

where k and the current-carrier momenta $k_j^{(\pm)}$ are determined by the Fermi energy and chemical potentials of the reservoirs and $N_\pm(k) = [k\kappa_{1\pm}^{-1}]$ are the number of propagating modes in the considered channels; analogous expressions can be written for conductances between other pairs of leads.

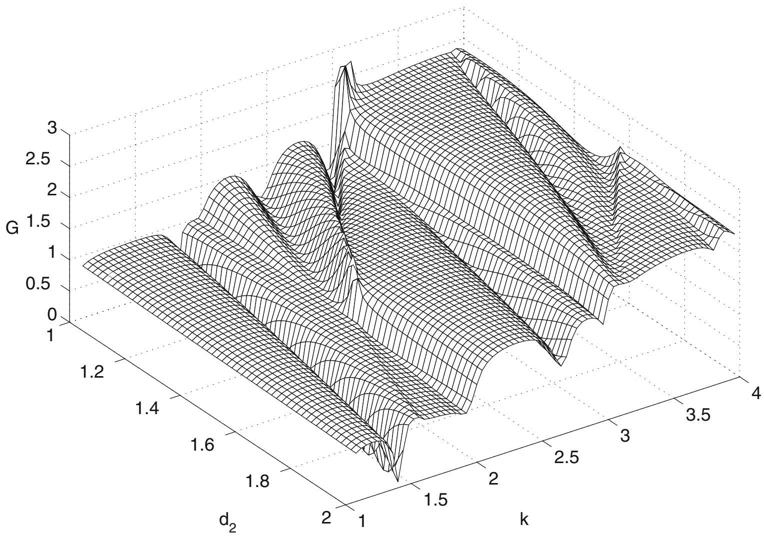

Fig. 2.1 A conductance plot for an asymmetric coupled waveguide system

As an illustration, we show in Fig. 2.1 the conductance plot for transport from the upper right to the upper left channel for $d_1 = \pi$ and $a = 1$ as a function of the momentum k and the lower channel width d_2. If the window was closed, the conductance $G_{l-,r-}(\cdot)$ would simply be a step function with a jump at every threshold. The general steplike pattern is preserved, being modified by the coupling, in particular, we observe pronounced resonances, the positions of which change with the channel width ratio.

2.3 Resonances from Perturbed Symmetry

One of the conspicuous effects in waveguides are scattering resonances, which we are going to discuss in this and the next section, because they typically entail sharp changes in transport properties. There are different mechanisms which can create resonances. The simplest one is based on symmetry violations. If a waveguide supports an eigenvalue embedded in the continuous spectrum which owes its existence to a particular symmetry, it is natural to expect that this eigenvalue turns into a resonance once the symmetry in question is perturbed.

Before discussing this mechanism in more detail, one has to make sure that its basic premise is not empty, i.e. that embedded eigenvalues can exist.

Examples 2.3.1 (a) Let $\Omega := \{\vec{x} \in \mathbb{R}^2 : -g(x) < y < g(x)\}$ be a symmetric strip with a protrusion. Specifically, suppose that g is a piecewise continuous function with $g(x) \geq \frac{1}{2}d$ and that there are sets $U \subset C \subset \mathbb{R}$, respectively open and compact, such that $g(x) > \frac{1}{2}d$ for $x \in U$ and $g(x) = \frac{1}{2}d$ for $x \in \mathbb{R} \setminus C$. By *Theorem* 1.4 we have $\sigma_{\mathrm{ess}}(-\Delta_D^\Omega) = [\epsilon_d, \infty)$. At the same time the operator decomposes into the even and odd part with respect to the strip axis, $y = 0$, the latter being unitarily equivalent to the Dirichlet Laplacian in the halfstrip $\Omega_+ := \{\vec{x} \in \mathbb{R}^2 : 0 < y < g(x)\}$. Consequently, if $-\Delta_D^{\Omega_+}$ has an eigenvalue in $(\epsilon_d, 4\epsilon_d)$, it is an embedded eigenvalue of the original operator (Problem 6).
(b) Let Ω be a pair of strips from Sect. 1.5.3 crossing at a right angle. The operator $-\Delta_D^\Omega$ has an embedded eigenvalue $\approx 3.72\epsilon_d$ (Problem 7).
(c) Similar conclusions can be made about local perturbations of the *Neumann* Laplacian $-\Delta_N^{\Omega_0}$ in the straight strip having $\sigma_{\mathrm{ess}}(-\Delta_N^{\Omega_0}) = [0, \infty)$. The operator H_a obtained by imposing an additional Neumann condition at a segment of the strip axis of length $2a$ has embedded eigenvalues for any $a > 0$ (Problem 3.2b).

Embedded eigenvalues can also be generated by a potential perturbation of a straight waveguide of the type discussed in Sect. 1.4. We shall now use this example to illustrate how the resonances emerge. We start from the unperturbed operator $-\Delta_D^{\Omega_0}$ referring to the straight strip $\Omega_0 = \mathbb{R} \times (-a, a)$ and put

$$H_\lambda := -\Delta_D^{\Omega_0} + V(x) + \lambda U(\vec{x}) , \tag{2.10}$$

where $V,\ U$ are real-valued functions on $\mathbb{R}$ and Ω_0, respectively, such that

(i) V is attractive, $V(x) \le 0$, and it does not vanish everywhere. Moreover, it is short-range, $|V(x)| \le \text{const}\, \langle x\rangle^{-2-\delta}$ for some $\delta > 0$, and it extends to a function analytic in the sector $\mathcal{M}_{\alpha_0} := \{ z \in \mathbb{C} : |\arg z| \le \alpha_0\}$ for some $\alpha_0 > 0$ and obeys the same bound there,

(ii) U is nonzero with similar properties, $|U(\vec{x})| \le \text{const}\, \langle x\rangle^{-2-\delta}$ for some $\delta > 0$ and all $\vec{x} = (x, y) \in \Omega$, and $U(\cdot, y)$ extends for any fixed $y \in (-a, a)$ to an analytic function in $\mathcal{M}_{\alpha_0}$ and satisfies the same bound there.

