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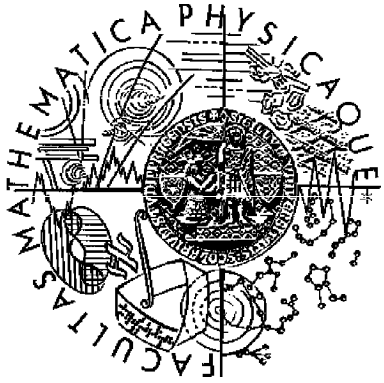

Spectral Properties of Straight Quantum Waveguides with a Parallel Semitransparent Barrier

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* * *

I declare that I completed this diploma programme myself and I used only the aforementioned literature.

* * *

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Chapter I

Introduction

I.1 Quantum Waveguides

Recent developments in semiconductor physics together with rapid progress in various fabrication techniques make possible to produce numerous tiny structures of a high pure crystalline matter. Let us mention some of them: *thin films* produced on an insulating surface by epitaxial techniques, *sandwiches* obtained by combining films of different semiconductor materials, sandwiches with variating layer thickness (*heterostructures*) and *quantum wires* obtained from semiconductor films by suitable masking and ion bombardment. By the last mentioned method one can create on the substrate various graphs and similarly one can produce many-probe *junctions* .

I.1.1 Basic Properties

Since such structures are large enough to be shaped by the experimentalist and at the same time so small that quantum effects are manifested on them, one often uses the term *mesoscopic physics* for experiments with them. As an experimental achievement made in this field, recall the manifestation of Aharonov-Bohm effect (*cf.* [1]) in heterostructures. Other experiments reveal a dependence of their conductivity properties on their form, on bendings or varying cross sections. For more details and a guide to physical literature see [11].

Let us summarize characteristic properties of the microstructures:

(a) small size (typically from tens to hundrends of nm),

(b) high purity (the particle mean free path can be a few μm or even larger),

(c) crystallic structure,

(d) the particle wavefunctions are usually suppressed at the boundaries between different semiconductor materials.

In fact, such a mesoscopic structure is still a complicated many-body system with a Hamiltonian describing its interaction with the lattice atoms including possible impurities. The mentioned properties allow us, however, to adopt several fundamentally simplifying assumptions.

I.1.2 Quantum Waveguides

It is obvious from (a) and (b) that the mean free path is typically two or three orders of magnitude greater than the size of the structure; hence the particle motion can be assumed in a resonable approximation as *ballistic*, *i.e.*, undisturbed by the scattering on impurities. Experimentalists are able to verify it by measuring interference effects which are excluded under other circumstances.

The most important simplification comes from the property (c). It is well known that a particle in a crystallic lattice moves as *free* with some effective mass m^*; from the mathematical point of view it follows from spectral properties of Schrödiger operators with periodic potentials (*cf.* [32], Sec. XIII.16.). The effective mass changes, of course, along the spectrum but one can regard it as a constant when we restrict our attention to the physically interesting part of the valence band. Next we recall that its value may differ substantially from the true particle mass (*cf.* Tab. 8.2 in [26]); for instance, one has $m^* = 0.07\, m_e$ for electron in GaAs which is the most common semiconductor material used in mesoscopic devices.

In combination with (d) we see that the particle motion inside the microstructure can be modelled as a free (spinless) particle living in the corresponding spatial region with the *Dirichlet condition* on its boundary.

If we denote the configuration space by Ω we may identify the particle Hamiltonian with the Dirichlet Laplacian (*cf.* [32], Sec. XIII.15), $H = -\Delta_D^\Omega$. This includes setting $\hbar^2/2m^\star = 1$ which we usually do if the values of the constants are not important. An interaction term must be added only if the whole structure is placed into an external field. In view of the natural analogy to the classical physics it is used to speak about the microstructures as *quantum waveguides*.

Introducing such a notation, one is naturally compelled to ask about the relations to the classical theory of acoustic and electromagnetic waveguides (for references, see the physical literature cited in [11]). The basic equations in the two cases, *i.e.*, the Schrödinger and wave equation are, of course, different but as far as one is concerned with the stationary problems only, both of them reduce to the Helmholz equation in the appropriate spatial region. The difference is then in the physical meaning of the spectral parameter, and also in the boundary conditions which are Neumann for the acoustic and TE-mode of the electromagnetic waveguides (in the quantum case, one can encounter the Neumann conditions when considering ballistic motion of electrons in metallic microstructures) while TM-modes correspond to Dirichlet boundary conditions.

This means that some results of the classical theory can be easily adapted to the quantum case. On the other hand, quantum mechanics and the classical theory

of waves use rather different mathematical methods so a mutual inspiration could be useful on both sides. For instance, using methods developed in the Schrödinger operator theory the authors of [17] demonstrate the existence of square integrable solutions (*i.e.* trapping modes) of the wave equation inside a curved electromagnetic waveguide with perfectly conducting walls.

I.1.3 Curved and Twisted Waveguides

In quantum waveguides there are effects which have no counterpart in classical situation. For instance, curved tubes have attracted a great attention since the authors of [16] proved the existence of at least one bound state for a particle living on a smooth curved planar strip of a constant width provided it is thin enough and its curvature decays sufficiently rapidly. The Birman-Schwinger technique in combination with the *minimax principle* was used there to obtain a lower bound on the critical width.

This result is very surprising since such regions have no closed classical trajectories with the exception of an obvious zero-measure set. Roughly speaking, there is nothing to prevent a classical particle from moving down the tube. In these two-dimensional systems, bound states do not arise from the "traditional" picture, where a binding potential creates classically allowed and forbidden regions. Here the boundary conditions give an effective confining potential which produce a minimum energy for continuum solutions. The curvature-induced bound states provide at the same time a warning example showing that an intuition based on semiclassical concepts may fail when dealing with quantum systems. As an analogous case we recall that low-dimensional Schrödinger operators have bound states for an arbitrarily small coupling constant as long as the potential is not repulsive in the mean and decays sufficiently fast at infinity.

The critical thickness is further studied in [10] and the decay assumption has been later substantially weakened in [14].

Another considerable progress was achieved in [23] where a suitably chosen trial function was used to demonstrate that all such strips possess at least one bound state, except for the strip which is straight everywhere. The proof does not require the tube to be in any sense narrow provided the curvature has compact support, or at least vanishes asymptotically.

The authors of [13] then applied the Goldstone's and Jaffe's variational proof also for the hollow tube threaded by an Aharonov-Bohm flux line and showed that the system has a bound state, unless the tube is perfectly straight.

However, one problem remained open: Into the postulates of all this work the condition had to be included that the boundary of the quantum waveguide has to be twice differentiable. The bound state in an L-shaped quantum waveguide determined explicitly in [19], however, suggested that this last condition is of purely technical nature. The computed bound-state energy has been verified experimentally in a flat electromagnetic waveguide in [8]. Another example of this type is a *bent pipe* discussed in [3] and [9].

An essential weakening of the regularity assumption was achieved in [33]. The argument given there does not require the curvature to be differentiable in order to prove the existence of bound states.

The paper [11] was devoted to a review and a further development of ideas formulated in the above mentioned papers. Moreover, a three-dimensional quantum waveguide is discussed there and using a trick known from Schrödinger operator theory (*cf.* [27]) an upper bound to the number of bound states in sufficiently thin tubes is derived too.

In [30] there is the specific case where the curved region is an arc of a circle numerically studied. The authors introduce a numerical method which permits high accuracy at high curvature and explore the dependence of these solutions on the curvature of the tube and angle of the bend.

Scattering problem of the bent tubes is studied in [12] and numerically in [30].

I.1.4 Other Geometries

There are other geometries provided analogous interesting quantum behaviour. For instance, a *cross* is in [3] handled with the same technique as the mentioned *bent pipes*.

The same variational proof of [23] demonstrates existence of a bound state in a straight Dirichlet strip with an arbitrarily small protrusion. An alternative proof of this result has been given in [7]; these authors also derived an asymptotic formula for the eigenvalue in terms of the protrusion volume.

Another kind of a waveguide is investigated in [20]: a pair of parallel straight strips coupled laterally through a window. This system is much like the one we shall study (it can be regarded as a limit case). The variational proof is performed there in order to demonstrate the existence of a bound state for any window width. Using the mode-matching method, the bound state and scattering problems are then discussed in more details.

A common feature observed in all mentioned geometries is the occurence of bound states with eigenvalues below the essential spectrum, which appear if the originally straight strip or layer is deformed, respectively a window between two of them is opened in a finite region; the eigenvalues depend continously on the deformation parameter.

In conclusion of the section we would like to mention of a randomly dented or bulged planar strip investigated in [29]. For this random quantum waveguide model, dense point spectrum with exponentially localized eigenfunctions near its fluctuation boundary at the bottom of the spectrum is established.

I.2 The Scope of Our Work

As was already mentioned above the geometry of the system we are going to study is similar to that of [20]. We consider the two infinite halfstrips but they are now

separated parallelly by a semitransparent barrier (the system is described more precisely in Section II.1).

The motivation for this problem is the following. While physically closely related, the two systems differ mathematically. In the case of a semitransparent boundary, the perturbed and unperturbed Hamiltonians have the same form domain. This makes it possible to employ other mathematical methods; in the first place the Birman-Schwinger technique to analyze the discrete spectrum.

I.2.1 δ-Interaction

The easiest way how to realize the partition is to suppose that it is supported by the common line only. Since the line is a set of Lebesgue measure zero, the notion of a δ-shaped potential along the line arises naturally as a model for the barrier.

Physical Motivation

For an obvious physical motivation one can figure a real waveguide with the partition which is supported on a very small range comparing to the other characteristic lenghths of the system, for instance, to the wavelength of the particle and the transverse proportions of the parallel strips.

On the other hand, the fact that the barrier support is "small" makes the model explicitly solvable.

Mathematical Handling

If the function α gives the shape of the barrier we could identify the Hamiltonian of our system with the formal expression $-\Delta + \alpha(x)\delta(y)$ (see Figure II.1 for specification of the coordinate system) used in the physics literature.

There are several equivalent ways of introducing the quantum Hamiltonian describing a δ-interaction in one dimension (our case, indeed) in a mathematically rigorous method as a self-adjoint extension of a suitable operator. We define it by means of the boundary conditions described in [2] (see (2.1)). For references to alternative definitions by scaling limits of short range potentials or by quadratic forms, see the literature cited there or in [6].

Resolvent

In Chapter III we modify the procedure performed in [6] for the Dirichlet Laplacian relative to $\mathbb{R}^d$ and derive the explicit expression for the resolvent of our Hamiltonian. The result is simplified and then modified to the case when the *effective coupling "constant"*, $\alpha - \alpha_0$, decays to zero at large distances. The resulting formula is useful for Birman-Schwinger analysis of the discrete spectrum subsequently made in Section IV.2.

I.2.2 Bound States and Scattering

Chapters IV and V are aimed at the investigation of the existence of the discrete spectrum and its dependence on various parameters.

Bound States

In Section IV.1 we exhibit the variational proof based on the idea of [23] to prove the existence of at least one isolated eigenvalue below threshold of the essential spectrum, provided the *effective coupling "constant"* is not repulsive in the mean and decays sufficiently fast at infinity.

In the next Section IV.2 we focus on the "adiabatic" limit when the perturbation of α_0 is small in the supremum norm. Using the Birman-Schwinger method well known from the theory of Schrödinger operators (*cf.*, *e.g.*, [34]) we find the perturbative expansion for the ground-state energy.

In Section IV.3 we find an analogous expansion in the case that the perturbation is small in the L^1-norm.

The numerical solution of the Schrödinger equation (Chapter V) is necessary in order to learn more about the dependence of the energies on the system's parameters. In particular, we shall investigate how the first eigenvalue emerges from the continuum.

Scattering

The scattering problem is handled only numerically in this thesis: the S-matrix and conductivity has been evaluated for a "rectangular-well" α by mode-matching.

An alternative is to modify the method of [12] to find – with help of the *complex scaling* (*cf.* [32], Sec. XIII.10) – a perturbative expansion for the resonances in the weakly coupled case. Using the *complex scaling* we could also find the resonances numerically. However, we did not manage to work out the complex scaling approach enough to include it into the thesis.

I.2.3 An Analogous Geometry

In Chapter VI we conclude the thesis by an example of a similar geometry (δ-interaction is supported by a line). We consider a cylindrical strip with a semi-transparent barrier placed parallelly to the cylinder axis.

However, we make the problem more complicated assuming that the cylinder is placed into a homogenous magnetic field (with the potential A), again parallel to the axis. This leads to interesting effects. The system is not sensitive to changes of the magnetic field corresponding to an integer multiple of the flux quantum. On the other hand, the "fractional" part "acts against" the attractive *effective potential*, $\alpha - \alpha_0$. As a consequence, we have no bound state for certain values of α_0 and A.

I.2.4 Some Open Problems

There are, of course, many other directions in which the above mentioned results can be extended.

For instance, if we were able to solve numerically the integral equation (4.7) we could compute the Hamiltonian's spectrum directly.

An open problem is also to find the way in which the other eigenvalues emerge from the continuum, *i.e.*, the problem of the "coupling-constant thresholds". (A similar problem was analyzed in [28] for the case of Schrödinger operators where a substantial dependence of the dimension was found.)

An entirely new class of effects opens when we replace the assumptions about the decay of the *coupling function* by a periodicity hypothesis or consider its random behaviour.

Chapter II

Preliminaries

II.1 Description of the Problem

The system we are going to study is sketched on Figure II.1. We consider a Schrödinger particle whose motion is confined to an infinite double waveguide consists of parallel strips of widths d_1, d_2, respectively, with the Dirichlet boundary conditions on one side and separated mutually by a δ-barrier. The coordinate system is chosen so that the x-axis merges with the barrier.

Denote $\mathcal{O} := \mathcal{O}_2 \cup \mathcal{O}_1 = (-d_2, 0) \cup (0, d_1)$ and $\Omega := \mathbb{R} \times \mathcal{O}$. Putting $\hbar^2/2m = 1$, we may identify the particle Hamiltonian H_α with the Laplace operator with the domain:

$$D(H_\alpha) := \left\{ \psi \in W_2^2(\Omega) |\ \forall x \in \mathbb{R} : \begin{array}{l} \psi(x, -d_2) = \psi(x, d_1) = 0 \\ \psi(x, 0+) = \psi(x, 0-) =: \psi(x, 0) \\ \psi_y(x, 0+) - \psi_y(x, 0-) = \alpha(x)\psi(x, 0) \end{array} \right\}. \quad (2.1)$$

The δ-interaction is in this way given by the standard boundary conditions described in [2], Chap.I.3. The piecewise continuous function $\alpha : \mathbb{R} \to \mathbb{R}$ gives the shape of the barrier and represents the x-dependent *coupling "constant"* of the interaction.

Remark II.1 For the sake of simplicity we exclude here the possibility $\alpha(x) = \infty$, *i.e.*, that a part of the barrier is represented by the Dirichlet boundary condition. This would make more complicated dealing with the form domain of the Hamiltonian.

The associated quadratic form is obtained by a simple integration of the Schrödinger equation by parts:

$$\begin{aligned} q_\alpha[\psi] &:= \int_{\mathbb{R}\times\bar{\mathcal{O}}} |\nabla\psi|^2(x, y)dxdy + \int_{\mathbb{R}} \alpha(x)|\psi(x, 0)|^2 dx \quad (2.2) \\ D(q_\alpha) &:= \{\psi \in W_2^1(\mathbb{R} \times (-d_2, d_1)) \mid \forall x \in \mathbb{R} : \psi(x, -d_2) = \psi(x, d_1) = 0\}. \end{aligned}$$

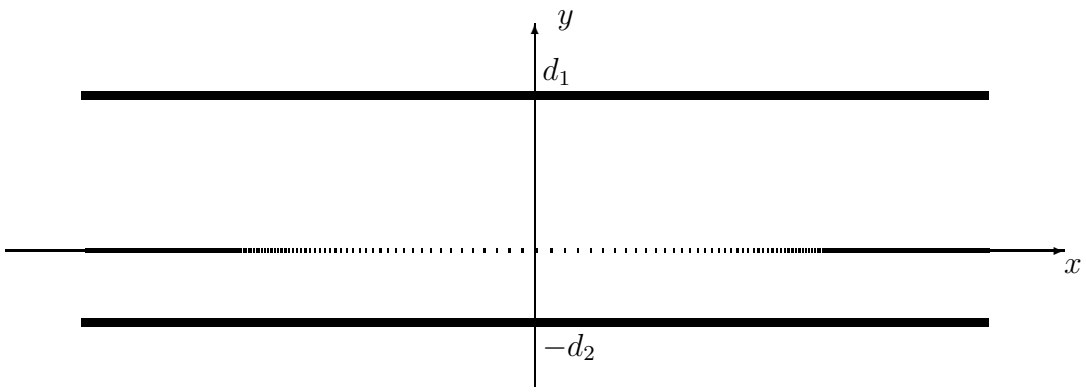

Figure II.1: Double waveguide with a δ-barrier

Hereafter we shall use the following notation:

$$\begin{aligned} d &:= \max\{d_1, d_2\} \\ D &:= d_1 + d_2 \\ \nu &:= \frac{\min\{d_1, d_2\}}{\max\{d_1, d_2\}}. \end{aligned} \tag{2.3}$$

Without loss of generality we may assume that $d_2 \leq d_1 = d$.

II.2 The Unperturbed System

If $\alpha(x) = \alpha$ is a constant function, we can solve the Schrödinger equation by separation of variables. To get the transverse eigenfunctions we have to match the solutions:

$$C_2 \sin k(y + d_2),\ C_1 \sin k(y - d_1).$$

If kd_1, kd_2 are not multiples of π the matching yields the condition to eigenvalues of the transverse operator

$$-\alpha = k(\cot kd_1 + \cot kd_2). \tag{2.4}$$

Remarks II.2 1. If d_1, d_2 are rationally related, *i.e.*, $\exists\, p, q \in \mathbb{N} \setminus \{0\}$ *relatively prime*: $\frac{d_1}{d_2} = \frac{p}{q}$, the solutions can be matched also with $k = \frac{\pi np}{d_1} = \frac{\pi nq}{d_2}, n \in \mathbb{N}\setminus\{0\}$. But such wave functions are zero at $y = 0$, and therefore independent of α. In this sense they represent a trivial part of the problem. A prime example is the symmetric waveguide pair, $d_1 = d_2$, where this concerns every solution antisymmetric w.r.t. $y{=}0$.

It is convenient to concentrate on the nontrivial part of the problem only. If $\nu \equiv \frac{d_2}{d_1} = \frac{p}{q}$, we denote by $\mathcal{G}_\nu$ the subspace in $L^2(-d_2, d_1)$ spanned by the above described solutions. Putting $\mathcal{H}_\nu := L^2(\mathbb{R}) \otimes \mathcal{G}_\nu^\perp$, we can restrict our attention to the

redefined operator $H_\alpha := H_\alpha \restriction \mathcal{H}_\nu$. The trivial part is clearly absent if ν is irrational. This restriction becomes essential in Chapter IV when one needs $\chi_1(0) \neq 0$.
2. For α large enough negative, $\alpha < \alpha_m := -(d_1^{-1} + d_2^{-1})$, there is a negative eigenvalue of the transverse operator given by $-\kappa^2$ with

$$-\alpha = \kappa(\coth \kappa d_1 + \coth \kappa d_2). \tag{2.5}$$

From the spectral condition (2.4) we get the increasing sequence of eigenvalues of (the nontrivial part of) the transverse operator; we denote it by $\{\nu_n(\alpha)\}_{n=1}^\infty$. The corresponding eigenfunctions will be:

$$\chi_n(y;\alpha) = \begin{cases} N_n \sin\sqrt{\nu_n} d_1 \sin\sqrt{\nu_n}(y+d_2) & \text{if} \quad y \in \mathcal{O}_2 \\ -N_n \sin\sqrt{\nu_n} d_2 \sin\sqrt{\nu_n}(y-d_1) & \text{if} \quad y \in \mathcal{O}_1. \end{cases} \tag{2.6}$$

N_n denotes the normalization factor chosen in such a way that χ_n would be a unit vector in $L^2(-d_2, d_1)$

$$N_n^2 = \frac{2\sqrt{\nu_n}}{\sqrt{\nu_n} d_1 \sin^2\sqrt{\nu_n} d_2 + \sqrt{\nu_n} d_2 \sin^2\sqrt{\nu_n} d_1 - \sin\sqrt{\nu_n} d_1 \sin\sqrt{\nu_n} d_2 \sin\sqrt{\nu_n} D} \tag{2.7}$$

Remark II.3 The eigenfunction corresponding to the solution of (2.5) can be formally obtained by the simple replacement $\sqrt{\nu_n} \mapsto -i\kappa$ in (2.6).

The extreme case, $\alpha = \alpha_m$, corresponds to a zero eigenvalue with the eigenfunction given by

$$\chi_1(y;\alpha_m) = \begin{cases} \frac{\sqrt{3}}{d_2\sqrt{D}}\,(y+d_2) & \text{if} \quad y \in \mathcal{O}_2 \\ \\ -\frac{\sqrt{3}}{d_1\sqrt{D}}\,(y-d_1) & \text{if} \quad y \in \mathcal{O}_1. \end{cases} \tag{2.8}$$

(We can get this result by means of the limit process $\sqrt{\nu_1} \to 0$ in (2.6) as well.)

Since the variables can be separated in the case of a constant α, the Green's function can be written down explicitly:

$$\begin{aligned} G_\alpha(x,y,x',y';k) &= \sum_{n=1}^\infty \frac{i}{2k_n} e^{ik_n|x-x'|} \chi_n(y;\alpha)\bar{\chi}_n(y';\alpha)\ ; \\ k_n &:= \sqrt{k^2 - \nu_n(\alpha)}. \end{aligned} \tag{2.9}$$

In the following we will use properties of the eigenvalues of the transverse operator which are collected below:

Proposition II.1

1. $\forall n \in \mathbb{N}\setminus\{0,1\}$:

$$\frac{\pi}{2d}(n-1) \leq \frac{\pi}{d} m_{n-1} < \sqrt{\nu_n} < \frac{\pi}{d} m_n \leq \frac{\pi}{d} n\,, \tag{2.10}$$

where the auxiliary sequence $\{m_i\}_{i=0}^\infty$ *arises from the arrangement of the elements of the sets* $\mathbb{N}, \nu^{-1}\mathbb{N}$ *into an increasing sequence.*

2. The function $\nu_n = \nu_n(\alpha)$ is strictly increasing and continuous for all $n \in \mathbb{N}\backslash\{0\}$.

PROOF: **1.** The inner inequalities follow from the analysis of the spectral condition (2.4). Putting

$$\begin{aligned} f(k) &:= -k(\cot kd + \cot k\nu d) \\ D(f) &:= \frac{\pi}{d} \bigcup_{n=2}^{\infty} (m_{n-1}, m_n), \end{aligned}$$

one can find roots of the equation (2.4) as the points where the function f is equal to α. The function f is discontinuous at the points $\frac{\pi}{d} m_n$. Between them it continuously increases and its range is all $\mathbb{R}$. Thus, the function f will be equal to α just once between the points of discontinuity.

The upper estimate on the elements of $\{m_i\}$ is clear from their definition. To clear up the lower, it is enough to realize that $\forall i \in \mathbb{N} : m_i \geq \tilde{m}_i$, where $\{\tilde{m}_i\}$ corresponds to some $\tilde{\nu} > \nu$. If $1 - \tilde{\nu}$ is small, the lower part of the sequence has a switching pattern $\tilde{m}_i = 0, 1, \tilde{\nu}^{-1}, 2, 2\tilde{\nu}^{-1}, 3, 3\tilde{\nu}^{-1}, \ldots$. Choosing $1 - \tilde{\nu}$ small enough, this part of $\{\tilde{m}_i\}$ can be made arbitrarily long and one can alternatively write for it

$$\tilde{m}_i = \begin{cases} \frac{i+1}{2} & \text{if } \ i \text{ is } \textit{odd} \\ \\ \frac{i}{2}\tilde{\nu}^{-1} & \text{if } \ i \text{ is } \textit{even} \end{cases}$$

and observe that $\frac{i+1}{2} > \frac{i}{2}$, $\frac{i}{2}\tilde{\nu}^{-1} \geq \frac{i}{2}$.

2. The second assertion follows by the implicit-function theorem (*cf.* [24], Kap. XIV.§1, for functions of two variables or [25], Kap. VIII.§1, for the general case). For $n \in \mathbb{N}\backslash\{0, 1\}$ we define

$$\begin{aligned} F(\alpha, k) &:= \alpha + k(\cot kd + \cot k\nu d) \\ D(F) &:= \mathbb{R} \times \frac{\pi}{d}(m_{n-1}, m_n). \end{aligned}$$

If k and α satisfy the spectral condition (2.4), $F(\alpha, k) = 0$ and

$$\begin{aligned} \frac{\partial F}{\partial \alpha} &= 1 \\ \frac{\partial F}{\partial k} &= \frac{\sin kd_1 \, \sin kd_2 \, \sin kD - k(d_1 \sin^2 kd_2 + d_2 \sin^2 kd_1)}{\sin^2 kd \, \sin^2 k\nu d} \equiv -2k\chi_n(0)^{-2} < 0\,, \end{aligned}$$

where χ_n is the eigenfunction corresponding to k^2. Thus, the function F is smooth on its domain, and since its partial derivative w.r.t. k is not equal to zero, $k = k(\alpha)$ is by the implicit-function theorem smooth too.

The monotonous behaviour of $k(\alpha)$ is then clear from the explicit expression of its first derivative

$$\frac{dk}{d\alpha} = -\frac{\frac{\partial F}{\partial \alpha}}{\frac{\partial F}{\partial k}} > 0. \tag{2.11}$$

The lowest transverse eigenvalue is determined by the different spectral conditions (2.4), (2.5). In particular, one has

$$\nu_1(\alpha) = \begin{cases} k^2 & \text{if} \quad \alpha > \alpha_m \\ 0 & \text{if} \quad \alpha = \alpha_m \\ -k^2 & \text{if} \quad \alpha < \alpha_m \end{cases} \tag{2.12}$$

where k is determined by the equation $F(\alpha, k) = 0$ with

$$F(\alpha, k) := \begin{cases} \alpha + k(\cot kd_1 + \cot kd_2) & \text{for } k \in \frac{\pi}{d}(0,1) \quad \text{if} \quad \alpha > \alpha_m \\ \alpha + k(\coth kd_1 + \coth kd_2) & \text{for } k \in (0,\infty) \quad \text{if} \quad \alpha < \alpha_m \,. \end{cases}$$

As before one can find that

$$\frac{\partial F}{\partial \alpha} = 1 \qquad \text{and} \qquad \frac{\partial F}{\partial k} = \begin{cases} -2k\chi_1(0)^{-2} < 0 & \text{if} \quad \alpha > \alpha_m \\ 2k\chi_1(0)^{-2} > 0 & \text{if} \quad \alpha < \alpha_m \,. \end{cases}$$

Comparing these results with (2.12) the proof is then completed by means of the implicit-function theorem and the fact that

$$\lim_{\substack{k\to 0+ \\ \alpha\to\alpha_m\pm}} F(\alpha, k) = 0 \,. \quad \blacksquare$$

Remark II.4 If ν is rational, $\mathbb{N}, \nu^{-1}\mathbb{N}$ will not be disjoint sets and we ought to arrange the elements of the sets $\mathbb{N}, \nu^{-1}\mathbb{N} \setminus \mathbb{N}$ instead, which bears on the restriction on $\mathcal{H}_\nu$ discussed in Remarks II.2 1.

If we denote by $\{a_i\}_{i=1}^{\infty}$ the increasing sequence of the elements of $\nu^{-1}\mathbb{N} \setminus \mathbb{N}$, we have:

$$m_0 = 0, \ m_1 = 1, \ m_2 = \min\{2, a_1\}, \ \textit{etc.}$$

Chapter III

Singularly Supported Interaction on a Subset of $\mathbb{R}^d$

We want to modify the consideration of [6] to the situation where $-\Delta$ is replaced by the Dirichlet Laplacian relative to a subset $\Omega \subset \mathbb{R}^d$; for the beginning we suppose only that Ω is open.

III.1 General Construction

Let m be a positive Radon measure on Ω, *i.e.*, the measure with the following properties (in fact, it is the abstraction of Lebesgue's (outer) measure for general topological spaces; *cf.* [31], Def. 2.3.9):

1. open sets are m-measurable
2. every compact set has a finite measure
3. $\forall A \subset \Omega$:
$$m(A) = \inf\{m(G) \,|\, G \supset A, G \text{ open}\}$$
4. $\forall B \in \mathcal{B}$ (the Borel σ-algebra):
$$m(B) = \sup\{m(C) \,|\, C \subset A, C \text{ compact and closed}\}.$$

Furthermore, consider a Borel measurable function $\alpha : \mathbb{R} \to \mathbb{R}$ such that

$$\int_\Omega |\psi(x)|^2 \left(1 + \alpha(x)^2\right) dm(x) \leq a \int_\Omega |\nabla\psi(x)|^2 dx + b \int_\Omega |\psi(x)|^2 dx \qquad (3.1)$$

for all $\psi \in C_0^\infty(\Omega)$ and some $a < 1$ and b. We are interested mainly in situation when m is a δ-measure but in general the regular case, $dm(x) = |V(x)|dx$, is also included.

By definition, $C_0^\infty(\Omega)$ is dense in the local Sobolev space $W_2^1(\Omega)$ (*cf.* [32], Sec. XIII.14), so there is a unique bounded linear operator

$$I_m : W_2^1(\Omega) \to L^2(m) := L^2(\Omega, dm)$$

such that

$$\forall \psi \in C_0^\infty(\Omega) : \ I_m \psi = \psi.$$

Remark III.1 The last relation means in fact $(I_m\psi)(x) = \psi(x)$ for $x \in \operatorname{supp} m$. We abuse notation employing the symbol ψ for

1. a continuous function ψ
2. the corresponding $L^2(\Omega)$ equivalent class
3. the corresponding $L^2(\Omega, dm)$ equivalent class.

By density, the inequality (3.1) holds for all $\psi \in W_2^1(\Omega)$ provided ψ is replaced by $I_m\psi$ on the left-hand-side.

Next we define the form

$$\begin{aligned} \mathcal{E}_{\alpha m}(\psi, \varphi) &:= \int_\Omega \overline{\nabla\psi(x)}.\nabla\varphi(x)dx + \int_\Omega \alpha(x) I_m\bar{\psi}(x) I_m\varphi(x)dx \qquad (3.2) \\ D(\mathcal{E}_{\alpha m}) &:= W_2^1(\Omega) \end{aligned}$$

It is well known (*cf.* [32], Sec. XIII.14) that the "free" form $\mathcal{E}_0$ is positive and closed on $L^2(\Omega)$; it gives rise to the Dirichlet Laplacian $-\Delta_D^\Omega$. By Kato–Lax–Lions–Milgram–Nelson theorem (*cf.* [32], Thm. X.17) and the extended version of inequality (3.1), $\mathcal{E}_{\alpha m}$ is lower semibounded and closed on $L^2(\Omega)$, and $C_0^\infty(\Omega)$ is a core for it. By the second representation theorem (*cf.* [5], Věta 7.5.8), there is a unique self-adjoint operator $H_{\alpha m}$ associated with $\mathcal{E}_{\alpha m}$.

Remarks III.2 1. The basic assumption (3.1) is satisfied, in particular, for measures m belonging to the generalized Kato class, *i.e.*

$$\begin{aligned} \lim_{\varepsilon\to 0+} \sup_{x\in\Omega} \int_{B(x,\varepsilon)\cap\Omega} \frac{dm(y)}{|x-y|^{d-2}} = 0 \qquad &\text{if} \quad d \geq 3 \\ \lim_{\varepsilon\to 0+} \sup_{x\in\Omega} \int_{B(x,\varepsilon)\cap\Omega} |\ln|x-y||\, dm(y) = 0 \qquad &\text{if} \quad d = 2 \\ \sup_{x\in\Omega} m([x, x+1]) < \infty \qquad &\text{if} \quad d = 1. \end{aligned}$$

($B(x,\varepsilon)$ denotes the ball with radius ε and center x.) In [6] one adopted the result by [35] by which (3.1) holds for such m and $\psi \in \mathcal{S}(\mathbb{R}^d)$ if $\Omega = \mathbb{R}^d$. The same is, *a fortiori*, true for $\psi \in C_0^\infty(\Omega)$ corresponding to an open $\Omega \subset \mathbb{R}^d$.

2. The δ-measure of our example belongs to the Kato class. It follows from Thm. 4.1 of [6], but one can check it also directly: We put $x = (x_1, x_2)$, $y = (y_1, y_2)$ and take $B(x,\varepsilon) \subset \Omega$; then

$$\begin{aligned} &\int_{B(x,\varepsilon)\cap\Omega} |\ln|x-y||\, dm(y) = \int_{|x-y|<\varepsilon} \left|\ln\sqrt{(x_1-y_1)^2 + x_2^2}\right| dy_1 \\ &\leq \int_{-\varepsilon}^{\varepsilon} \left|\ln\sqrt{u_1^2 + x_2^2}\right| du_1 \leq 2\int_0^\varepsilon |\ln u| du = 2\varepsilon(1 - \ln\varepsilon) \to 0 \end{aligned}$$

as $\varepsilon \to 0+$. The same is true for a δ-measure supported by a smooth planar curve.