Here $\langle x\rangle := \sqrt{1+x^2}$; since the potentials are by assumption continuous and bounded, the right-hand side in (2.10) is well defined. The unperturbed operator H_0 admits a separation of variables and the longitudinal part $h^V := -\partial_x^2 + V(x)$ has in view of *(i)* a nonempty and finite discrete spectrum,

$$\mu_1 < \mu_2 < \cdots \mu_N < 0\,;$$

the normalized eigenfunctions $\phi_n \in L^2(\mathbb{R}),\ n = 1, \dots, N$, associated with these simple eigenvalues are exponentially decaying. On the other hand, the transverse spectrum consists of the eigenvalues $\nu_j = \kappa_j^2 = (\pi j/2a)^2,\ j \in \mathbb{N}$, corresponding to the eigenfunctions (1.10), hence the spectrum of H_0 consists of the continuous part, $\sigma_{\text{ess}}(H_0) = \sigma_{\text{ac}}(H_0) = [\nu_1, \infty)$, and an infinite family of eigenvalues,

$$\sigma_{\text{p}}(H_0) = \left\{ \mu_n + \nu_j : n = 1, \dots, N\,,\ j = 1, 2, \dots \right\}.$$

Among these a finite subset is isolated, while the rest satisfying the condition

$$\nu_1 < \mu_n + \nu_j \ne \nu_k\,, \quad k = 2, 3, \dots\,, \tag{2.11}$$

are embedded in the continuous spectrum away from the thresholds. We rewrite the Hamiltonian (2.10) as an infinite matrix differential operator $\{H_{jk}(\lambda)\}$ on $L^2(\mathbb{R})$ with the elements

$$H_{jk}(\lambda) := \mathcal{J}_j^* H_\lambda \mathcal{J}_k = \left(h^V + \nu_j\right) \delta_{jk} + \lambda U_{jk}(x)\,, \tag{2.12}$$

where in the last term $U_{jk}(x) := \int_{-a}^{a} U(x, y)\, \overline{\chi}_j(y)\chi_k(y)\, \mathrm{d}y$ and we use the embeddings $\mathcal{J}_k : L^2(\mathbb{R}) \to L^2(\Omega_0)$ and their adjoints $\mathcal{J}_k^* : L^2(\Omega_0) \to L^2(\mathbb{R})$ which act as

$$(\mathcal{J}_k\, u)(x, y) = u(x)\, \chi_k(y)\,, \quad (\mathcal{J}_k^*\, f)(x) = \int_{-a}^{a} f(x, y)\chi_k(y)\, \mathrm{d}y\,.$$

Speaking of resonances we have in mind the most common definition which is based on analytical continuation of the Hamiltonian resolvent across the cut(s) associated with the continuous spectrum into a domain on another sheet of the corresponding energy surface, conventionally to the lower complex halfplane. A ***resonance*** is then identified with a pole in this analytic continuation; it is physically important if the pole is close to the real axis and the respective residue is not negligible. This concept naturally requires a sort of analyticity hypothesis, for instance such as we have made in the above assumptions.

One of the most efficient methods to determine resonances of Schrödinger operators is based on the so-called ***complex scaling***. With a small modification this technique can also be applied to waveguides. In this case one has to scale only the longitudinal variable as we shall now illustrate on the example in question. We begin with the family of unitary operators

$$S_\theta : \ (S_\theta\psi)(x, y) = \mathrm{e}^{\theta/2}\psi(\mathrm{e}^\theta x, y) , \quad \theta \in \mathbb{R} , \tag{2.13}$$

on $L^2(\mathbb{R})$ and extend this scaling transformations analytically to $\mathcal{M}_{\alpha_0}$. This is made possible by assumptions *(i), (ii)* according to which the transformed Hamiltonians are of the form

$$\begin{aligned} H_{\theta,\lambda} &:= S_\theta H_\lambda S_\theta^{-1} = H_{\theta,0} + \lambda U_\theta , \\ H_{\theta,0} &:= \mathrm{e}^{-2\theta}(-\partial_x^2) - \partial_y^2 + V_\theta(x) , \end{aligned}$$

where $V_\theta(x) := V(\mathrm{e}^{\theta x})$ and $U_\theta(x, y) := U(\mathrm{e}^\theta x, y)$. The operators $H_{\theta,0}$ with $\theta \in \mathcal{M}_{\alpha_0}$ clearly constitute a type (A) analytic family of m-sectorial operators. It is straightforward to check that U_θ is relatively bounded with respect to $H_{\theta,0}$, thus the operators $H_{\theta,\lambda}$ with the same θ and $|\lambda|$ small enough constitute again a type (A) analytic family. The free part of the transformed operator still separates variables, hence its spectrum equals

$$\sigma\left(H_{\theta,0}\right) = \bigcup_{j=1}^{\infty} \left\{ \nu_j + \sigma\left(h_\theta^V\right)\right\} ,$$

where $h_\theta^V := -\mathrm{e}^{-2\theta}\partial_x^2 + V_\theta(x)$. Since the potential V is dilation analytic by assumption, the discrete spectrum of h_θ^V is independent of θ; we have

$$\sigma\left(h_\theta^V\right) = \mathrm{e}^{-2\theta}\mathbb{R}_+ \cup \{\mu_1, \dots, \mu_N\} \cup \{\rho_1, \rho_2, \dots\} .$$

Here μ_n are eigenvalues of h^V which will turn into resonances as a result of the perturbation. On the other hand, the ρ_r are the "intrinsic" resonances, i.e. complex poles of the resolvent of h_θ^V uncovered by the rotation of the essential spectrum; in view of assumption *(i)* there is at most a finite number of them in any finite part of the lower complex halfplane (see the notes). The two pole types are easily distinguished by their behavior in the limit $\lambda \to 0$ because only the former ones tend to the real axis as the perturbation is removed.