Lemma 2.1 of [6] is abstract and we adopt it:

Lemma III.1 *Let $\mathcal{E}$ be a lower semibounded densely defined closed quadratic form on the complex Hilbert space $\mathcal{H}$ with inner product $(\cdot\,,\cdot)$, and let H be the unique self-adjoint operator on $\mathcal{H}$ associated with $\mathcal{E}$. Finally, let $R : \mathcal{H} \to D(\mathcal{E})$ be an arbitrary map and $z \in \mathbb{C}$. Then the following statements are equivalent.*

(i) $z \in \rho(H)$ *and* $(H - z)^{-1} = R$.
(ii) $\forall\, \psi \in \mathcal{H}, \varphi \in D(\mathcal{E})\ :\quad \mathcal{E}(R\psi, \varphi) = (zR\psi + \psi, \varphi)$.

Given $k \in \mathbb{C}, \operatorname{Im} k > 0$, we denote by $G_0(\cdot, \cdot; k)$ the free resolvent kernel corresponding to the Dirichlet Laplacian $-\Delta_D^\Omega$. The main difference with respect to [6] is that for $\Omega \neq \mathbb{R}^d$ the kernel depends on both arguments, not only on their difference.

Let μ, ν be positive Radon measures without a discrete component (*i.e.* $\forall a \in \Omega : \mu(a) = \nu(a) = 0$). We denote by $R^k_{\mu,\nu}$ the integral operator from $L^2(\mu) := L^2(\Omega, d\mu)$ to $L^2(\nu)$ with the kernel $G_0(\cdot, \cdot; k)$. In particular, we have

$$(R^k_{\mu,\nu}\psi)(x) = \int_\Omega G_0(x, y; k)\psi(y)d\mu(y) \tag{3.3}$$

for all $\psi \in D(R^k_{\mu,\nu}) \subset L^2(\mu)$. (Since we agreed to the mentioned abuse of notation, there is no ν in the definition; we compute the right-hand-side and interpret it as values of a function in $L^2(\nu)$.) We also denote

$$\mathbb{C}^+ := \{k \in \mathbb{C} \,|\, \operatorname{Im} k > 0\}.$$

Henceforth $(\cdot\,,\cdot)$ denotes the inner product on $L^2(\Omega)$.

Lemma III.2 *Let $k \in \mathbb{C}^+$ and $\psi \in L^2(m)$. Then $R^k_{m,dx}\psi \in W^1_2(\Omega)$ and*

$$\forall \varphi \in W^1_2(\Omega) :\qquad \mathcal{E}_0(R^k_{m,dx}\psi, \varphi) - (k^2 R^k_{m,dx}\psi, \varphi) = \int_\Omega \bar\psi(y)(I_m\varphi)(y)dm(y) \tag{3.4}$$

In particular, $R^k_{m,dx}$ is injective.

Proof: The injectivity follows from the equality in the above lemma and density of Ran I_m in $L^2(m)$.

(a) Assume first $k^2 < 0$, *i.e.*, k is purely imaginary. Then

$$\forall \psi, \varphi \in W^1_2(\Omega) :\quad \langle \psi, \varphi\rangle_k := \mathcal{E}_0(\psi, \varphi) - k^2(\psi, \varphi) \tag{3.5}$$

defines an inner product on $W^1_2(\Omega)$ and the corresponding norm is equivalent to the usual Sobolev norm ($k^2 = -1$). Take a fixed $\psi \in L^2(m)$. Using Schwarz inequality and the fact that I_m is bounded we infer

$$\begin{aligned}\left|\int_\Omega \bar\psi(y)(I_m\varphi)(y)dm(y)\right|^2 &\le \int_\Omega |\psi(y)|^2 dm(y) \int_\Omega |(I_m\varphi)(y)|^2 dm(y)\\ &\le c\,\langle\varphi, \varphi\rangle_k \qquad \forall \varphi \in W^1_2(\Omega)\end{aligned}$$

for some constant c depending on ψ. Hence the linear functional

$$\varphi \mapsto \int_\Omega \bar{\psi}(y)(I_m\varphi)(y)dm(y)$$

on the Hilbert space $(W_2^1(\Omega), \langle\cdot\,,\cdot\rangle_k)$ is bounded, and by Riesz's lemma, there is a unique $\psi_m^k \in W_2^1(\Omega)$ such that

$$\forall \varphi \in W_2^1(\Omega): \quad \left\langle \psi_m^k, \varphi \right\rangle_k = \int_\Omega \bar{\psi}(y)(I_m\varphi)(y)dm(y). \tag{3.6}$$

Hence it is sufficient to show that

$$\forall \psi \in L^2(\Omega): \quad (R_{m,dx}^k\psi)(x) \equiv \int_\Omega G_0(x,y;k)\psi(y)dm(y) = \psi_m^k(x) \qquad dx-\text{a.e.}$$

If $k^2 < 0$, the Green's function $G_0(x,y;k)$ is known to be positive for all $x, y \in \Omega, x \neq y$ (*cf.* [32], App. 1 to Sec. XIII.12). Moreover, for a non-compact Ω the kernel is dx-integrable (in fact, exponentially decaying) and

$$\forall\, y \in \Omega, \varphi \in C_0^\infty(\Omega): \quad \int_\Omega G_0(x,y;k)(-\Delta_D^\Omega - k^2)\varphi(x)dx = \varphi(y).$$

(a1) Suppose now, in addition, that $\psi \in L^1(m) \cap L^2(m)$. Then

$$\int_\Omega |\psi(y)| \left| \int_\Omega G_0(y,x;k)(-\Delta_D^\Omega - k^2)\varphi(x)dx \right| dm(y) \leq c \int_\Omega |\psi(y)|dm(y)$$

is finite by assumption. By Fubini theorem,

$$\int_\Omega G_0(\cdot,y;k)|\psi(y)|dm(y) \in L^1(\Omega)$$

and

$$\begin{aligned}
&\int_\Omega \overline{\left(\int_\Omega G_0(x,y;k)\psi(y)dm(y)\right)}(-\Delta_D^\Omega - k^2)\varphi(x)\,dx \\
&\quad = \int_\Omega \bar{\psi}(y) \left(\int_\Omega G_0(y,x;k)(-\Delta_D^\Omega - k^2)\varphi(x)\,dx \right) dm(y) \\
&\quad = \int_\Omega \bar{\psi}(y)\varphi(y)\,dm(y) \qquad \forall \varphi \in C_0^\infty(\Omega).
\end{aligned}$$

(We have used here the fact that G_0 is real-valued for $k^2 < 0$.) By (3.6) and the second representation theorem, we have

$$\begin{aligned}
\int_\Omega \overline{\psi_m^k}(-\Delta_D^\Omega - k^2)\varphi(x)\,dx &= \left\langle \psi_m^k, \varphi \right\rangle_k \\
&= \int_\Omega \bar{\psi}(y)\varphi(y)\,dm(y) \qquad \forall \varphi \in C_0^\infty(\Omega)
\end{aligned}$$

Since $-\Delta_D^\Omega - k^2$ maps $C_0^\infty(\Omega)$ onto itself, it follows that

$$\psi_m^k = R_{m,dx}^k\psi \qquad dx-\text{a.e.}$$

(a2) For a nonnegative $\psi \in L^2(m)$ we use a standard approximation argument choosing an increasing sequence $\{\tilde\psi_n\}_{n=1}^\infty$ in this way:

$$\begin{aligned}
&\{\tilde\psi_n\} \in L^1(m) \cap L^2(m) \\
&0 \le \tilde\psi_1 \le \tilde\psi_2 \le \cdots \le \tilde\psi_n \le \cdots \quad m-\text{a.e.} \\
&\lim_{n\to\infty} \tilde\psi_n = \psi \quad m-\text{a.e.}
\end{aligned}$$

Then

$$\forall \varphi \in W_2^1(\Omega): \quad \left\langle R^k_{m,dx}\tilde\psi_n, \varphi \right\rangle_k = \int_\Omega \overline{\tilde\psi_n(y)} (I_m\varphi)(y)\, dm(y)$$

By the dominated convergence theorem, it follows that

$$\forall \varphi \in W_2^1(\Omega): \quad \left\langle R^k_{m,dx}\tilde\psi_n, \varphi \right\rangle_k \to \int_\Omega \bar\psi(y) (I_m\varphi)(y)\, dm(y) = \left\langle R^k_{m,dx}\psi, \varphi \right\rangle_k$$

as $n \to \infty$, *i.e.*, the sequence $\{R^k_{m,dx}\tilde\psi_n\}$ converges weakly to $R^k_{m,dx}\psi$ in the Hilbert space $(W_2^1(\Omega), \langle\cdot\,,\cdot\rangle_k)$. By the *diagonal trick* (*cf.* [32], Sec. I.5) we may thus assume (selecting a subsequence if necessary) that

$$R^k_{m,dx}\psi_n \to R^k_{m,dx}\psi \quad \text{as} \quad n \to \infty \tag{3.7}$$

strongly in $W_2^1(\Omega)$, where $\psi_n := \frac{1}{n}\sum_{j=1}^n \tilde\psi_j$. Since $G_0(\cdot,\cdot;k)$ is nonnegative and the sequence $\{\psi_n\}$ is nondecreasing again, the monotone convergence theorem implies

$$\forall x \in \Omega: \quad \int_\Omega G_0(x,y;k)\psi(y)\, dm(y) = \lim_{n\to\infty} (R^k_{m,dx}\psi_n)(x) \le \infty.$$

The relation (3.7) then gives

$$\int_\Omega G_0(\cdot,y;k)\psi(y)\, dm(y) = R^k_{m,dx}\psi \qquad dx-\text{a.e.}$$

By linearity, the validity of this result extends to all $\psi \in L^2(m)$.

(b) To establish the sought identity for an arbitrary $k \in \mathbb{C}^+$ we employ the first resolvent relation which gives

$$R^{\tilde k}_{m,dx} = R^k_{m,dx} + (\tilde k^2 - k^2) R^{\tilde k}_0 R^k_{m,dx},$$

where we have denoted $R^k_0 := R^k_{dx,dx}$. In combination with the preceeding Lemma III.1 it yields

$$\begin{aligned}
&\mathcal{E}_0(R^{\tilde k}_{m,dx}\psi, \varphi) - (\tilde k^2 R^{\tilde k}_{m,dx}\psi, \varphi) \\
&\quad = \mathcal{E}_0(R^k_{m,dx}\psi, \varphi) - (\tilde k^2 R^k_{m,dx}\psi, \varphi) \\
&\qquad + \mathcal{E}_0((\tilde k^2 - k^2) R^{\tilde k}_0 R^k_{m,dx}\psi, \varphi) - (\tilde k^2 (\tilde k^2 - k^2) R^{\tilde k}_0 R^k_{m,dx}\psi, \varphi) \\
&\quad = \mathcal{E}_0(R^k_{m,dx}\psi, \varphi) - (\tilde k^2 R^k_{m,dx}\psi, \varphi) + (\tilde k^2 (\tilde k^2 - k^2) R^{\tilde k}_0 R^k_{m,dx}\psi, \varphi)
\end{aligned}$$

$$+((\tilde{k}^2-k^2)R^k_{m,dx}\psi,\varphi)-(\tilde{k}^2(\tilde{k}^2-k^2)R^{\tilde{k}}_0R^k_{m,dx}\psi,\varphi)$$

$$=\mathcal{E}_0(R^k_{m,dx}\psi,\varphi)-(\tilde{k}^2R^k_{m,dx}\psi,\varphi)+((\tilde{k}^2-k^2)R^k_{m,dx}\psi,\varphi)$$

$$=\mathcal{E}_0(R^k_{m,dx}\psi,\varphi)-(k^2R^k_{m,dx}\psi,\varphi).\quad\blacksquare$$

The lemmas have several important consequences.

Corollary III.1 *Let $k\in\mathbb{C}^+$. Suppose that the operator $I+\alpha I_mR^k_{m,dx}$ is invertible on $L^2(m)$ and the operator*

$$R^k:=R^k_0-R^k_{m,dx}(I+\alpha I_mR^k_{m,dx})^{-1}\alpha I_mR^k_0$$

is defined everywhere in $L^2(\Omega)$. Then $k^2\in\rho(H_{\alpha m})$ and

$$(H_{\alpha m}-k^2)^{-1}=R^k.$$

PROOF: Take $\psi\in L^2(\Omega)$ and $\varphi\in W^1_2(\Omega)\equiv D(\mathcal{E}_{\alpha m})$. By assumption, the operator R^k is defined on $L^2(\Omega)$. The free resolvent maps $L^2(\Omega)$ into $W^1_2(\Omega)$; the same is true for the second term in view of the assumed invertibility and the preceding Lemma III.2. Thus $R^k\psi\in W^1_2(\Omega)$, and by Lemma III.1, we have to check that

$$\mathcal{E}_{\alpha m}(R^k\psi,\varphi)-(k^2R^k\psi,\varphi)=(\psi,\varphi)$$

for all ψ,φ from the indicated sets.

Dividing the left-hand-side into the "free" and "interaction" parts and denoting

$$\chi:=(I+\alpha I_mR^k_{m,dx})^{-1}\alpha I_mR^k_0\psi,$$

we can rewrite it as

$$\begin{aligned}&\mathcal{E}_0(R^k_0\psi,\varphi)-(k^2R^k_0\psi,\varphi)\\&-\mathcal{E}_0(R^k_{m,dx}\chi,\varphi)+(k^2R^k_{m,dx}\chi,\varphi)+\int_\Omega\alpha(x)(I_m\overline{R^k\psi})(x)(I_m\varphi)(x)\,dm(x)\end{aligned}$$

The first two terms equal (ψ,φ) by Lemma III.1, the other two are

$$-\int_\Omega\bar{\chi}(x)(I_m\varphi)(x)\,dm(x)$$

by Lemma III.2. Since the relation should hold for all $\varphi\in W^1_2(\Omega)$ we have therefore to check that

$$\forall\psi\in L^2(\Omega):\quad\alpha I_mR^k\psi=\chi$$

This follows from algebraic manipulations

$$\begin{aligned}\alpha I_mR^k\psi&=\alpha I_mR^k_0\psi-\alpha I_mR^k_{m,dx}\chi\\&=(I+\alpha I_mR^k_{m,dx}\psi)\underbrace{(I+\alpha I_mR^k_{m,dx}\psi)^{-1}\alpha I_mR^k_0\psi}_{\chi}-\alpha I_mR^k_{m,dx}\chi=\chi.\quad\blacksquare\end{aligned}$$

As usual the resolvent formula works for energies large enough negative.

Corollary III.2

$$\exists \kappa_0 > 0 \;\; \forall \kappa, \kappa_0 \leq \kappa < \infty : \quad \|\alpha I_m R^{i\kappa}_{m,dx}\| < 1$$

PROOF: In view of our basic assumption (3.1) and the boundedness of the operator I_m we can choose $a < 1$ and $0 < b < \infty$ so that

$$\begin{aligned} \forall \varphi \in W^1_2(\Omega) : \quad \int_\Omega |I_m \varphi(x)|^2 (1 + \alpha(x)^2)\, dm(x) &\leq a\mathcal{E}_0(\varphi,\varphi) + b(\varphi,\varphi) \\ &= a \left\langle \varphi, \varphi \right\rangle_{i\kappa_0} \end{aligned}$$

where $\kappa_0 := \sqrt{\frac{b}{a}}$ and $\langle \cdot\,, \cdot \rangle$ is defined as in the proof of Lemma III.2. We denote by S_κ the unit sphere in $(W^1_2(\Omega), \langle \cdot\,, \cdot \rangle_{i\kappa})$ and choose $\kappa \geq \kappa_0$ and $\psi \in L^2(m)$; then the above inequality gives

$$\begin{aligned} \int_\Omega \alpha(x)^2 |(I_m R^{i\kappa}_{m,dx}\psi)(x)|^2 dm(x) &\leq a \left\langle R^{i\kappa}_{m,dx}\psi, R^{i\kappa}_{m,dx}\psi \right\rangle_{i\kappa_0} \leq a \left\langle R^{i\kappa}_{m,dx}\psi, R^{i\kappa}_{m,dx}\psi \right\rangle_{i\kappa} \\ &= a \sup_{\varphi \in S_\kappa} \left| \left\langle R^{i\kappa}_{m,dx}\psi, \varphi \right\rangle_{i\kappa} \right|^2 . \end{aligned}$$

The last expression can be rewritten using Lemma III.2 as

$$\begin{aligned} a \sup_{\varphi \in S_\kappa} \left| \int_\Omega \bar{\psi}(y)(I_m\varphi)(y)\, dm(y) \right|^2 \quad a &\leq \int_\Omega |\psi(y)|^2 dm(y) \sup_{\varphi \in S_\kappa} \underbrace{\int_\Omega |(I_m\varphi)(y)|\, dm(y)}_{\leq a\langle \varphi,\varphi\rangle_{i\kappa}} \\ &\leq a^2 \int_\Omega |\psi(y)|^2 dm(y) \end{aligned}$$

where we have used Schwarz inequality and the assumption (3.1) again. Consequently, $\|\alpha I_m R^{i\kappa}_{m,dx}\| < a$ holds for all $\kappa \geq \kappa_0$. ∎

A part of the generalized Birman-Schwinger analysis we are constructing here is an expression for the number of eigenvalues of $H_{\alpha m}$.

Corollary III.3

$$\forall k \in \mathbb{C}^+ : \quad \dim \mathrm{Ker}(H_{\alpha m} - k^2) = \dim \mathrm{Ker}(I + \alpha I_m R^k_{m,dx})$$

PROOF: **(a)** Suppose that $\psi \in L^2(m)$ satisfies $\psi + \alpha I_m R^k_{m,dx}\psi = 0$. By Lemma III.2 we have

$$\begin{aligned} &\mathcal{E}_{\alpha m}(R^k_{m,dx}\psi, \varphi) - (k^2 R^k_{m,dx}\psi, \varphi) \\ &\quad = \int_\Omega \bar{\psi}(y)(I_m\varphi)(y)\, dm(y) + \int_\Omega \alpha(y)(I_m \overline{R^k_{m,dx}\psi})(y)(I_m\varphi)(y)\, dm(y) = 0 \end{aligned}$$

for all $\varphi \in W^1_2(\Omega) \equiv D(\mathcal{E}_{\alpha m})$. By the second representation theorem, it follows that $R^k_{m,dx}\psi \in D(H_{\alpha m})$ and $H_{\alpha m} R^k_{m,dx}\psi = k^2 R^k_{m,dx}\psi$. Since $R^k_{m,dx}$ is injective by Lemma III.2, we get

$$\dim \mathrm{Ker}(I + \alpha I_m R^k_{m,dx}) \leq \dim \mathrm{Ker}(H_{\alpha m} - k^2).$$

(b) On the other hand, let $\varphi \in D(H_{\alpha m})$ with $H_{\alpha m}\varphi = k^2\varphi$. In view of the above argument, it is sufficient to show that $\varphi = R^k_{m,dx}\psi$ for some $\psi \in L^2(m)$ such that $\psi + \alpha I_m R^k_{m,dx}\psi = 0$. We put $\psi := -\alpha I_m\varphi$; then by Lemma III.2, we have

$$\forall\chi \in W^1_2(\Omega): \quad \mathcal{E}_0(R^k_{m,dx}\psi,\chi) - (k^2 R^k_{m,dx}\psi,\chi) = -\int_\Omega \alpha(x)(I_m\bar\varphi)(x)(I_m\chi)(x)\,dm(x)$$

By the second representation theorem and the assumption $H_{\alpha m}\varphi = k^2\varphi$ we have $\mathcal{E}_{\alpha m}(\varphi,\chi) - (k^2\varphi,\chi) = 0$, so

$$\begin{aligned}\mathcal{E}_0(\varphi,\chi) - (k^2\varphi,\chi) &= \mathcal{E}_{\alpha m}(\varphi,\chi) - (k^2\varphi,\chi) - \int_\Omega \alpha(x)(I_m\bar\varphi)(x)(I_m\chi)(x)\,dm(x) \\ &= -\int_\Omega \alpha(x)(I_m\bar\varphi)(x)(I_m\chi)(x)\,dm(x) \qquad \forall\chi \in W^1_2(\Omega).\end{aligned}$$

Comparing the two expressions, we find $\varphi = R^k_{m,dx}\psi$, and therefore $\psi + \alpha I_m R^k_{m,dx}\psi = \psi + \alpha I_m\varphi = 0$. ∎

III.2 Birman-Schwinger Analysis in Our Case

To make the BS analysis more convenient, we want to prove another expression for the resolvent known to be valid for $\Omega = \mathbb{R}^d$ (*cf.* [6], Lemma 2.3). We do it for our case where $\Omega := \mathbb{R}\times(-d_2,d_1)$ and m is supported by the x-axis.

Lemma III.3 (i) $\forall k \in \mathbb{C}^+:\ I_m R^k_{m,dx} = R^k_{m,m}$ *and* $I_m R^k_0 = R^k_{dx,m}$
(ii) $I + \alpha R^{i\kappa}_{m,m}$ *has a bounded inverse on* $L^2(m)$ *for all* $\kappa > 0$ *large enough.*
(iii) *Suppose that* $I + \alpha R^k_{m,m}$ *is invertible and the operator*

$$R^k := R^k_0 - R^k_{m,dx}(I + \alpha R^k_{m,m})^{-1}\alpha R^k_{dx,m}$$

on $L^2(m)$ *is everywhere defined. Then* $k^2 \in \rho(H_{\alpha m})$ *and* $(H_{\alpha m} - k^2)^{-1} = R^k$.
(iv) $\forall k \in \mathbb{C}^+:\ \dim\mathrm{Ker}(H_{\alpha m} - k^2) = \dim\mathrm{Ker}(I + \alpha I_m R^k_{m,m})$.

Proof: Since the assertions (ii)–(iv) are easy consequences of (i) and the above corollaries, it is sufficient to check (i).

The Green's function for Ω in our case was calculated in [15]. In particular, we have

$$\begin{aligned}G_0(\vec x,\vec x';i\kappa) &= \frac{1}{D}\sum_{n=1}^\infty \frac{e^{-\kappa_n|x-x'|}}{\kappa_n}\sin\frac{\pi n}{D}(y+d_2)\sin\frac{\pi n}{D}(y'+d_2)\,; \\ \kappa_n &:= \sqrt{\kappa^2 + \left(\frac{\pi n}{D}\right)^2}\end{aligned}$$

for $\kappa > 0$, where $\vec x := (x,y)$. We know that $G_0(\vec x,\vec x';i\kappa) > 0$, smooth in each argument, exponentially decaying as $|x-x'|\to\infty$ and has a logarithmic singularity as $\vec x' \to \vec x$. As in [6], we need a smooth approximation to G_0. We employ the fact that

$$G_0(\vec x,\vec x';i\kappa) = -\frac{1}{2\pi}\ln|\vec x - \vec x'| + \Gamma(\vec x,\vec x')$$

where Γ is a C^∞ function which is zero at $y,y' = d_1,-d_2$. We take

- a C^∞ function $\xi : (0,\infty) \to [1,\infty)$ such that

$$\begin{aligned} & \xi(0) = 1 \\ \forall x > 0 : \quad & \xi'(x) > 0 \\ \forall x \geq 2 : \quad & \xi(x) = x \end{aligned}$$

- an increasing sequence $\{\eta_n\}_{n=1}^\infty \in C_0^\infty(\Omega)$ such that

$$\forall \vec{x} \in \Omega : \quad \lim_{n\to\infty} \eta_n(\vec{x}) = 1$$

and put

$$G_n(\vec{x},\vec{x}';i\kappa) := \left[-\frac{1}{2\pi} \ln \frac{\xi(n|\vec{x}-\vec{x}'|)}{n} + \Gamma(\vec{x},\vec{x}') \right] \eta_n(\vec{x}).$$

Clearly,

$$\begin{aligned} &\text{(i)} && G_n(\cdot,\vec{x};i\kappa) \in C_0^\infty(\Omega) \\ &\text{(ii)} && \forall \vec{x},\vec{x}' \in \Omega : \quad G_n(\vec{x},\vec{x}';i\kappa) \leq G_{n+1}(\vec{x},\vec{x}';i\kappa) \\ &\text{(iii)} && \exists c_1 > 0 \ \forall \vec{x},\vec{x}' \in \Omega, \vec{x} \neq \vec{x}' : \quad |\nabla_x G_n(\vec{x},\vec{x}';i\kappa)| \leq \frac{c_1}{|\vec{x}-\vec{x}'|} \\ &\text{(iv)} && \exists c_2, c_3 > 0 \ \forall \vec{x},\vec{x}' \in \Omega, |\vec{x}-\vec{x}'| \textit{ large enough} : \\ & && \qquad |G_n(\vec{x},\vec{x}';i\kappa)| + |\nabla_x G_n(\vec{x},\vec{x}';i\kappa)| \leq c_2 e^{-c_3|x-x'|} \end{aligned}$$

We use a common notation μ for m, dx. Take an arbitrary $\psi \in L^2(\mu)$ and $\varphi_n := R^{n,i\kappa}_{\mu,dx}\psi$, *i.e.*

$$\varphi_n = \int_\Omega G_n(\vec{x},\vec{x}';i\kappa)\psi(\vec{x})\, d\mu(\vec{x}').$$

Each $\varphi_n \in W_2^1(\Omega)$ by definition. Furthermore, by the construction of the regularized Green's function, we have also $\varphi_n \in C_0^\infty(\Omega)$. Next we have to estimate the Sobolev norm of φ_n. In view of (iii) we have

$$\begin{aligned} \int_\Omega \left| \nabla_x \int_\Omega G_n(\vec{x},\vec{x}';i\kappa)\psi(x')\, d\mu(x') \right|^2 dx &= \int_\Omega \left| \int_\Omega \nabla_x G_n(\vec{x},\vec{x}';i\kappa)\psi(x')\, d\mu(x') \right|^2 dx \\ &\leq \int_\Omega \left| \int_\Omega \frac{c_1}{|\vec{x}-\vec{x}'|}\psi(x')\, d\mu(x') \right|^2 dx \\ &\leq \int_{\mathbb{R}^2} \left| \int_{\mathbb{R}^2} \frac{c_1}{|\vec{x}-\vec{x}'|}\psi(x')\, d\mu(x') \right|^2 dx \end{aligned}$$

where ψ in the last expression means a trivial extension from Ω to $\mathbb{R}^2$. The integral was shown to be finite in the proof of Lemma 2.3 in [6]. As for the nonderivative part we notice that G_0 has a bound as a consequence of the fact that $R^{i\kappa}_{\mu,dx}\psi \in W_2^1(\Omega) \subset L^2(\Omega)$.

Summing the above considerations, we have demonstrated that $\{\varphi_n\}$ is a bounded sequence in the local Sobolev space $W_2^1(\Omega)$. Then we proceed as above:

we construct $\chi_n := \frac{1}{n}\sum_{j=1}^n \varphi_j$ and using the *diagonal trick* to show that (a subsequence of) $\{\chi_n\}$ converges strongly in $W_2^1(\Omega)$. By the property (ii) and monotone convergence theorem

$$\forall \vec{x} \in \Omega : \quad \lim_{n\to\infty} \chi_n(\vec{x}) = (R^{i\kappa}_{\mu,dx}\psi)(\vec{x}),$$

so $\chi_n \to R^{i\kappa}_{\mu,dx}\psi$ in $W_2^1(\Omega)$ as $n \to \infty$. From the definition of I_m,

$$I_m\chi_n \to I_m R^{i\kappa}_{\mu,dx}\psi \quad \text{in } L^2(m)$$

as $n \to \infty$. Since $I_m\chi_n \in C_0^\infty(\Omega)$ by construction, we have $I_m\chi_n = \chi_n \quad m-$a.e., and therefore

$$I_m R^{i\kappa}_{\mu,dx}\psi = R^{i\kappa}_{\mu,dx}\psi \quad m-\text{a.e.}$$

This proves the desired relations for k purely imaginary. The result extends to any $k \in \mathbb{C}^+$ by means of the Hilbert identity as in the proof of Lemma III.2. ∎

Let now α be as above a Borel measurable function $\mathbb{R} \to \mathbb{R}$ and $\alpha_0 \in \mathbb{R}$; by abuse of notation we denote by α_0 also a constant function $\mathbb{R} \to \mathbb{R}$, $\alpha_0(x) = \alpha_0$. By the preceding result, we have

$$\begin{aligned} R^k(\alpha) &= R_0^k - R^k_{m,dx}(I + \alpha R^k_{m,m})^{-1}\alpha R^k_{dx,m} \\ R^k(\alpha_0) &= R_0^k - R^k_{m,dx}(I + \alpha_0 R^k_{m,m})^{-1}\alpha_0 R^k_{dx,m}, \end{aligned}$$

so

$$\begin{aligned} R^k(\alpha) - R^k(\alpha_0) &= R^k_{m,dx}\left[(I + \alpha_0 R^k_{m,m})^{-1}\alpha_0 - (I + \alpha R^k_{m,m})^{-1}\alpha\right] R^k_{dx,m} \\ &= R^k_{m,dx}(I + \alpha R^k_{m,m})^{-1}\left[\alpha_0(I + \alpha R^k_{m,m}) - \alpha(I + \alpha_0 R^k_{m,m})\right] \\ &\quad (I + \alpha_0 R^k_{m,m})^{-1} R^k_{dx,m} \\ &= R^k_{m,dx}(I + \alpha R^k_{m,m})^{-1}(\alpha_0 - \alpha)(I + \alpha_0 R^k_{m,m})^{-1} R^k_{dx,m} \qquad (3.8) \end{aligned}$$

where in the second relation we have used the fact that α_0 is a number and thus commutes with $I + \alpha R^k_{m,m}$.

Next we compute traces of $R^k(\alpha_0)$. By Lemma III.3, we have

$$\begin{aligned} R^k_{dx,m}(\alpha_0) &= R^k_{dx,m} - R^k_{m,m}(I + \alpha_0 R^k_{m,m})^{-1}\alpha_0 R^k_{dx,m} \\ &= (I + \alpha_0 R^k_{m,m})^{-1} R^k_{dx,m}. \end{aligned}$$

On the other hand, $(R^k_{\mu,\nu})^*$ maps $L^2(\nu)$ into $L^2(\mu)$ and $(R^k_{\mu,\nu})^* = R^{\bar{k}}_{\nu,\mu}$. This yields

$$\begin{aligned} R^k_{m,dx}(\alpha_0) &= R^k_{m,dx} - R^k_{m,dx}(I + \alpha_0 R^k_{m,m})^{-1}\alpha_0 R^k_{m,m} \\ &= R^k_{m,dx}(I + \alpha_0 R^k_{m,m})^{-1}. \end{aligned}$$

Applying once more Lemma III.3, we get also

$$R^k_{m,m}(\alpha_0) = (I + \alpha_0 R^k_{m,m})^{-1} R^k_{m,m} = R^k_{m,m}(I + \alpha_0 R^k_{m,m})^{-1}.$$

Let us now proceed with the calculation of the resolvent difference (3.8). With this preliminary it equals (up to the sign)

$$R^k_{m,dx}(\alpha_0)(I+\alpha_0 R^k_{m,m})(I+\alpha R^k_{m,m})^{-1}(\alpha-\alpha_0)R^k_{dx,m}(\alpha_0)$$

and the central expression can be further rewritten as follows

$$\begin{aligned}
&(I+\alpha_0 R^k_{m,m})(I+\alpha R^k_{m,m})^{-1}(\alpha-\alpha_0)\\
&\quad=\left[\left(I+\alpha_0 R^k_{m,m}+(\alpha-\alpha_0)R^k_{m,m}\right)(I+\alpha_0 R^k_{m,m})^{-1}\right]^{-1}(\alpha-\alpha_0)\\
&\quad=\left[I+(\alpha-\alpha_0)R^k_{m,m}(\alpha_0)\right]^{-1}(\alpha-\alpha_0)\\
&\quad=(\alpha-\alpha_0)^{\frac12}(\alpha-\alpha_0)^{-\frac12}\left[I+(\alpha-\alpha_0)^{\frac12}|\alpha-\alpha_0|^{\frac12}R^k_{m,m}(\alpha_0)\right]^{-1}(\alpha-\alpha_0)^{\frac12}|\alpha-\alpha_0|^{\frac12}\\
&\quad=(\alpha-\alpha_0)^{\frac12}\left[(\alpha-\alpha_0)^{-\frac12}\left(I+(\alpha-\alpha_0)^{\frac12}|\alpha-\alpha_0|^{\frac12}R^k_{m,m}(\alpha_0)\right)(\alpha-\alpha_0)^{\frac12}\right]^{-1}|\alpha-\alpha_0|^{\frac12}\\
&\quad=(\alpha-\alpha_0)^{\frac12}\left[I+|\alpha-\alpha_0|^{\frac12}R^k_{m,m}(\alpha_0)(\alpha-\alpha_0)^{\frac12}\right]^{-1}|\alpha-\alpha_0|^{\frac12}\,. \qquad (3.9)
\end{aligned}$$

We have introduced here the common notation $(\alpha-\alpha_0)^{\frac12}:=|\alpha-\alpha_0|^{\frac12}\,\mathrm{sgn}(\alpha-\alpha_0)$.