The main insight of the complex scaling method is that moving the essential spectrum we turn the embedded eigenvalues into isolated ones whose perturbation can be treated by usual methods; it is easy when the perturbation is relatively bounded as in our case. Any fixed eigenvalue $\epsilon_0 = \mu_n + \nu_j$ of $H_{\theta,0}$ has a neighborhood containing none of the points $\rho_k + \nu_{j'}$ in which we choose a contour encircling it; for the sake of simplicity we consider only the non-degenerate case, i.e. we suppose that $\mu_n + \nu_j \neq \mu_{n'} + \nu_{j'}$ holds for different pairs of indices.

It is sufficient to consider a purely imaginary scaling parameter, $\theta = i\beta$ with $\beta > 0$. Let P_θ be the projection onto the eigenspace associated with such an ϵ_0 and let $R_\theta(z) := (H_{\theta,0} - z)^{-1}$, then we set

$$S_\theta^{(p)} := \frac{1}{2\pi i} \int_{\mathcal{C}} \frac{R_\theta(z)}{(\epsilon_0 - z)^p} \, \mathrm{d}z$$

for $p \geq 0$, in particular, $P_\theta = -S_\theta^{(0)}$ and $S_\theta^{(1)} = \hat{R}_\theta(\epsilon_0)$ is the reduced resolvent value at the point ϵ_0. The assumption *(ii)* implies the existence of a positive c_θ such that $\max_{z\in\mathcal{C}} \|U_\theta R_\theta(z)\| \leq c_\theta$, and it follows that

$$\left\| U_\theta S_\theta^{(p)} \right\| \leq c_\theta \, \frac{|\mathcal{C}|}{2\pi} \left[\mathrm{dist}\,(\mathcal{C}, \epsilon_0)\right]^{-p}$$

holds for any $p \geq 0$. Thus we can justify the existence of the perturbation expansion,

$$\epsilon(\lambda) = \mu_n + \nu_j + \sum_{m=1}^{\infty} \epsilon_m(\lambda)\,, \tag{2.14}$$

where

$$\epsilon_m(\lambda) = \sum_{p_1+\dots+p_m=m-1} \frac{(-\lambda)^m}{m} \,\mathrm{tr} \prod_{i=1}^{m} U_\theta S_\theta^{(p_i)}\,,$$

because $\epsilon_m(\lambda) = \mathcal{O}(\lambda^m)$ and the convergence of the series (2.14) is checked in the same way as in Problem 1.28.

Let us next determine what the leading terms in the expansion look like. The first-order correction, $\epsilon_1(\lambda) = \mathrm{tr}\,(\lambda U_\theta P_\theta)$, is real-valued,

$$\epsilon_1(\lambda) = \left(\overline{\phi_n^\theta \otimes \chi_j}, \lambda U_\theta\, \phi_n^\theta \otimes \chi_j\right) = \left(\phi_n \otimes \chi_j, \lambda U \phi_n \otimes \chi_j\right) = \lambda \left(\phi_n, U_{jj}\phi_n\right)\,,$$

where ϕ_n is the eigenvector of h^V associated with μ_n. Thus, as usual in such situations, it does not contribute to the resonance width. The second-order term is conventionally computed by taking the limit $\beta \to 0$. In this way we get

$$\epsilon_2(\lambda) = -\lambda^2 \,\mathrm{tr}\left(P_{j,n} U \hat{R}_1(\epsilon_0 - i0)\, U P_{j,n}\right) = -\lambda^2 \sum_{k=1}^{\infty} \left(U_{jk}\phi_n, \hat{\mathcal{R}}_k U_{jk}\phi_n\right)\,,$$

where $P_{j,n}$ is the projection onto the subspace spanned by $\phi_n \otimes \chi_j$ and $\hat{\mathcal{R}}_k$ is the shorthand for the reduced resolvent obtained by subtracting the pole term from $(h^V - \epsilon_0 + \nu_k - i0)^{-1}$. We are interested primarily in the imaginary part of $\epsilon_2(\lambda)$ which determines the resonance width in the leading order.

Notice first that the imaginary part of the last series is in fact a finite sum. We put $k(\epsilon_0) := \max\{k : \epsilon_0 - \nu_k > 0\}$; if the unperturbed eigenvalue is embedded we have $k(\epsilon_0) \geq 1$, otherwise the set is empty and we put $k(\epsilon_0) = 0$ by definition. It is clear that $\hat{\mathcal{R}}_k^* = \hat{\mathcal{R}}_k$ holds for $k > k(\epsilon_0)$, hence we have

$$\operatorname{Im} \epsilon_2(\lambda) = -\lambda^2 \sum_{k=1}^{k(\epsilon_0)} \left(U_{jk}\phi_n, (\operatorname{Im} \hat{\mathcal{R}}_k)\, U_{jk}\phi_n \right) .$$

To write the right-hand side explicitly we need to express $\operatorname{Im} \hat{\mathcal{R}}_k$. The imaginary part and the relation between the free and full resolvent can be rewritten using the resolvent identities; in this way we get for any $\epsilon > 0$ the formula

$$\operatorname{Im} (h^V - \epsilon - i0)^{-1} = \omega(\epsilon + i0)^* \operatorname{Im} (-\partial_x^2 - \epsilon - i0)^{-1} \omega(\epsilon + i0) \tag{2.15}$$

(Problem 8) in which $\omega(z) := \left(I + V(-\partial_x^2 - z)^{-1}\right)^{-1}$ is the inverse to

$$\omega^{-1}(z) : \left(\omega^{-1}(z)\phi\right)(x) = \phi(x) + \frac{iV(x)}{2\sqrt{z}} \int_{\mathbb{R}} \mathrm{e}^{i\sqrt{z}|x-x'|}\, \phi(x')\, \mathrm{d}x' .$$