Summing up the discussion, we get

Theorem III.1 *Under the above stated assumptions, the resolvent of $H_{\alpha m}$ can be expressed by means of that of the reference operator $H_{\alpha_0 m}$ as*

$$\begin{aligned}
R^k(\alpha) \;&=\; R^k(\alpha_0)-R^k_{m,dx}(\alpha_0)\,(\alpha-\alpha_0)^{\frac12}\cdot\\
&\quad\cdot\left[I+|\alpha-\alpha_0|^{\frac12}\,R^k_{m,m}(\alpha_0)\,(\alpha-\alpha_0)^{\frac12}\right]^{-1}|\alpha-\alpha_0|^{\frac12}R^k_{dx,m}(\alpha_0) \qquad (3.10)
\end{aligned}$$

for any $k\in\mathbb{C}^+$.

One of the most interesting situations is when $\lim_{|x|\to\infty}\alpha(x)=\alpha_0$, so the *effective coupling "constant"* $\alpha(x)$–α_0 decays to zero at large x-distances. In the same way as above we can derive the following assertions which are the basis of Birman-Schwinger analysis in the present case.

Corollary III.4 (i) $I+|\alpha-\alpha_0|^{\frac12}\,R^{i\kappa}_{m,m}(\alpha_0)\,(\alpha-\alpha_0)^{\frac12}$ *has a bounded inverse on $L^2(m)$ for all $\kappa>0$ large enough.*
(ii) $\forall k\in\mathbb{C}^+:\ \dim\mathrm{Ker}(H_{\alpha m}-k^2)=\dim\mathrm{Ker}\left(I+|\alpha-\alpha_0|^{\frac12}\,R^k_{m,m}(\alpha_0)\,(\alpha-\alpha_0)^{\frac12}\right)$.

Remark III.3 From the third line of (3.9) it is clear that the resolvent can also be expressed as

$$R^k(\alpha)=R^k(\alpha_0)-R^k_{m,dx}(\alpha_0)\left[I+(\alpha-\alpha_0)R^k_{m,m}(\alpha_0)\right]^{-1}(\alpha-\alpha_0)R^k_{dx,m}(\alpha_0)\,. \qquad (3.11)$$

This formula can be used as a basis of the Birman-Schwinger analysis in analogy with [6]. We have followed this path in the first version of Chapter IV. It is a pleasure to thank Walter Renger who pointed to us advantages of a symmetrized expression.

The inverted term in (3.10) gives arise to the integral operator K_α^k with the kernel given by (4.8). An analogous operator corresponding to (3.11) provides, of course, the same eigenvalues (as the solutions of the integral equation $K_\alpha^k\psi = -\psi$, *cf.* Theorem IV.2), however, its nonsymmetric form would force us to assume that $\alpha - \alpha_0$ has a compact support in order to perform the weak coupling analysis in Section. IV.2. This strong requirement becomes unnecessary if the former is regarded. Really, its kernel is analogous in dependency on the coupling function to the one in classical Birman-Schwinger principle (compare (4.8) with (1) in [34]).

Chapter IV

Bound States

IV.1 Existence

In [20] it is proved that an arbitrary "window" leads to the existence of a bound state. Here we shall show that it is sufficient to make the *coupling "constant"* smaller in the mean in order to create a locally stronger tunelling between the both channels.

This general existence result is given by the following theorem. Its variational proof is based on the idea of [23], Sec. II. (see also Thm.2.1. of [11] and [20], Sec. III).

Denote by α_0 a constant function $\mathbb{R} \to \mathbb{R}$ which represents here the unperturbed system discussed in Section II.2. Then we have

Theorem IV.1 *Assume*

$$\begin{array}{ll} \text{(i)} & \alpha - \alpha_0 \in L^1_{loc}(\mathbb{R}) \\ \text{(ii)} & \alpha(x) - \alpha_0 = \mathcal{O}(|x|^{-1-\varepsilon}) \quad \textit{for some } \varepsilon > 0 \textit{ as } |x| \to \infty. \end{array}$$

If $\int_{\mathbb{R}} (\alpha(x) - \alpha_0) dx < 0$*, then* H_α *has at least one isolated eigenvalue below its essential spectrum,* $\sigma_{ess}(H_\alpha) = [\nu_1(\alpha_0), \infty)$*.*

Proof: **(a)** We must first determine $\sigma_{ess}(H_\alpha)$. This can be done by a simple bracketing argument (as in [20], Sec. II) employing the *minimax principle* (*cf.* [32], Sec. XIII.1).

Assumption (ii) tells us that $\lim_{|x|\to\infty} |x|^{1+\varepsilon}(\alpha(x) - \alpha_0) = 0$, *i.e.*,

$$\forall \delta > 0 \; \exists a > 1 : |x| > a \Rightarrow |\alpha(x) - \alpha_0| < \frac{\delta}{|x|^{1+\varepsilon}} < \frac{\delta}{a^{1+\varepsilon}} =: \delta'. \tag{4.1}$$

Cutting now Ω by the additional Neumann or Dirichlet boundaries parallel to the y-axis at $x = \pm a$, we get

$$H^{(N)}_{\alpha,t} \oplus H^{(N)}_{\alpha,c} \leq H_\alpha \leq H^{(D)}_{\alpha,t} \oplus H^{(D)}_{\alpha,c}, \tag{4.2}$$

where the *"tail"* part corresponds to the two halfstrips ($|x| > a$) and the rest to the *central* part with the Neumann and Dirichlet condition on the vertical boundaries,

respectively. Next we denote

$$\begin{aligned}\alpha_{min}(a) &:= \min\left\{\alpha_0, \inf_{|x|>a}\alpha(x)\right\}\\ \alpha_{max}(a) &:= \max\left\{\alpha_0, \sup_{|x|>a}\alpha(x)\right\}.\end{aligned}$$

Since $\sigma_{ess}(H^{(j)}_{\alpha_{min},t}) = [\nu_1(\alpha_{min}),\infty)$ and $\sigma_{ess}(H^{(j)}_{\alpha_{max},t}) = [\nu_1(\alpha_{max}),\infty)$, $j = N, D$, and

$$H^{(j)}_{\alpha_{min},t} \le H^{(j)}_{\alpha,t} \le H^{(j)}_{\alpha_{max},t},$$

in the sense of quadratic forms, we get the following two-sided bound of the bottom of the *"tail"* essential spectrum

$$\nu_1(\alpha_{min}) \le \underbrace{\inf\sigma_{ess}(H^{(j)}_{\alpha,t})}_{=:\nu_{ess}} \le \nu_1(\alpha_{max}).$$

The Hamiltonians of the *central* part, $H^{(j)}_{\alpha,c}$, have clearly discrete spectrum because of the boundaries. By (4.2) and the *minimax principle* it follows that the essential spectrum of H_α is determined by the essential spectrum of the *"tail"* Hamiltonians only and thus $\inf\sigma_{ess}(H_\alpha) = \nu_{ess}$ as well.

Since the assertion (4.1) yields

$$\alpha_0 - \delta' < \alpha_{min} \le \alpha_0 \le \alpha_{max} < \alpha_0 + \delta',$$

and by Proposition II.1 2. ν_1 is an increasing function of α, we eventually have

$$\nu_1(\alpha_0 - \delta') < \nu_{ess} < \nu_1(\alpha_0 + \delta').$$

In addition, by the same proposition $\nu_1 = \nu_1(\alpha)$ is a continuous function, hence $\nu_{ess} = \nu_1(\alpha_0)$.

(b) After localizing the essential spectrum, we shall prove now the claim of the theorem. For any $\Psi \in D(q_\alpha)$ we put

$$Q_\alpha[\Psi] := q_\alpha[\Psi] - \nu_1(\alpha_0)\|\Psi\|_2^2. \tag{4.3}$$

Since the essential spectrum of H_α starts at $\nu_1(\alpha_0)$, we have to find a trial function Ψ such that $Q_\alpha[\Psi]$ is negative.

To make the longitudinal contribution to the kinetic energy small, we use an exterior scaling. We choose an interval $\mathcal{A} := [-a, a]$ for some $a > 1$ and the function $\varphi \in \mathcal{S}(\mathbb{R})$ in such a way that $\varphi(x) = 1$ on $\mathcal{A}$. Furthermore, we define the family $\{\varphi_\sigma : \sigma \in \mathbb{R}\}$ by a scaling exterior to $\mathcal{A}$:

$$\varphi_\sigma(x) := \begin{cases} \varphi(x) & \text{if} \quad |x| \le a \\ \varphi(\pm a + \sigma(x \mp a)) & \text{if} \quad \pm x > a \end{cases} \tag{4.4}$$

such that $\forall x \in \mathbb{R} : |\varphi_\sigma(x)| \leq 1$.

Now we set $\Psi(x,y) := \varphi_\sigma(x)\chi_1(y;\alpha_0)$ and since $\|\dot\varphi_\sigma\|_2^2 = \sigma\|\dot\varphi\|_2^2$ and

$$\begin{aligned} q_\alpha[\Psi] &= q_{\alpha_0}[\Psi] + \int_{\mathbb{R}} (\alpha(x)-\alpha_0)|\Psi(x,0)|^2 dx \\ q_{\alpha_0}[\Psi] &= \|\dot\varphi_\sigma\|_2^2 + \nu_1(\alpha_0)\|\varphi_\sigma\|_2^2\,, \end{aligned}$$

(It is quite tedious to check the second equality while the first follows directly from (2.2).) we obtain

$$Q_\alpha[\Psi] = \sigma\|\dot\varphi\|_2^2 + |\chi_1(0;\alpha_0)|^2 \int_{\mathbb{R}} (\alpha(x)-\alpha_0)|\varphi_\sigma(x)|^2 dx. \tag{4.5}$$

We split now the branch of the integration into two mutually disjoint regions: $\mathcal{A}, \mathbb{R}\setminus\mathcal{A}$ and the application of (4.1) together with the properties of φ_σ then yields:

$$Q_\alpha[\Psi] < \sigma\|\dot\varphi\|_2^2 + \frac{4\delta|\chi_1(0;\alpha_0)|^2}{\varepsilon a^\varepsilon} + |\chi_1(0;\alpha_0)|^2 \int_{\mathbb{R}} (\alpha(x)-\alpha_0)\, dx. \tag{4.6}$$

If the assumption $\int_{\mathbb{R}}(\alpha(x)-\alpha_0) < 0$ holds we can choose δ and σ sufficiently small to make the quadratic form $Q_\alpha[\Psi]$ negative. ∎

IV.2 Weak Coupling

In this section we will study the existence of bound states in the case that $\alpha(x)$ differs from α_0 slightly, *i.e.*, we replace $\alpha(x)$–α_0 by $\lambda(\alpha(x)$–$\alpha_0)$ and consider the limit $\lambda \to 0$. We use the results of the previous chapter as the basis of Birman-Schwinger analysis and similarly as in [34], [4], [16], Sec. V., [14] and [11], Thm. 4.2., we find necessary and sufficient conditions for H_α to have a (unique) bound state for all sufficiently small positive λ. In addition we shall derive expansion of the bound-state energy at $\lambda = 0$.

Let us already now list our requirements on $\alpha(x)$:

(a1) $\alpha(x)-\alpha_0 \in L^{1+\varepsilon}(\mathbb{R}, dx)$ for some small $\varepsilon > 0$,

(a2) $\alpha(x)-\alpha_0 \in L^1(\mathbb{R}, |x|\, dx)$.

As a consequence of *(a1), (a2)*; the function $\alpha(x)-\alpha_0$ belongs to $L^1(\mathbb{R}, dx)$ too.

IV.2.1 Introduction

Recall the results of the previous chapter (*cf.* Theorem III.1 and Corollary III.4) which we shall need for investigation of the discrete spectrum:

Theorem IV.2

$$k^2 \in \sigma_{disc}(H_\alpha) \Leftrightarrow K_\alpha^k \psi = -\psi, \tag{4.7}$$

where K_α^k is an integral operator on $L^2(\mathbb{R})$ with the kernel

$$K_\alpha(x,x';k) = |\alpha(x)-\alpha_0|^{\frac{1}{2}}\, G_{\alpha_0}(x,0,x',0;k)\, (\alpha(x')-\alpha_0)^{\frac{1}{2}}.$$

The Green's function G_{α_0} is given by (2.9). Since we are interested in the discrete spectrum, we must take the Green's function for $k^2 < \nu_1(\alpha_0)$. Thus we have

$$K_\alpha(x,x';k) = |\alpha(x)-\alpha_0|^{\frac{1}{2}} \sum_{n=1}^{\infty} \frac{|\chi_n(0;\alpha_0)|^2}{2\kappa_n} e^{-\kappa_n|x-x'|} (\alpha(x')-\alpha_0)^{\frac{1}{2}}, \tag{4.8}$$

where $\kappa_n := \sqrt{\nu_n(\alpha_0) - k^2}$.

Before we start to investigate the properties of the operator K^k_α, notice the following trivial fact. Denote $\Lambda := \|\alpha-\alpha_0\|_1$, then we have

Proposition IV.1 *Assume (a1), (a2), then*

$$\lim_{\Lambda\to 0} k^2 = \nu_1 \qquad \text{(i.e. } \kappa_1 \to 0) \tag{4.9}$$

PROOF: Using the expression of the quadratic form (2.2), we have for a normalized $\psi \in D(q_\alpha) = D(q_{\alpha_0})$:

$$\begin{aligned} k^2 &= \min_\psi q_\alpha[\psi] = \min_\psi q_{\alpha_0}[\psi] + \min_\psi \int_{\mathbb{R}} (\alpha(x)-\alpha_0)|\psi(x,0)|^2 dx \\ &= \nu_1 + \min_\psi \int_{\mathbb{R}} (\alpha(x)-\alpha_0)|\psi(x,0)|^2 dx, \end{aligned}$$

$$\begin{aligned} |k^2-\nu_1| &\le \int_{\mathbb{R}} |\alpha(x)-\alpha_0||\psi(x,0)|^2 dx \\ &\le \Lambda d\,(\|\nabla\psi\|_2^2 + \|\psi\|_2^2) \to 0 \end{aligned}$$

as $\Lambda \to 0$. In the last inequality we have used the basic Sobolev type estimate

$$\|\psi\|_\infty \le a\|\nabla\psi\|_2 + b\|\psi\|_2$$

holds for any $a > 0$ and some b (*cf.* [32], Thm. IX.28). ∎

As a consequence we have

Corollary IV.1 *Assume (a1), (a2), then*

$$\lim_{\lambda\to 0} k^2 = \nu_1 \tag{4.10}$$

IV.2.2 Analysis of K_α

The key idea of the further process is that K^k_α has a well-behaved limit as $k^2 \to \nu_1$ except for a divergent rank-one piece. The singularity is contained in the first term of the expansion (4.8) and can be singled out by taking (as in [34] or [16])

$$K^k_\alpha = L_\alpha + P_\alpha = L_\alpha + M_\alpha + N_\alpha,$$

where

$$\begin{aligned} L_\alpha(x,x') &= |\alpha(x)-\alpha_0|^{\frac{1}{2}}\,\frac{|\chi_1(0)|^2}{2\kappa_1}\,(\alpha(x')-\alpha_0)^{\frac{1}{2}} \\ M_\alpha(x,x') &= |\alpha(x)-\alpha_0|^{\frac{1}{2}}\,\frac{|\chi_1(0)|^2}{2\kappa_1}\,(e^{-\kappa_1|x-x'|}-1)\,(\alpha(x')-\alpha_0)^{\frac{1}{2}} \\ N_\alpha(x,x') &= |\alpha(x)-\alpha_0|^{\frac{1}{2}}\sum_{n=2}^{\infty}\frac{|\chi_n(0)|^2}{2\kappa_n}\,e^{-\kappa_n|x-x'|}\,(\alpha(x')-\alpha_0)^{\frac{1}{2}}\,. \end{aligned} \tag{4.11}$$

This decomposition would lead to a BS-analysis requirement $\alpha(x)-\alpha_0 \in L^2(\mathbb{R},|x|^2\,dx)$; however, one can manage with *(a2)* by replacing the above by more sophisticated method of [4], [14], [11]:

$$K_\alpha^k = Q_\alpha + P_\alpha = Q_\alpha + A_\alpha + N_\alpha$$

with

$$\begin{aligned} Q_\alpha(x,x') &= |\alpha(x)-\alpha_0|^{\frac{1}{2}}\,e^{-\kappa_1|x|}\,\frac{|\chi_1(0)|^2}{2\kappa_1}\,e^{-\kappa_1|x'|}\,(\alpha(x')-\alpha_0)^{\frac{1}{2}} \\ A_\alpha(x,x') &= |\alpha(x)-\alpha_0|^{\frac{1}{2}}\,\frac{|\chi_1(0)|^2}{\kappa_1}\,e^{-\kappa_1|x|_>}\sinh\kappa_1|x|_<\,(\alpha(x')-\alpha_0)^{\frac{1}{2}}\,. \end{aligned} \tag{4.12}$$

Here we have introduced

$$\begin{aligned} |x|_< &:= \max\{0,\min\{|x|,|x'|\}\operatorname{sgn}(xx')\} \\ |x|_> &:= \max\{|x|,|x'|\}\,. \end{aligned}$$

According to [4] the latter decomposition is very natural because it arises from replacing the Green's function in K_α^k by the Green's function in which a zero boundary condition is imposed at the origin. The advantage of the former decomposition is that it results in a simpler implicit equation for κ_1 (compare our (4.17) with (7) of [34]).