By assumption *(i)* which ensures, in particular, that h^V has no positive eigenvalues, the operator $\omega(\epsilon + i0)$ is well defined. Furthermore, we have

$$\operatorname{Im} (-\partial_x^2 - \epsilon - i0)^{-1} = \frac{\pi}{2\sqrt{\epsilon}} \sum_{\sigma=\pm} \tau_\sigma(\epsilon)^* \tau_\sigma(\epsilon) \tag{2.16}$$

for any $\epsilon > 0$ where $\tau_\sigma(\epsilon) : H^1(\mathbb{R}) \to \mathbb{C}$ on the right-hand side is the trace map acting as $\tau_\sigma(\epsilon)\phi = \hat{\phi}(\sigma\sqrt{\epsilon})$ with $\hat{\phi}$ being the Fourier transform of ϕ (Problem 8). The above discussion can be summarized in the following way.

Theorem 2.4 *Assume (i), (ii). Moreover, let $\epsilon_0 = \mu_n + \nu_j$ be a simple eigenvalue of H_0 satisfying conditions (2.11). Then ϵ_0 is also a simple eigenvalue of the operator $H_{\theta,0}$ and a weak potential perturbation $\lambda U(\vec{x})$ in (2.10) moves it to $\epsilon(\lambda)$ with*

$$\operatorname{Im} \epsilon(\lambda) = -\frac{\lambda^2}{2} \sum_{k=1}^{k(\epsilon_0)} \sum_{\sigma=\pm} \frac{\pi}{\sqrt{\epsilon_0 - \nu_k}} \left| \tau_\sigma(\epsilon_0 - \nu_k)\, \omega(\epsilon_0 - \nu_k + i0)\, U_{jk}\phi_n \right|^2 + \mathcal{O}(\lambda^3) ,$$

as $\lambda \to 0$. If the second-order coefficient is nonzero, then $\epsilon(\lambda)$ describes a resonance of the operator H_λ.

Remarks 2.3.1 (a) The imaginary part given above is non-positive for small λ. It may happen, of course, that ϵ_0 persists as an eigenvalue. A trivial example is represented by a potential which preserves the symmetry, $U(\vec{x}) = U_1(x) + U_2(y)$ with suitable functions of which U_1 can be added to the potential V; notice that $k(\epsilon_0) < j$ so the diagonal elements of the matrix potential do not contribute. The leading coefficient may also accidentally vanish for potentials which do not decompose, however, then higher terms of the series may be nonzero.
(b) Notice that the ω introduced above is in fact a wave operator for the pair $(h^V, -\partial_x^2)$. It follows that the squared numbers in the above formula can be formally written as $|(\psi_{\pm\sqrt{\epsilon_0-\nu_k}}, U_{jk}\phi_k)|^2$, where ψ_m is the generalized eigenfunction of h^V with the momentum m. This shows that the leading term of the resonance width expansion is in this case given by ***Fermi's golden rule***.

2.4 Resonances in Thin Bent Strips

The symmetry violation is not the only mechanism which can give rise to resonances. Let us now return to one of our basic examples, a curved planar strip, and discuss it from the present point of view; the role of the perturbation parameter will be played by the strip width d. To explain the idea, we express the Hamiltonian H introduced in Sect. 1.1 in terms of the transverse modes, similarly as we did earlier in *Theorem* 1.6 where, however, we only singled out the lowest transverse mode, or in the previous section using the embedding operators $\mathcal{J}_j$ and their adjoints.

If the strip is asymptotically straight, i.e. the curvature decays fast enough, the spectrum of $-\partial_s^2 - \frac{1}{4}\gamma(s)^2$ consists of a continuous part which is the positive halfline and a nonempty family $\{\lambda_n\}$ of simple negative eigenvalues. Let us define the operator

$$H^0 := A - \partial_u^2, \qquad A := -\partial_s^2 + V^0, \quad V^0 = -\frac{1}{4}\gamma(s)^2 \tag{2.17}$$

acting on the Hilbert space $\mathcal{H} = L^2(\mathbb{R} \times (0, d), \mathrm{d}s\, \mathrm{d}u)$ with Dirichlet conditions at $u = 0, d$. Since the spectrum of the transverse part of H^0 is discrete with the eigenvalues $\nu_j = \kappa_j^2$, $j \in \mathbb{N}$, it is clear that for any $j \geq 2$ and d small enough the numbers $\lambda_n + \nu_j$ are eigenvalues embedded in the continuous spectrum of H^0. If we regard the original operator $-\Delta_D^\Omega$ as a result of perturbing H^0, as we did when discussing the discrete spectrum in Sect. 1.6, one expects that these embedded eigenvalues can turn into resonances provided we impose suitable analyticity assumptions on the curvature, for instance,

(i) γ extends to an analytic function, denoted by the same symbol, in $\mathcal{M}_{\alpha_0,\eta_0} := \{z \in \mathbb{C} :\ |\arg z| \leq \alpha_0 \text{ or } |\mathrm{Im}\, z| < \eta_0\}$ with $\alpha_0 < \pi/2$ and $\eta_0 > 0$,
(ii) to each $\alpha \in (0, \alpha_0)$ and $\eta \in (0, \eta_0)$ one can find positive $c_{\alpha,\eta}$ and δ such that the inequality $|\gamma(z)| < c_{\alpha,\eta}(1+|z|)^{-1-\delta}$ holds in $\mathcal{M}_{\alpha_0,\eta_0}$.

Proceeding as in the previous section, we can then derive an expansion for the resonance pole position and to estimate the first nonzero contribution to its imaginary part, i.e. the resonance width (cf. Problem 10 and the notes).

Theorem 2.5 *Let H be given by (1.7). Suppose that the strip Ω does not intersect itself and assumptions (i), (ii) are valid. Then for all sufficiently small widths d each eigenvalue $\lambda_n + \nu_j$ of H^0 with $j \geq 2$ gives rise to a resonance $\epsilon_{j,n}(d)$ of H the position of which is given by a convergent series,*

$$\epsilon_{j,n}(d) = \mu_n + \nu_j + \sum_{m=1}^{\infty} \epsilon_m^{(j,n)}(d)\,,$$

where $\epsilon_m^{(j,n)}(d) = \mathcal{O}(d^m)$ as $d \to 0$. The first-order term is real-valued and the second-order term satisfies the estimate

$$0 \leq \mathrm{Im}\,\epsilon_2^{(j,n)}(d) \leq c_{\eta,j}\,\mathrm{e}^{-2\pi\eta\sqrt{2j-1}/d}$$

for any $\eta \in (0, \eta_0)$ and some positive $c_{\eta,j}$ depending on η and j.

The second claim of the theorem shows that $\epsilon_m^{(j,n)}(d)$ may tend to zero much faster than the $\mathcal{O}(d^m)$ rate which such a straightforward argument gives. It is not *a priori* clear whether the lowest order term are dominant as $d \to 0$, however, one can prove similar bounds on the total resonance width:

Theorem 2.6 *Suppose that the strip Ω does not intersect itself and assumptions (i), (ii) are valid. Then for any $\eta \in (0, \eta_0)$, $j \geq 2$, and $n = 1, \dots, N$ there exists a $c_{n,\eta} > 0$ such that*

$$0 \;\leq\; -\mathrm{Im}\,\epsilon_{j,n}(d) \;\leq\; c_{\eta,j}\,\mathrm{e}^{-2\pi\eta\sqrt{2j-1}/d} \tag{2.18}$$

holds for all d small enough.

Sketch of the proof: As in the previous case, to demonstrate *Theorem* 2.6 one has to treat the resonances of H as perturbations of a suitable operator with eigenvalues embedded in the continuous spectrum; we write therefore $H = H^0 + W$, where H^0 is given by (2.17) and W is the perturbation. The spectrum of the operator H^0 is of the form

$$\sigma(H^0) = \left\{\lambda + E \;:\; \lambda \in \sigma(A),\; E \in \sigma(-\partial_u^2)\right\},$$

where

$$\sigma(A) = \{\lambda_j\}_{j=1}^{N} \cup [0, \infty)\,, \quad \sigma(-\partial_u^2) = \left\{\nu_j\right\}_{j=1}^{\infty}\,,$$

with $\nu_j := \kappa_j^2,\ \kappa_j := \pi j/d$. Since Ω is not straight, $\gamma \neq 0$, the discrete spectrum of A is nonempty and the eigenvalues λ_j are simple. Moreover, from assumption (ii) it follows that their number N is finite. Then the eigenvalues

$$E^0_{j,n} = \lambda_n + \nu_j$$

with $j \geq 2$ are embedded in the continuous spectrum of H^0 for d small enough and we expect them to give rise to resonances of the full operator H.

We pass to the unitary equivalent operator by performing the inverse Fourier transformation in the s variable, denoted by F_s^{-1}. We introduce

$$p := F_s^{-1} i\partial_s F_s\,, \qquad D := -i\partial_p = F_s^{-1} s F_s$$

and with a slight abuse of notation we shall employ the usual symbols for all other transformed operators,

$$H = p\, b(D,u)p - \partial_u^2 + V(D,u). \tag{2.19}$$

As in Sect. 2.3 above, we are going to use a complex scaling, this time an *exterior* one defined as

$$p_\theta(t) := \begin{cases} t & \text{if} \quad t \in \Omega_i := (-\omega, \omega) \\ \\ \pm\omega + e^\theta (t \mp \omega) & \text{if} \quad t \in \Omega_e := \mathbb{R} \setminus \bar{\Omega}_i \end{cases} \tag{2.20}$$

where ω is a positive number to be determined later. First we consider $\theta \in \mathbb{R}$ and associate with a given closed operator T the family of operators

$$T_\theta := U_\theta T\, U_\theta^{-1}, \quad U_\theta \varphi := p_\theta^{1/2} \varphi \circ p_\theta\,.$$

If the function $\theta \mapsto T_\theta$ has an analytic continuation to some strip $\{\theta \in \mathbb{C} \,:\, |\operatorname{Im}\theta| < \alpha\}$, we are able to define complex deformations of T. In particular, the family of complex deformations of the Hamiltonian (2.19) is given by

$$H_\theta = H_\theta^0 + W_\theta, \quad H_\theta^0 = A_\theta \otimes I + I \otimes (-\partial_u^2), \tag{2.21}$$

where

$$W_\theta = p_\theta (b-1)_\theta p_\theta + (V - V^0)_\theta.$$

Under the premises of the theorem the operators H_θ and H_θ^0 form self-adjoint analytic families of type (A). From now we set for simplicity $\theta = i\beta$ with $\beta > 0$. It is not hard to check that the spectrum of $H_{i\beta}^0$ equals

$$\sigma(H^0_{i\beta}) = \left\{\lambda + \nu_j \;:\; \lambda \in \left(\{\lambda_n\}_{n=1}^N \cup \varrho \cup \sigma(p^2_{i\beta})\right),\; j = 1, 2, \dots\right\}, \tag{2.22}$$

where ϱ denotes the (possibly empty) set of resonances of the operators $A_{i\beta}$.