First we shall collect the properties of A_α, N_α, which we will use in the proof of the main result of the chapter, Theorem IV.3. We will often employ the notation $z := \kappa_1$.

Properties of A_α

Let A_0 be an integral operator given by its kernel

$$A_0(x,x') := |\alpha(x)-\alpha_0|^{\frac{1}{2}}\,|\chi_1(0)|^2\,|x|_<\,(\alpha(x')-\alpha_0)^{\frac{1}{2}}\,,$$

then one has:

Proposition IV.2 *Assume that the hypothesis (a2) is valid, then*

$$\lim_{\kappa_1\to 0}\|A_\alpha - A_0\|_{HS} = 0\,. \tag{4.13}$$

PROOF: A_0 is Hilbert-Schmidt since

$$\begin{aligned}\|A_0\|_{HS}^2 &= \int_{\mathbb{R}^2} |A_0(x,x')|^2\,dx\,dx' \\ &= |\chi_1(0)|^4 \int_{\mathbb{R}^2} |\alpha(x)-\alpha_0|\;|x|_<^2\;|\alpha(x')-\alpha_0|\,dx\,dx' \\ &\le |\chi_1(0)|^4 \left(\int_{\mathbb{R}} |x|\;|\alpha(x)-\alpha_0|\,dx\right)^2 < \infty\end{aligned}$$

by assumption (the estimate follows from $|x|_<^2 \le |x||x'|$). Next we have

$$\begin{aligned}\lim_{\kappa_1\to 0} A_\alpha &= A_0 \\ |A_\alpha(x,x';\kappa_1)| &\le |A_0(x,x')| \qquad (\Leftarrow \forall x \ge 0 : \sinh x \le x e^x)\,.\end{aligned}$$

This ensures that the assumptions of the dominated convergence theorem are valid, and thus

$$\int_{\mathbb{R}^2} |(A_\alpha - A_0)(x,x')|^2\,dx\,dx' \to 0\,. \quad \blacksquare$$

We will also need the boundedness of A_α for complex κ_1.

Lemma IV.1

$$\forall z \in \mathbb{C}, \operatorname{Re} z \ge 0, |z| < \frac{\pi}{2} :\ |A_\alpha(z)| \le \sqrt{2}\,|A_0|. \tag{4.14}$$

PROOF: Obviously it is sufficient to prove the inequality $|e^{-z}-1| \le \sqrt{2}|z|$. If we put $z = \rho e^{i\varphi}$, then (by the inequality $\cos x \ge 1 - \frac{x^2}{2}$)

$$\begin{aligned}|e^{-z}-1|^2 &= 1 + e^{-2\rho\cos\varphi} - 2e^{-\rho\cos\varphi}\cos(\rho\sin\varphi) \\ &\le 1 + e^{-2\rho\cos\varphi} - 2e^{-\rho\cos\varphi}\cos\rho \\ &\le 1 + e^{-2\rho\cos\varphi} - 2e^{-\rho\cos\varphi} + \rho^2 e^{-\rho\cos\varphi} \\ &\le \rho^2\cos^2\varphi + \rho^2 e^{-\rho}\cos\varphi \le 2\rho^2\end{aligned}$$

holds for $\varphi \in [-\frac{\pi}{2}, \frac{\pi}{2}], \rho < \frac{\pi}{2}$. $\blacksquare$

Properties of N_α

Now define

$$N_0(x,x') := |\alpha(x)-\alpha_0|^{\frac{1}{2}} \sum_{n=2}^{\infty} \frac{|\chi_n(0)|^2}{2}\;\frac{e^{-\sqrt{\nu_n-\nu_1}|x-x'|}}{\sqrt{\nu_n-\nu_1}}\;(\alpha(x')-\alpha_0)^{\frac{1}{2}}\,,$$

and similarly as above:

Proposition IV.3 *Assume that the hypotheses (a1), (a2) are valid, then*

$$\lim_{\kappa_1\to 0} \|N_\alpha - N_0\|_{HS} = 0\,. \tag{4.15}$$

PROOF: If $x \neq x'$ the sum in N_0 converges (note that by Proposition II.1 1 the sequence $\{\sqrt{\nu_n}\}$ grows linearly with n as $n \to \infty$) while it has a logarithmic singularity as $x' \to x$. In particular, by means of the proposition we have

$$\sum_{n=2}^{\infty} \frac{|\chi_n(0)|^2}{2} \, \frac{e^{-\sqrt{\nu_n-\nu_1}|x-x'|}}{\sqrt{\nu_n-\nu_1}} \geq C \sum_{n=1}^{\infty} \frac{e^{-\frac{\pi}{d}\, n\,|x-x'|}}{n} = -C \, \ln\left(1-e^{-\frac{\pi}{d}\,|x-x'|}\right) \to \infty$$

as $x' \to x$.

Nevertheless, its Hilbert-Schmidt norm is still finite because by Hölder inequality and the above mentioned proposition we have

$$\begin{aligned}
\|N_0\|^2_{HS} &= \sum_{m,n=2}^{\infty} \frac{|\chi_n(0)\,\chi_m(0)|^2}{4\sqrt{\nu_n-\nu_1}\sqrt{\nu_m-\nu_1}} \int_{\mathbb{R}^2} |\alpha(x)-\alpha_0| \; e^{-\frac{1}{2}(\sqrt{\nu_n-\nu_1}+\sqrt{\nu_m-\nu_1})|x-x'|} \cdot \\
&\qquad \cdot |\alpha(x')-\alpha_0| \; e^{-\frac{1}{2}(\sqrt{\nu_n-\nu_1}+\sqrt{\nu_m-\nu_1})|x-x'|} \, dx\, dx' \\
&\leq C(\varepsilon)\, \|\alpha-\alpha_0\|^2_{1+\varepsilon} \sum_{m,n=2}^{\infty} \frac{1}{\sqrt{\nu_n-\nu_1}\sqrt{\nu_m-\nu_1}\,(\sqrt{\nu_n-\nu_1}+\sqrt{\nu_m-\nu_1})^{2\varepsilon'}} \\
&\leq C(\varepsilon)\, \|\alpha-\alpha_0\|^2_{1+\varepsilon} \left[\Sigma + \left(\frac{2d}{\pi}\right)^3 \sum_{m,n=4}^{\infty} \frac{1}{(n-3)(m-3)(m+n-6)^{2\varepsilon'}}\right].
\end{aligned}$$

The monotone convergence theorem justifies the interchange of summation and integration we have made. Σ denotes the sum for $m, n = 2, 3$ of the unapproximated expression from the third line and ε' is the abbreviation for $\frac{\varepsilon}{1+\varepsilon} > 0$.

After the substitution $(m, n) \mapsto (m+3, n+3)$, the remaining sum can be next estimated as follows

$$\sum_{m,n=1}^{\infty} \frac{1}{m\,n\,(m+n)^{2\varepsilon'}} \leq \frac{1}{2^{\varepsilon'}} \sum_{m,n=1}^{\infty} \frac{1}{m^{1+\varepsilon'}\, n^{1+\varepsilon'}} \leq \left(\sum_{n=1}^{\infty} \frac{1}{n^{1+\varepsilon'}}\right)^2 < \infty\,.$$

The assumptions of the dominated convergence theorem are fulfilled again because

$$\begin{aligned}
\lim_{\kappa_1 \to 0} N_\alpha &= N_0 \\
|N_\alpha(x, x'; \kappa_1)| &\leq |N_0(x, x')|\,,
\end{aligned}$$

and thus

$$\int_{\mathbb{R}^2} |(N_\alpha - N_0)(x, x')|^2 \, dx\, dx' \to 0\,. \quad \blacksquare$$

To have a HS bound for N_α independent of a complex κ_1, it is useful to introduce an operator N_0^β, $\beta > 0$:

$$N_0^\beta(x, x') := |\alpha(x)-\alpha_0|^{\frac{1}{2}} \sum_{n=2}^{\infty} \frac{|\chi_n(0)|^2}{2} \, \frac{e^{-\beta\sqrt{\nu_n-\nu_1}|x-x'|}}{\beta\sqrt{\nu_n-\nu_1}} \, (\alpha(x')-\alpha_0)^{\frac{1}{2}}\,.$$

It has a finite HS norm (the proof would follow by mimicking the proof for N_0 from the previous proposition) and the following estimate holds:

Lemma IV.2

$$\exists C,\beta>0 \quad \forall z\in\mathbb{C},\mathrm{Re}\, z\geq 0, |z|<\sqrt{\nu_n-\nu_1}:\ |N_\alpha(z)|\leq C|N_0^\beta|. \tag{4.16}$$

PROOF: Put again $z=\rho e^{i\varphi}$. For any $0<\gamma<1$ we take $\rho:=\gamma\sqrt{\nu_n-\nu_1}<\sqrt{\nu_n-\nu_1}$. If in addition $\varphi\in[-\frac{\pi}{2},\frac{\pi}{2}]$, we get the estimates:

$$\begin{aligned}
|\kappa_n(z)|^2 &= \sqrt{(\nu_n-\nu_1)^2+\rho^4+2\rho^2(\nu_n-\nu_1)\cos 2\varphi} \\
&\geq \sqrt{(\nu_n-\nu_1)^2+\rho^4-2\rho^2(\nu_n-\nu_1)} \\
&= |\gamma^2-1|(\nu_n-\nu_1)\,,
\end{aligned}$$

$$\begin{aligned}
\left|e^{-|x-x'|\sqrt{\nu_n-\nu_1+\rho^2e^{2i\varphi}}}\right|^2 &= e^{-|x-x'|\sqrt{\nu_n-\nu_1+\rho^2e^{2i\varphi}}+\sqrt{\nu_n-\nu_1+\rho^2e^{-2i\varphi}}} \\
&\leq e^{-2|x-x'|(\sqrt{\nu_n-\nu_1}+\rho\cos 2\varphi)} \\
&\leq e^{-2|x-x'|(\sqrt{\nu_n-\nu_1}-\rho)} \\
&= e^{-2(1-\gamma)\sqrt{\nu_n-\nu_1}|x-x'|}\,.
\end{aligned}$$

To complete the proof it is sufficient to take $\beta:=2(1-\gamma)$ and $C:=\frac{2}{1+\gamma}$. ∎

IV.2.3 The Main Theorem

In this section we want to prove the following theorem.

Theorem IV.3 *Assume that the hypotheses (a1), (a2) are valid. Then, for λ small, H_α has at most one simple eigenvalue $E(\lambda)<\nu_1$, and this happens if and only if*

$$\sqrt{\nu_1-E}\equiv\kappa_1=-\frac{\lambda}{2}\,|\chi_1(0)|^2\left(e^{-\kappa_1|\cdot|}\,(\alpha-\alpha_0)^{\frac{1}{2}},(I+\lambda P_\alpha)^{-1}\,e^{-\kappa_1|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}\right) \tag{4.17}$$

has a solution $\kappa_1>0$.

PROOF: By Corollary IV.1 κ_1 must go to zero as $\lambda\to 0$. From the proves of Proposition IV.2 and IV.3 it is clear that

$$\|P_\alpha\|\leq\|A_\alpha\|+\|N_\alpha\|\leq\|A_\alpha\|_{HS}+\|N_\alpha\|_{HS}\leq\|A_0\|_{HS}+\|N_0\|_{HS}<\infty,$$

and thus for λ sufficiently small $\|\lambda P_\alpha\|<1$, so $I+\lambda P_\alpha$ is invertible and we may write

$$(I+\lambda K_\alpha^k)^{-1}=\left[I+(I+\lambda P_\alpha)^{-1}\lambda Q_\alpha\right]^{-1}(I+\lambda P_\alpha)^{-1}.$$

Hence λK_α has eigenvalue -1 if and only if the same is true for $(I+\lambda P_\alpha)^{-1}\lambda Q_\alpha$. Since Q_α is a rank-one operator (see (4.12)),

$$(I+\lambda P_\alpha)^{-1}\lambda Q_\alpha=(\psi,\cdot)\,\varphi$$

with

$$\begin{aligned}\psi &:= \lambda\,\frac{|\chi_1(0)|^2}{2\kappa_1}\,e^{-\kappa_1|\cdot|}\,(\alpha(\cdot)-\alpha_0)^{\frac{1}{2}}\\ \varphi &:= (I+\lambda P_\alpha)^{-1}\,e^{-\kappa_1|\cdot|}\,|\alpha(\cdot)-\alpha_0|^{\frac{1}{2}}\,,\end{aligned}$$

it has just one eigenvalue (ψ,φ). Putting it equal to -1 we get the condition (4.17). (To get this result we could also have employed the theory of modified determinants as in the proof of Theorem 2.3 in [34].)

This proves the entire theorem except for the assertion that (4.17) has *at most* one positive solution for λ small and fixed. Since there is a one-to-one correspondence between eigenvalues of H_α and solutions of (4.17) and the number of eigenvalue can only go up with replacement $\alpha-\alpha_0 \mapsto -|\alpha-\alpha_0|$, we need only show that (4.17) has at most one solution when $\alpha-\alpha_0 \le 0$. In this case, (4.17) is equivalent to:

$$\begin{aligned} z &= G(z,\lambda),\\ G(z,\lambda) &:= \tfrac{\lambda}{2}\,|\chi_1(0)|^2\left(\,e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}, (I+\lambda P_\alpha)^{-1}\,e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}\,\right)\end{aligned} \tag{4.18}$$

($z \equiv \kappa_1$).

To complete the proof, we need the following lemmas.

Auxiliary Results

Lemma IV.3 *If $\alpha-\alpha_0 \not\equiv 0$, then $|z|^{-1} \le C_1\lambda^{-1}$ for λ small.*

PROOF: From (4.18), we see that any solution z for λ small must obey

$$z = \frac{\lambda}{2}|\chi_1(0)|^2\int_{\mathbb{R}}|\alpha(x)-\alpha_0|\,dx + \mathcal{O}(\lambda^2),$$

what gives us the assertion provided $\alpha-\alpha_0$ is not identically zero. ∎

Lemma IV.4 *For sufficiently small z,*

$$\left\|\frac{\partial P_\alpha}{\partial z}\right\| < \frac{C_2}{|z|}\,.$$

PROOF: Let us choose a contour in complex plane, $\varphi : s = z + ze^{it}\ ; t \in [0,2\pi]$. The operator-valued fuction $P_\alpha(z)$ is real-analytic in the region $\mathrm{Re}\,z > 0$ and has a bounded limit as $z \to 0+$. Hence Cauchy integral formula gives

$$\begin{aligned} P_\alpha(z) &= \frac{1}{2\pi i}\int_\varphi \frac{P_\alpha(s)}{s-z}\,ds\\ \frac{\partial P_\alpha}{\partial z}(z) &= \frac{1}{2\pi i}\int_\varphi \frac{P_\alpha(s)}{(s-z)^2}\,ds\end{aligned}$$

and by Lemmas IV.1 and IV.2 we get

$$\left|\frac{\partial P_\alpha}{\partial z}\right| = \left|\frac{1}{2\pi i}\int_0^{2\pi}\frac{P_\alpha(s)\,i\,z\,e^{it}dt}{z^2\,e^{2it}}\right| \leq \frac{\sqrt{2}|A_0|+C|N_0^\beta|}{|z|}\,,$$

$$\left\|\frac{\partial P_\alpha}{\partial z}\right\| \leq \left\|\frac{\partial P_\alpha}{\partial z}\right\|_{HS} \leq \frac{C_2}{|z|}\,,$$

because A_0, N_0^β have a finite HS norm. ∎

Lemma IV.5 $\forall z_0 \in \mathbb{R} \quad \exists C_3 > 0 \quad \forall z \in [0, z_0]$:

$$\left|\left(\, e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}, \left[2\,|\cdot| + \frac{\partial P_\alpha}{\partial z}\right] e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}\,\right)\right| \leq C_3$$

PROOF: We recall that $P_\alpha = A_\alpha + N_\alpha$. An explicit calculation shows that

$$\begin{aligned}
\frac{\partial N_\alpha}{\partial z}(x,x') &= -|\alpha(x)-\alpha_0|^{\frac{1}{2}}\sum_{n=2}^{\infty} z\,\frac{|\chi_n(0)|^2}{2\kappa_n^2}\,\frac{1+\kappa_n|x-x'|}{\kappa_n}\,e^{-\kappa_n|x-x'|}\,(\alpha(x')-\alpha_0)^{\frac{1}{2}} \\
\frac{\partial A_\alpha}{\partial z}(x,x') &= -|\chi_1(0)|^2\,|\alpha(x)-\alpha_0|^{\frac{1}{2}}\,(\alpha(x')-\alpha_0)^{\frac{1}{2}}\,e^{-z\,(|x|_>-|x|_<)}\,. \\
&\quad \cdot\,\frac{1-e^{-2z|x|_<}+z\,(|x|_>-|x|_<)-z\,(|x|_>+|x|_<)\,e^{-2z|x|_<}}{2z^2}\,.
\end{aligned}$$

(a) The sum in the first expression converges because

$$\frac{1+\kappa_n|x-x'|}{\kappa_n}e^{-\kappa_n|x-x'|} \leq \left(|x-x'| + \frac{1}{\sqrt{\nu_2-\nu_1}}\right)$$

and by using Proposition II.1 1. we get the estimates:

$$\sum_{n=2}^{\infty}\frac{|\chi_n(0)|^2}{\kappa_n^2} \leq \sum_{n=2}^{\infty}\frac{K}{\nu_n-\nu_1} \leq \sum_{n=2}^{3}\frac{K}{\nu_n-\nu_1} + \left(\frac{2d}{\pi}\right)^2\sum_{n=4}^{\infty}\frac{K}{(n-3)^2} < \infty\,.$$

Since $e^{-z|\cdot|} \leq 1$ the integrals then converge because of the hypotheses *(a1), (a2)*; so the term containing the derivative of N_α is bounded by a term which is proportional to $|z|$.

(b) Since $|x|_> \geq |x|_<$ and $\forall x \geq 0 : 1 - e^{-x} - xe^{-x} \leq x^2$, the other term with the derivative is bounded by a term which is independent of z and stays finite after integration by the hypotheses.

(c) The term without derivative is finite by the hypotheses as well. ∎

Lemma IV.6

$$\exists C_4 > 0 \;: \qquad \left|\left(\, e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}, \left[\,|\cdot|\,|P_\alpha+P_\alpha|\cdot|\,\right] e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}\,\right)\right| \leq \frac{C_4}{|z|}$$

PROOF: Since $\forall x > 0 : x\,e^{-x} \leq e^{-1}$, using Schwarz inequality we infer that the expression is bounded by

$$\frac{e^{-1}}{|z|}\,\|\alpha-\alpha_0\|_1\,\|P_\alpha\|_{HS}\,. \quad ∎$$

Completion of the Proof

By the elementary inequality

$$(I+\lambda P_\alpha)^{-1} \leq \frac{1-\lambda P_\alpha}{1-\lambda} \leq d\,(1-\lambda P_\alpha)$$

held for λ small enough and by the preceding lemmas we have for all small λ:

$$\begin{aligned}
\left|\frac{\partial G}{\partial z}\right| &= \left|\frac{\lambda}{2}\,|\chi_1(0)|^2\Big(e^{-z\,|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}, \Big[-|\cdot|\,(I+\lambda P_\alpha)^{-1}+\right.\\
&\quad \left.+\,(I+\lambda P_\alpha)^{-1}\,\lambda\,\frac{\partial P_\alpha}{\partial z}\,(I+\lambda P_\alpha)^{-1}-(I+\lambda P_\alpha)^{-1}\,|\cdot|\Big]\;e^{-z\,|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}\Big)\right|\\
&\leq d\,\frac{\lambda}{2}\,|\chi_1(0)|^2\,\Bigg\{\;\left|\left(e^{-z\,|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}, \left[2\,|\cdot|+\frac{\partial P_\alpha}{\partial z}\right]\;e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}\right)\right|\\
&\quad +\lambda\left|\left(e^{-z\,|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}, \left[\;|\cdot|\,P_\alpha+P_\alpha\,|\cdot|\;\right]e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}\right)\right|\\
&\quad +\lambda\left|\left(e^{-z\,|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}, \left[P_\alpha\frac{\partial P_\alpha}{\partial z}+\frac{\partial P_\alpha}{\partial z}P_\alpha\right]\;e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}\right)\right|\\
&\quad +\lambda^2\left|\left(e^{-z\,|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}, P_\alpha\,\frac{\partial P_\alpha}{\partial z}\,P_\alpha\,e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}}\right)\right|\;\Bigg\}\\
&\leq d'\,\Bigg\{\;C_3\,\lambda+\frac{C_4}{|z|}\,\lambda^2+\lambda^2\,\|\alpha-\alpha_0\|_1\,\|P_\alpha\|_{HS}\,\left\|\frac{\partial P_\alpha}{\partial z}\right\|_{HS}+\\
&\quad +\lambda^3\,\|\alpha-\alpha_0\|_1\,\|P_\alpha\|_{HS}^2\,\left\|\frac{\partial P_\alpha}{\partial z}\right\|_{HS}\;\Bigg\}\\
&\leq d'(C_3\,\lambda+C_1C_4\,\lambda+C_1C_2d_1\,\lambda+C_1C_2d_2\,\lambda^2)\leq C\lambda\,. \qquad (4.19)
\end{aligned}$$

Let z_1, z_2 are two solutions of $z=G(z,\lambda)$. Because they have to fulfil

$$|z_1-z_2|=\left|\int_{z_1}^{z_2}\frac{\partial G}{\partial z}dz\right|\leq\left|\int_{z_1}^{z_2}\left|\frac{\partial G}{\partial z}\right|dz\right|\leq C\lambda|z_1-z_2|,$$

we have the uniqueness ensured for $\lambda < C^{-1}$. ∎

IV.2.4 Condition for a Bound State

In this section we introduce necessary and sufficient condition for there to be a bound state when λ is small.

Theorem IV.4 *Let α obeys hypotheses (a1), (a2) and $\alpha-\alpha_0 \not\equiv 0$. Then H_α has an eigenvalue $E(\lambda)<\nu_1$ for all small $\lambda>0$ if and only if*

$$\int_{\mathbb{R}}(\alpha(x)-\alpha_0)\,dx \leq 0. \qquad (4.20)$$

If this condition holds, then the eigenvalue is unique and simple and obeys

$$\begin{aligned}\sqrt{\nu_1 - E(\lambda)} = &-\frac{\lambda}{2}\,|\chi_1(0)|^2 \int_{\mathbb{R}} (\alpha(x)-\alpha_0)\,dx \\ &-\frac{\lambda^2}{4}\Bigg\{ |\chi_1(0)|^4 \int_{\mathbb{R}^2} (\alpha(x)-\alpha_0)\,|x-x'|\,(\alpha(x')-\alpha_0)\,dx\,dx' \\ &-|\chi_1(0)|^2 \sum_{n=2}^{\infty} |\chi_n(0)|^2 \int_{\mathbb{R}^2} (\alpha(x)-\alpha_0)\,\frac{e^{-\sqrt{\nu_n-\nu_1}|x-x'|}}{\sqrt{\nu_n-\nu_1}}\,(\alpha(x')-\alpha_0)\,dx\,dx'\Bigg\} \\ &+\mathcal{O}(\lambda^3). \end{aligned} \tag{4.21}$$

PROOF: The expansion follows by the implicit-function theorem. In particular, denoting (*cf.* (4.17))

$$F(z,\lambda) := z + \frac{\lambda}{2}\,|\chi_1(0)|^2 \left(e^{-z|\cdot|}\,(\alpha-\alpha_0)^{\frac{1}{2}}, (I+\lambda P_\alpha)^{-1}\, e^{-z|\cdot|}\,|\alpha-\alpha_0|^{\frac{1}{2}} \right)$$

we have

$$\begin{aligned} \frac{\partial F}{\partial z}(0,0) &= 1 \\ \frac{\partial F}{\partial \lambda}(0,0) &= \frac{1}{2}\,|\chi_1(0)|^2 \left((\alpha-\alpha_0)^{\frac{1}{2}}, |\alpha-\alpha_0|^{\frac{1}{2}} \right) \\ \frac{\partial^2 F}{\partial z^2}(0,0) &= 0 \\ \frac{\partial^2 F}{\partial \lambda^2}(0,0) &= |\chi_1(0)|^2 \left((\alpha-\alpha_0)^{\frac{1}{2}}, P_0\,|\alpha-\alpha_0|^{\frac{1}{2}} \right) \\ \frac{\partial^2 F}{\partial \lambda \partial z}(0,0) &= -|\chi_1(0)|^2 \left((\alpha-\alpha_0)^{\frac{1}{2}}, |\cdot|\,|\alpha-\alpha_0|^{\frac{1}{2}} \right) ; \end{aligned}$$

since $F(0,0) = 0$ and

$$\dot z = -\frac{\frac{\partial F}{\partial \lambda}}{\frac{\partial F}{\partial z}} \qquad \text{and} \qquad \ddot z = -\frac{\frac{\partial^2 F}{\partial \lambda^2} + 2\dot z \frac{\partial^2 F}{\partial \lambda \partial z} + \dot z^2 \frac{\partial^2 F}{\partial z^2}}{\frac{\partial F}{\partial z}},$$

we see that, by the implicit-function theorem, (4.17) has a unique solution for λ small and it is given by (4.21).

It remains to prove that such solution is strictly positive for λ small. It is clearly fulfilled, if $\int(\alpha(x)-\alpha_0)dx < 0$. If this integral is zero, the first term of order λ in the expansion (4.21) vanishes and we have to prove then that the term of order λ^2 is strictly positive. One can do it by the following trick:

$$\begin{aligned} &-\int_{\mathbb{R}^2} (\alpha(x)-\alpha_0)|x-x'|(\alpha(x')-\alpha_0)dxdx' \\ &\qquad = \lim_{\xi\to 0+} 2\int_{\mathbb{R}^2} (\alpha(x)-\alpha_0)\frac{e^{-\xi|x-x'|}-1}{2\xi}(\alpha(x')-\alpha_0)dxdx' \end{aligned}$$

$$= \lim_{\xi\to 0+} 2\int_{\mathbb{R}^2} (\alpha(x)-\alpha_0)\frac{e^{-\xi|x-x'|}}{2\xi}(\alpha(x')-\alpha_0)dxdx'$$
$$= \lim_{\xi\to 0+} 2\int_{-\infty}^{\infty} |\widehat{(\alpha-\alpha_0)}(k)|^2 \frac{dk}{k^2+\xi^2}$$
$$= 2\int_{-\infty}^{\infty} |\widehat{(\alpha-\alpha_0)}(k)|^2 \frac{dk}{k^2} > 0.$$

The third equality follows from the fact that $\int(\alpha(x)-\alpha_0)dx = 0$. The assumption of the theorem, $\alpha-\alpha_0 \not\equiv 0$, justifies the strict inequality.

Analogically for the second term of order λ^2:

$$\int_{\mathbb{R}^2} (\alpha(x)-\alpha_0)\frac{e^{-\sqrt{\nu_n-\nu_1}|x-x'|}}{\sqrt{\nu_n-\nu_1}}(\alpha(x')-\alpha_0)dxdx'$$
$$= 2\int_{-\infty}^{\infty} |\widehat{(\alpha-\alpha_0)}(k)|^2 \frac{dk}{k^2+\nu_n-\nu_1} > 0. \quad \blacksquare$$

Remark IV.1 The assertion of the theorem holds for *all* $\lambda > 0$, provided $\alpha(x) < \alpha_0$ a.e. in $\mathbb{R}$. This is because, if $q_{\tilde\alpha} \le \nu_1$ and the *barrier function* satisfies $\alpha(x) < \tilde\alpha(x)$ a.e. in $\mathbb{R}$, then $H_\alpha < H_{\tilde\alpha}$ holds in the form sense, $q_\alpha < q_{\tilde\alpha} \le \nu_1$. Thus, by the *minimax principle*, the number of eigenvalues below ν_1 increases.

IV.3 Scaling Behaviour

IV.3.1 Motivation

Suppose that $\int(\alpha(x)-\alpha_0)\,dx < 0$. In the previous section we have found the behaviour of the ground-state energy if the *coupling "constant"* $\alpha-\alpha_0$ is small in the supremum norm. Indeed, the asymptotic formula (4.21) tells us that

$$E(\lambda) = \nu_1 - c\lambda^2 + \mathcal{O}(\lambda^3)\,, \qquad c := \frac{|\chi_1(0)|^4}{4}\left(\int_{\mathbb{R}}(\alpha(x)-\alpha_0)\,dx\right)^2. \tag{4.22}$$

One can compare this with the similar "weak coupling" result in [7] (Thm. 1.2.) where a straight Dirichlet strip with an arbitrarily small protrusion is investigated.

A different situation appears in [20]. The authors studied numerically the rate at which the ground-state energy emerges from the continuum in a quantum waveguide coupled laterally through a boundary window (this corresponds formally to $\alpha_0 = \infty$ in the present notation) and observed (*cf.* Sec. VI.1 of [20]) that

$$E(\ell) = \left(\frac{\pi}{d}\right)^2 - c(\nu)\ell^4 + \mathcal{O}(\ell^5), \tag{4.23}$$

where ℓ is the window width and d, ν coincide with our notation (2.3). In [21] it is proved that there are positive c_1, c_2 such that

$$-c_1\ell^4 \le E(\ell) - \left(\frac{\pi}{d}\right)^2 \le -c_2\ell^4.$$

An analogous result was obtained for bent pipes studied in [3]: for small angles, the binding energy is found to be quartic with respect to the bending angle.

We have excluded the possibility $\alpha(x) = \infty$ in Remark II.1 and therefore we cannot apply the results of Chap. III to the mentioned "window situation". However, we would like to study the bound state problem if $\mathrm{supp}(\alpha - \alpha_0) \to 0$ for $\|\alpha - \alpha_0\|_\infty$ fixed. More specifically, we regard the scaling Hamiltonian given by scaling of the *coupling function*:

$$\alpha_\sigma(x) := \alpha\left(\frac{x}{\sigma}\right) \tag{4.24}$$

with the scaling parameter $\sigma \in (0, 1]$ and consider the limit $\sigma \to 0+$.

We shall proceed in the similar way as above. The main tool for investigation of the discrete spectrum is again Theorem IV.2 which stays valid after the scaling.

However, as Remarks IV.2 1. below shows, one cannot apply the implicit-function theorem in order to derive an expansion analogous to (4.21). To obtain an asymptotic formula for κ_1 yet, we employ the simpler decomposition (4.11) which requires

(a2') $\quad \alpha(x) - \alpha_0 \in L^1(\mathbb{R}, |x|^2\, dx)$.

Nevertheless, the sought assertions are given by a slight modification of the claims of the previous section and are summarized below.

IV.3.2 Summary of the Modified Results

The next corollary immediately follows from Proposition IV.1 and the fact that $\|\alpha_\sigma - \alpha_0\|_1 = \sigma \|\alpha - \alpha_0\|_1$.