As before the resonances of H are identified with the complex eigenvalues of the non-selfadjoint operator $H_{i\beta}$, and their positions can be estimated with the help of the regular perturbation theory, where the role of the unperturbed operator is played by $H^0_{i\beta}$ and the perturbation is represented by $W_{i\beta}$. We choose a fixed eigenvalue $E^0_{n,j} = \lambda_n + \nu_j,\; j \ge 2$, of $H^0_{i\beta}$ and define

$$\Gamma := \left\{z \in \mathbb{C} \;:\; |z - E^0_{n,j}| = r\right\}, \quad r = \frac{1}{2}\,\mathrm{dist}(\lambda_n, \sigma(A) \setminus \{\lambda_n\})$$

to be a circular contour around $E^0_{n,j}$ such that no other eigenvalue of $H^0_{i\beta}$ lies within Γ. It is convenient to use the transverse mode decomposition of $H^0_{i\beta}$,

$$H^0_{i\beta} = \sum_{k\ge1} \mathcal{J}_k H^{0,k}_{i\beta} \mathcal{J}^*_k \qquad \text{with} \quad H^{0,k}_{i\beta} = \mathcal{J}^*_k H^0_{i\beta} \mathcal{J}_k \;\text{ in }\; L^2(\mathbb{R}, \mathrm{d}p)$$

where the $\mathcal{J}_k$'s are the natural embedding operators introduced in the previous section. Assume now that $E = E_{n,j}$ is the resonance arising from $E^0_{n,j}$ and that $\phi_{i\beta}$ is the associated eigenfunction,

$$H_{i\beta}\,\phi_{i\beta} = E\,\phi_{i\beta}\,. \tag{2.23}$$

This equation is equivalent to the system

$$\begin{aligned}\left(P_j H_{i\beta} P_j - P_j W_{i\beta} \hat{R}^j_{i\beta}(E) W_{i\beta} P_j\right) \phi_{i\beta} &= E\; P_j \phi_{i\beta}, \\ Q_j\, \phi_{i\beta} &= -\hat{R}^j_{i\beta}(E) W_{i\beta} P_j \phi_{i\beta},\end{aligned}$$

where $P_j := \mathcal{J}_j \mathcal{J}^*_j$, $Q_j := I - P_j$, and $\hat{R}^j_{i\beta}(E) := Q_j \left(Q_j(H_{i\beta} - E)Q_j\right)^{-1} Q_j$. Moreover, it is easy to see that the first equation is further equivalent to

$$\left(H^j_{i\beta} - B^j_{i\beta}(E)\right) \phi^j_{i\beta} = E\,\phi^j_{i\beta}\,, \quad B^j_{i\beta}(E) := \mathcal{J}^*_j W_{i\beta} \hat{R}^j_{i\beta}(E) W_{i\beta} \mathcal{J}_j\,, \tag{2.24}$$

in $L^2(\mathbb{R})$, where $H^j_{i\beta} := P_j H_{i\beta} P_j$ and $\phi^j_{i\beta} := P_j\,\phi_{i\beta}$. Taking the imaginary part of equation (2.24) we get

$$\mathrm{Im}\, E\, \|\phi^j_{i\beta}\|^2 = (\mathrm{Im}\,(H^j_{i\beta} - B^j_{i\beta}(E))\phi^j_{i\beta}, \phi^j_{i\beta}). \tag{2.25}$$

Using next the identity $\mathrm{Im}\,(ABA) = 2\,\mathrm{Re}\,(\mathrm{Im}\,(A)BA) + A^*\mathrm{Im}\,(B)A$ in combination with the resolvent equation, we can write $\mathrm{Im}\, B^j_{i\beta}$ as

$$\begin{aligned}\mathrm{Im}\, B^j_{i\beta} &= Z_{i\beta} + \mathrm{Im}\, E\, |\hat{R}^j_{i\beta} W_{i\beta} \mathcal{J}_j|^2 \\ Z_{i\beta} &:= \mathcal{J}^*_j \left\{ 2\mathrm{Re}\, \left(\mathrm{Im}\, (W_{i\beta} \hat{R}^j_{i\beta} W_{i\beta} \right) - W^*_{i\beta} (\hat{R}^j_{i\beta})^* \mathrm{Im}\, (Q_j H_{i\beta} Q_j) \hat{R}^j_{i\beta} W_{i\beta} \right\} \mathcal{J}_j .\end{aligned}$$

Inserting this into Eq. (2.25) we obtain

$$\mathrm{Im}\, E \left(\|\phi^j_{i\beta}\|^2 + \|\hat{R}^j_{i\beta} W_{i\beta} \mathcal{J}_j \phi^j_{i\beta}\|^2 \right) = \|P_j \phi_{i\beta}\|^2_{\mathcal{H}} + \|Q_j \phi_{i\beta}\|^2_{\mathcal{H}} = \|\phi_{i\beta}\|^2_{\mathcal{H}}$$

and since the eigenfunction $\phi_{i\beta}$ is supposed to be normalized, we arrive at

$$\mathrm{Im}\, E = ((\mathrm{Im}\, H^j_{i\beta} - Z_{i\beta}) \phi^j_{i\beta}, \phi^j_{i\beta}) . \tag{2.26}$$

This equation will yield the desired bound (2.18); to this end we need a couple of definitions. We choose ω in the scaling relation (2.20) to be

$$\omega := \frac{\pi}{d} \sqrt{(2j-1)(1-\xi d)} ,$$

where ξ is a positive parameter. Moreover, we define the function

$$\rho(p) := \eta \int_{\min\{0,p\}}^{\max\{0,p\}} \chi_{\Omega_i \setminus \Omega_*}(t)\, \mathrm{d}t ,$$

where $\Omega_* = (-p_*, p_*)$ and p_* is a suitable positive constant independent of d. Then one can prove (see the notes) that there exists a number C_η such that

$$\left\| \langle p \rangle^{-1} e^{-\rho} (\mathrm{Im}\, H^j_{i\beta} - Z_{i\beta}) \langle p \rangle^{-1} e^{-\rho} \right\| \le C_\eta\, e^{-\rho(\omega)} , \tag{2.27}$$

where

$$\langle p \rangle = (p^2 + \tau)^{1/2}, \quad \tau := \sup \left\{ \|e^\rho\, V^0_{i\beta}\| \, : \, |\beta| \le \alpha_0 \right\} .$$

Since $\mathrm{Im}\, E$ cannot be positive, insertion of (2.27) into equation (2.26) gives

$$0 \le -\mathrm{Im}\, E \le C_\eta\, e^{-\rho(\omega)} \left(\|p\, e^\rho\, \phi^j_{i\beta}\|^2 + \tau \|e^\rho\, \phi^j_{i\beta}\|^2 \right) . \tag{2.28}$$

At this point we have to take into account the exponential decay of the complex scaled resonance eigenvectors $\phi^j_{i\beta}$. Indeed, with our definition of the function ρ we have

$$\|p\, e^\rho\, \phi^j_{i\beta}\|^2 \le 2, \quad \|e^\rho\, \phi^j_{i\beta}\|^2 \le 2\, p_* ,$$

see again the notes for more details. Using now the fact that

$$e^{-2\,\rho(\omega)} = \exp\left\{-\frac{2\pi\eta}{d}\sqrt{2j-1}\,\left(1+\mathcal{O}(\xi d)\right)\right\} \quad \text{as} \quad d \to 0$$

we get the upper bound (2.18) from (2.28). ∎

2.5 Notes

Section 2.1 The smooth perturbation method used in the proof of *Theorem* 2.1 is due to Kato [Ka66]—see, e.g., Sect. 8.7 of [RS], or [Sch], Chap. 10. The abstract result we refer to here is contained in Theorem 10.2.2 of [Sch].

Mourre's method naturally does not require the Hilbert space to be $L^2(\Omega_0)$. The idea to use positive commutators is based on an analogy with the classical Poison bracket of some coordinate q and the Hamiltonian H_{cl}. If one can show that for some trajectory $\{q, H_{\mathrm{cl}}\} = \partial_t q \geq \delta > 0$, then the motion along this trajectory is extended in the coordinate q. The simplest application in quantum mechanics yields a criterium for the absence of eigenvalues. Indeed, if ψ is an eigenfunction of the Hamiltonian H, then by the virial theorem $(\psi, [i\Pi, H]\psi) = 0$ holds for any self-adjoint operator Π satisfying certain regularity properties. E. Mourre proved in [Mou81] that under yet stronger regularity assumptions the positivity of the commutator implies not only $\sigma_{\mathrm{p}}(H) \cap I = \emptyset$ but also the absence of the entire singular spectrum of H in the interval I, that is, the version of *Theorem* 2.2 with $\alpha = 1$. For a proof and further generalizations see the monographs [ABG,CFKS]. *Theorem* 2.3 is taken from [KrT04], where the result is also extended to bent tubes in any dimensions provided δ is large enough. Mourre's method has also recently been applied to the analysis of scattering in twisted three-dimensional waveguides, see [BKR14] for details.

Section 2.2 It is a matter of convention whether we regard threshold states, i.e. those with $\nu_n^{(j)} = k^2$, as propagating modes in the definition of $N_j(k)$. The example discussed here comes from [EŠTV96], in a similar way one can treat scattering in a double waveguide separated by a leaky barrier of Sect. 1.5.2 (Problem 5). Many other examples of waveguide scattering treated by mode matching can be found in [LCM].

The relation between the conductance of a perturbed channel and the corresponding quantum mechanical scattering problem was first formulated by R. Landauer [La70], later extended by M. Büttiker [Bü88] to systems with an arbitrary finite number of outgoing channels. In practical applications one usually adds a factor of two which accounts for the spin states of the electron, in other words the right-hand side of (2.9) is multiplied in the standard units by $2e^2/h$. A rigorous derivation of the Landauer-Büttiker formula together with a bibliography can be found in [CJM05]. Let us add that such a description of transport contains two simplifying assumptions. First, it supposes that the potential difference between the heat baths connected by the waveguide is infinitesimally small—one usually speaks in this connection about *linear response theory* – and secondly, the transport occurs at temperature zero. More generally, the current flowing through the guide is expressed by the formula

$$I = \frac{2e^2}{h} \int_{\mathbb{R}} \left[f_\beta(k^2 - \mu_2) - f_\beta(k^2 - \mu_1) \right] |t(k)|^2 \mathrm{d}k^2 \,,$$

where $f_\beta(\epsilon) = (\mathrm{e}^{\beta\epsilon} + 1)^{-1}$ is the Fermi-Dirac distribution function at temperature β^{-1}, μ_j are the chemical potentials in the reservoirs, and for simplicity we left out the factor describing the possibly different incoming and outgoing velocities; differentiating this expression and putting $\beta = \infty$ we get the conductance mentioned above.

Mode matching also offers other insights into the scattering process. Using the Ansatz (2.7) with the coefficients obtained by solving the matching conditions (2.8) we find what the generalized eigenvectors at energy k^2 look like. Then one can compute, in particular, the probability flow distribution $\vec{j}(\vec{x}) := -i\bar{\psi}(\vec{x})\vec{\nabla}\psi(\vec{x})$, for examples see again [EŠTV96], [EKr99], [LCM]. The flow patterns can reveal some features of the scattering, for example, a pronounced vortex suggests the existence of a resonance. On the other hand, vortices in transport of charged particles give rise to a nonzero magnetic moment which is in principle measurable [ESŠF98].

Section 2.3 The embedded eigenvalue in the crossed strips of Example 2.3.1b was noticed first in [SRW89]. On the other hand, the conclusion of Example 2.3.1c extends to a class of more general symmetric obstacles in *Neumann* waveguides —see [ELV94] and [DP98] where some conditions for the nonexistence of such eigenvalues were also derived. Resonances coming from mirror symmetry violations in strips with rectangular protrusions were investigated by mode matching in [AVD95], the analogous question for obstacle-induced eigenvalues in a Neumann waveguide was addressed in [APV00]. For an analysis of resonances coming from symmetry breaking associated with twisting of a three-dimensional waveguide we refer to [KS07].

The resonance system with the Hamiltonian (2.10) is a modification of Nöckel's model [Nö92] which will be discussed in Sect. 7.1.3; the material is taken from [DEM01]. Similar conclusions can be made if a hard-wall strip is replaced by a "soft" waveguide in which the confinement is due to a transverse potential (Problem 9). The most common definition of a resonance used here, in terms of poles of an analytically continued resolvent, is discussed in many places—see, e.g., Chap. 3 of [Ex] and the bibliography given there. Alternatively one can associate resonances, for instance, with poles of the analytically continued scattering matrix. Since the former definition expresses a property of the Hamiltonian alone while the latter concerns a pair of operators which we compare, it is clear that the objects they describe are in general different. On the other hand, it is true that for a "natural" choice of the free and full dynamics both types of resonances usually coincide, but this is a fact which one has to check it in each particular case.

The complex scaling method was formulated in the paper [AC71]. With several modifications and generalizations, cf. Chap. 8 of [CFKS], it developed into a powerful method for treating resonances in atomic and molecular systems—for a review with a bibliography see [Mo98]. The application of longitudinal complex scaling to resonances in waveguides was proposed in [DEŠ95]. For the definition and properties of analytic operator families see Chap. 7 of [Ka]. The "intrinsic" singularities coming from resonances of h^V do not accumulate in $\mathcal{M}_{\alpha_0}$; under the assumption *(i)* this follows from [AC71] or [Je78]. The method used here to evaluate the second-order coefficient in *Theorem* 2.4 is standard—see, e.g., Sect. 8.6 in [RS].

Section 2.4 *Theorem* 2.5 comes from [DEŠ95]. The bound on the imaginary part of the pole positions corresponds to the heuristic semiclassical picture – see [LL], Sect. 7.51—according to which the rate of exponential decay is proportional to

$$2\,\mathrm{Im}\int_0^{i\eta_0}\left(\sqrt{\epsilon - V_{0,j}(\zeta)} - \sqrt{\epsilon - V_{0,j-1}(\zeta)}\right)\mathrm{d}\zeta = \frac{2\pi\eta_0}{d}\sqrt{2j-1} + \mathcal{O}(d^0)\,,$$

where $V_{0,j} = \frac{1}{4}\gamma^2 + \nu_j$ and $\epsilon = \lambda_n + \nu_j + \mathcal{O}(d)$. *Theorem* 2.6 showing that the total resonance width has the same exponential bound as the lowest nontrivial term in the expansion of *Theorem* 2.5 comes from [DEM98], an analogous result was proved in [Ne97]. We refer to these papers for some technical statements made in the proof.

2.6 Problems

1. Fill in the details of the proof of *Theorem* 2.1.
Hint: Compute the integral $\int_0^\infty p^{2l}[(p^2+\mu)^2+\eta^2]^{-1}\mathrm{d}p$.

2. Modify *Theorem* 2.1 for the case when H refers to a bent tube in $\mathbb{R}^3$ satisfying Tang's condition (1.18) together with the other assumptions of Sect. 1.3.

3. Let H be the self-adjoint operator associated with quadratic form (1.24). Suppose that the potential V satisfies the assumptions of *Proposition* 1.4.1 and in addition, that $|V(\vec{x})| < c|x|^{-1-\varepsilon}$ holds if $|x| > x_0$ for some positive c, x_0, and ε. Then the wave operators $\Omega_\pm(H, H_0)$ exist, are complete, and $\sigma_{sc}(H) = \emptyset$.
Hint: Proceed as in the proof of *Theorem* 2.1.

4. Check the asymptotic completeness for the pair H, H_0 where H is associated with the form (1.26) and the function $\rho(\cdot)-1$ has a compact support.

5. Find by mode matching the on-shell S-matrix for double waveguides of Sect. 1.5.2.
Hint: Modify the argument of Sect. 2.2—cf. [EKr99].

6. Suppose that the protrusion in Example 2.3.1a is of rectangular shape, $g(x) = \frac{1}{2}d_1 \in (\frac{1}{2}d, d)$ for $|x| \le \frac{1}{2}L$ and $g(x) = \frac{1}{2}d$ otherwise. Check that $-\Delta_D^\Omega$ has an embedded eigenvalue whenever $L > dd_1/\sqrt{d_1^2 - d^2}$. Show that to a given $n \in \mathbb{N}$ one can find a protruded strip Ω such that $-\Delta_D^\Omega$ has at least n embedded eigenvalues.
Hint: Use bracketing estimates.

7. Prove that the crossed strips of Example 2.3.1b support an embedded eigenvalue.
Hint: Use the symmetry of the problem and *Proposition* 1.2.3.

8. Prove relations (2.15) and (2.16).
Hint: For the latter use the momentum representation.
9. The conclusions of Sect. 2.3 can be modified to the case of a potential confinement, i.e. for the operator $H_\lambda := -\Delta + V(x) + W(y) + \lambda U(\vec{x})$ on $L^2(\mathbb{R}^2)$, where U, V are similar as before and W satisfies, e.g., the inequality $W(y) \geq cy^2$ for some $c > 0$.
10. Prove *Theorem* 2.5.
Hint: To estimate the imaginary part of $\epsilon_2^{(j,n)}(d)$ use the analytic continuation of the group of shifts in the longitudinal variable—cf. [DEŠ95].

http://www.springer.com/978-3-319-18575-0

Quantum Waveguides
Exner, P.; Kovařík, H.
2015, XXII, 382 p. 9 illus., 3 illus. in color., Hardcover
ISBN: 978-3-319-18575-0