Proposition IV.4

$$\lim_{\sigma \to 0} k^2 = \nu_1 \qquad (\text{i.e. } \kappa_1 \to 0) \tag{4.25}$$

We put

$$K^k_{\alpha_\sigma} = L_{\alpha_\sigma} + P_{\alpha_\sigma} = L_{\alpha_\sigma} + M_{\alpha_\sigma} + N_{\alpha_\sigma}$$

with kernels

$$\begin{aligned}
L_{\alpha_\sigma}(x, x') &= |\alpha_\sigma(x) - \alpha_0|^{\frac{1}{2}}\, \frac{|\chi_1(0)|^2}{2\kappa_1}\, (\alpha_\sigma(x') - \alpha_0)^{\frac{1}{2}} \\
M_{\alpha_\sigma}(x, x') &= |\alpha_\sigma(x) - \alpha_0|^{\frac{1}{2}}\, \frac{|\chi_1(0)|^2}{2\kappa_1}\, (e^{-\kappa_1|x-x'|} - 1)\, (\alpha_\sigma(x') - \alpha_0)^{\frac{1}{2}} \qquad (4.26) \\
N_{\alpha_\sigma}(x, x') &= |\alpha_\sigma(x) - \alpha_0|^{\frac{1}{2}} \sum_{n=2}^{\infty} \frac{|\chi_n(0)|^2}{2\kappa_n}\, e^{-\kappa_n|x-x'|}\, (\alpha_\sigma(x') - \alpha_0)^{\frac{1}{2}} .
\end{aligned}$$

Next we define

$$\begin{aligned}
M_{0_\sigma}(x, x') &:= -|\alpha_\sigma(x) - \alpha_0|^{\frac{1}{2}}\, \frac{|\chi_1(0)|^2}{2}\, |x - x'|\, (\alpha_\sigma(x') - \alpha_0)^{\frac{1}{2}} \qquad (4.27) \\
N_{0_\sigma}(x, x') &:= |\alpha_\sigma(x) - \alpha_0|^{\frac{1}{2}} \sum_{n=2}^{\infty} \frac{|\chi_n(0)|^2}{2}\, \frac{e^{-\sqrt{\nu_n - \nu_1}|x-x'|}}{\sqrt{\nu_n - \nu_1}}\, (\alpha_\sigma(x') - \alpha_0)^{\frac{1}{2}} . \qquad (4.28)
\end{aligned}$$

In analogy to Propositions IV.2 and IV.3, we have

Proposition IV.5 *Assume that the assumptions (a1), (a2') are valid, then*

$$\lim_{\kappa_1\to 0}\|M_{\alpha_\sigma}-M_{0_\sigma}\|_{HS}=0 \qquad \text{and} \qquad \lim_{\kappa_1\to 0}\|N_{\alpha_\sigma}-N_{0_\sigma}\|_{HS}=0\,. \tag{4.29}$$

Proof: One should check the first assertion (the second one is exactly the claim of Proposition IV.3), however, M_{0_σ} is Hilbert-Schmidt since

$$\|M_0\|^2_{HS}\le\sigma^4\,\frac{|\chi_1(0)|^4}{4}\int_{\mathbb{R}^2}|\alpha(x)-\alpha_0|\;(|x|^2+|x'|^2)\;|\alpha(x')-\alpha_0|\,dx\,dx'<\infty$$

and

$$\begin{aligned}\lim_{\kappa_1\to 0}M_{\alpha_\sigma} &= M_{0_\sigma}\\ |M_{\alpha_\sigma}(x,x';\kappa_1)| &\le |M_{0_\sigma}(x,x')| \qquad (\Leftarrow\forall x\ge 0: 1-e^{-x}\le x)\,,\end{aligned}$$

and thus by the dominated convergence theorem,

$$\int_{\mathbb{R}^2}|(M_{\alpha_\sigma}-M_{0_\sigma})(x,x')|^2\,dx\,dx'\to 0\,. \quad \blacksquare$$

It is easy to check that the norms of the operators $M_{\alpha_\sigma}, N_{\alpha_\sigma}$ can be made arbitrarily small by choosing σ small enough because

$$\|M_{\alpha_\sigma}\|^2_{HS}\le K_1\,\sigma^4 \qquad \text{and} \qquad \|N_{\alpha_\sigma}\|^2_{HS}\le K_2\,\sigma\,. \tag{4.30}$$

Lemmas IV.1 and IV.2 remain valid without any changes. Since the latter is rather algebraic, it holds for the operator M_{α_σ} as well.

Finally, we have to modify Lemmas IV.3–IV.5. But it is very simple to check the following results.

Lemma IV.7 *If $\alpha-\alpha_0\not\equiv 0$, then $|z|^{-1}\le C_1\sigma^{-1}$ for σ small.*

Lemma IV.8 *For sufficiently small z,*

$$\left\|\frac{\partial P_{\alpha_\sigma}}{\partial z}\right\|<C_2\frac{\sqrt{\sigma}}{|z|}.$$

Lemma IV.9

$$\forall z_0\in\mathbb{R}\quad\exists C_3>0\quad\forall z\in[0,z_0]\;:\;\left|\left(|\alpha_\sigma-\alpha_0|^{\frac12},\frac{\partial P_\alpha}{\partial z}\,|\alpha_\sigma-\alpha_0|^{\frac12}\right)\right|\le C_3\sigma^2$$

Proof: Here one has only to show that

$$\frac{\partial M_{\alpha_\sigma}}{\partial z}(x,x')=-\frac{|\chi_1(0)|^2}{2}\,|\alpha_\sigma(x)-\alpha_0|^{\frac12}\,(\alpha_\sigma(x')-\alpha_0)^{\frac12}\,\frac{e^{-z|x-x'|}+z\,|x-x'|\,e^{-z|x-x'|}-1}{z^2}$$

remains bounded as $z\to 0+$ but it is clear from the elementary inequality $\forall x\ge 0: 1-e^{-x}-xe^{-x}\le x^2$. The rest of the proof follows by a simple modification of the proof of Lemma IV.5 and by the rescaling of the integral's variables, $(x,x')\mapsto\sigma(x,x')$. $\blacksquare$

With such preliminaries we can now formulate and prove the theorem analogous to Theorem IV.3.

IV.3.3 The Main Theorem

Theorem IV.5 *Assume that the assumption (a1), (a2') are valid. Then, for σ small, H_{α_σ} has at most one simple eigenvalue $E(\sigma) < \nu_1$, and this happens if and only if*

$$\sqrt{\nu_1 - E} \equiv \kappa_1 = -\frac{|\chi_1(0)|^2}{2} \left((\alpha_\sigma - \alpha_0)^{\frac{1}{2}}, (I + P_{\alpha_\sigma})^{-1} |\alpha_\sigma - \alpha_0|^{\frac{1}{2}} \right) \tag{4.31}$$

has a solution $\kappa_1 > 0$.

Proof: By means of the claims of the previous section we can now follow by mimicking the proof of Theorem IV.3. Since $\|P_{\alpha_\sigma}\| < 1$ holds for small enough σ, we may write

$$(I + K^k_{\alpha_\sigma})^{-1} = \left[I + (I + P_{\alpha_\sigma})^{-1} L_{\alpha_\sigma} \right]^{-1} (I + P_{\alpha_\sigma})^{-1}.$$

$(I + P_{\alpha_\sigma})^{-1} L_{\alpha_\sigma}$ has just one eigenvalue (ψ, φ) with

$$\begin{aligned} \psi &:= \frac{|\chi_1(0)|^2}{2\kappa_1} \, (\alpha_\sigma(\cdot) - \alpha_0)^{\frac{1}{2}} \\ \varphi &:= (I + P_{\alpha_\sigma})^{-1} \, |\alpha_\sigma(\cdot) - \alpha_0|^{\frac{1}{2}} \, . \end{aligned}$$

Putting it equal to -1 we get the implicit equation (4.31).

As above, we can introduce

$$G(z, \sigma) := \frac{|\chi_1(0)|^2}{2} \left(|\alpha_\sigma - \alpha_0|^{\frac{1}{2}}, (I + P_{\alpha_\sigma})^{-1} |\alpha_\sigma - \alpha_0|^{\frac{1}{2}} \right) \tag{4.32}$$

and obtain the estimate

$$\begin{aligned} \left| \frac{\partial G}{\partial z} \right| \;\leq\; & d \, \frac{|\chi_1(0)|^2}{2} \left\{ \left| \left(|\alpha_\sigma - \alpha_0|^{\frac{1}{2}}, \frac{\partial P_{\alpha_\sigma}}{\partial z} |\alpha_\sigma - \alpha_0|^{\frac{1}{2}} \right) \right| \right. \\ & + \left| \left(|\alpha_\sigma - \alpha_0|^{\frac{1}{2}}, \left[P_{\alpha_\sigma} \frac{\partial P_{\alpha_\sigma}}{\partial z} + \frac{\partial P_{\alpha_\sigma}}{\partial z} P_{\alpha_\sigma} \right] |\alpha_\sigma - \alpha_0|^{\frac{1}{2}} \right) \right| \\ & \left. + \left| \left(|\alpha_\sigma - \alpha_0|^{\frac{1}{2}}, P_{\alpha_\sigma} \frac{\partial P_{\alpha_\sigma}}{\partial z} P_{\alpha_\sigma} |\alpha_\sigma - \alpha_0|^{\frac{1}{2}} \right) \right| \right\} < C \, \sigma^2 \, . \end{aligned}$$

It means that the uniqueness of the solution is now ensured for $\sigma < C^{-1/2}$. ∎

IV.3.4 Condition for a Bound State

With these preliminaries, we can formulate and prove now a necessary and sufficient condition for the existence of a bound state in case of small σ.

Theorem IV.6 *Let α satisfies the assumptions (a1), (a2') and $\alpha-\alpha_0 \not\equiv 0$. Then H_{α_σ} has an eigenvalue $E(\sigma) < \nu_1$ for all σ small enough if and only if*

$$\int_{\mathbb{R}} (\alpha(x)-\alpha_0)\, dx \leq 0\,. \tag{4.33}$$

If this condition holds, then the eigenvalue is unique and simple and obeys

$$\begin{aligned}\sqrt{\nu_1 - E(\sigma)} = &-\frac{\sigma}{2}\,|\chi_1(0)|^2 \int_{\mathbb{R}} (\alpha(x)-\alpha_0)\, dx \\ &+\frac{\sigma^2}{4}\,|\chi_1(0)|^2 \sum_{n=2}^{\infty} |\chi_n(0)|^2 \int_{\mathbb{R}^2} (\alpha(x)-\alpha_0)\, \frac{e^{-\sigma\sqrt{\nu_n-\nu_1}|x-x'|}}{\sqrt{\nu_n-\nu_1}}\, (\alpha(x')-\alpha_0)\, dx\, dx' \\ &+\mathcal{O}(\sigma^3)\,. \end{aligned} \tag{4.34}$$

PROOF: Writing

$$(I + P_{\alpha_\sigma})^{-1} = I - P_{0_\sigma} - (P_{\alpha_\sigma} - P_{0_\sigma}) + P_{\alpha_\sigma}^2 (I + P_{\alpha_\sigma})^{-1}, \tag{4.35}$$

we see that (4.31) has a unique solution for σ small and it is given by (4.34). (It is only important to notice that although σ does not take place in the expansion (4.35) explicitly, it appears after putting (4.35) into (4.31) because of the integration. That is also why we can be sure that the last term in (4.35) does not contributes to the leading terms in (4.34).)

The proof of the strict positivity of such a solution is exactly the same as in the case of Theorem IV.4. ∎

Remarks IV.2 1. We cannot expand the exponential in the second leading term of (4.34) because of the convergence of the sum.
2. Now we would like to make the limit $\alpha_0 \to \infty$ (note that $\chi_n(0)$ decay like $\mathcal{O}(\alpha_0^{-1})$ as $\alpha_0 \to \infty$) for $\alpha \equiv 0$ to get the behaviour (4.23). The first term in (4.34) vanishes after that but it seems that we cannot interchange the summation and limitation in the next one!

Chapter V

Numerical Solution

To learn more about the bound states and scattering in our system, one has to solve the corresponding Schrödinger equation numerically. To employ the mode-matching method we take the *barrier function* α so that the waveguide consists of several rectangular regions. We restrict our attention to the situation

$$\alpha(x) := \begin{cases} \alpha_1 & \text{if} \quad |x| < a \\ \\ \alpha_0 & \text{if} \quad |x| \leq a \end{cases}$$

with $a > 0$, $\alpha_1, \alpha_0 \in \mathbb{R}$ and $-(d_1^{-1} + d_2^{-1}) < \alpha_1 < \alpha_0$. The choice $\alpha_1 = 0$ and α_0 large enough will then enable us to approach some results of the "window" situation in [20]. Henceforth, we shall denote the corresponding transverse eigenvalues as $\nu_n^s := \nu_n(\alpha_s)$, $s := 0, 1$, $n \in \mathbb{N}\setminus\{0\}$.

In view of the natural mirror symmetry with respect to the y-axis we may consider separately the symmetric and antisymmetric solutions, *i.e.* regard the halfstrip with the Neumann or Dirichlet conditions at $x = 0$, respectively.

Before we write down formulae for the numerical solution, we mimic the process introduced in Preliminaries of [20] and derive in this way some useful estimates.

V.1 Preliminaries

The bracketing procedure in the proof of Theorem IV.1 enabled us to localize the essential spectrum of our Hamiltonian H_α for the general shape of α (specified only by the decay assumptions (i), (ii)). We can apply this result to the present situation, *i.e.*, $\sigma_{ess}(H_\alpha) = [\nu_1^0, \infty)$.

Moreover, one can now show that H_α has bound states for a large enough even without the variational proof given in the mentioned theorem. Isolated eigenvalues of H_α are squeezed between those of $H_{\alpha,c}^{(j)}$ ($j = N, D$), the *central* part Hamiltonians (see (4.2)). The Neumann estimate tells us that $\inf \sigma(H_\alpha) \geq \nu_1^1$. On the other hand, H_α has an eigenvalue below ν_1^1 provided $H_{\alpha,c}^{(D)}$ does, which is true if $\nu_1^1 + \left(\frac{\pi}{2a}\right)^2 \leq \nu_1^0$;

this shows that a sufficient condition for H_α to have at least a bound state is

$$a \geq \frac{\pi}{2\sqrt{\nu_1^0 - \nu_1^1}}. \tag{5.1}$$

More generally, the number of eigenvalues of $H_{\alpha,c}^{(D)}$ is $N_D := \left[\frac{2a}{\pi}\sqrt{\nu_1^0 - \nu_1^1}\right]$, where $[\cdot]$ denotes the entire part, while the number of the "Neumann" eigenvalues is $N_N := N_D + 1$; this means that the number of bound states of H_α satisfies the inequality $N_D \leq N \leq 1 + N_D$.

In the same way, one finds that the n-th eigenvalue E_n of H_α is estimated by

$$\nu_1^1 + \left(\frac{(n-1)\pi}{2a}\right)^2 \leq E_n \leq \nu_1^1 + \left(\frac{n\pi}{2a}\right)^2, \tag{5.2}$$

and that the critical a_n at which n-th eigenvalue appears satisfies the bounds

$$\frac{(n-1)\pi}{2\sqrt{\nu_1^0 - \nu_1^1}} \leq a_n \leq \frac{n\pi}{2\sqrt{\nu_1^0 - \nu_1^1}}. \tag{5.3}$$

V.2 Bound States

V.2.1 The Symmetric Case

Consider first the situation $\nu = 1$ ($d_1 = d_2 = d$). The Hamiltonian then decouples into an orthogonal sum of the even and the odd part, the spectrum of the latter being clearly trivial (*cf.* Remarks II.2 1).

This and the mentioned mirror symmetry w.r.t. the y-axis allow us to restrict ourselves to the part of Ω in the first quadrant, with Neumann or Dirichlet condition in the segment $(0, d)$ of the y-axis, and take the transverse eigenvalues determined by the spectral conditions

$$\begin{aligned} -\alpha_0 &= 2k \cot kd \qquad \text{if} \quad x \geq a \\ -\alpha_1 &= 2k \cot kd \qquad \text{if} \quad 0 \leq x < a. \end{aligned}$$

The corresponding transverse eigenfunctions are

$$\chi_n := -N_n^0 \sin\sqrt{\nu_n^0}(y-d) \qquad \text{if} \quad x \geq a \tag{5.4}$$

$$\phi_n := -N_n^1 \sin\sqrt{\nu_n^1}(y-d) \qquad \text{if} \quad 0 \leq x < a. \tag{5.5}$$

N_n^s denotes the norm so that χ_n, ϕ_n would be unit vectors in $L^2(0,d)$

$$(N_n^s)^2 = \frac{4\sqrt{\nu_n^s}}{2\sqrt{\nu_n^s}d - \sin 2\sqrt{\nu_n^s}d}\ . \tag{5.6}$$

The overlap integrals of the two bases are easily seen to be

$$(\chi_m, \phi_n) = \frac{N_m^0 N_n^1}{\nu_m^0 - \nu_n^1}(\sqrt{\nu_n^1}\sin\sqrt{\nu_m^0}d\cos\sqrt{\nu_n^1}d - \sqrt{\nu_m^0}\sin\sqrt{\nu_n^1}d\cos\sqrt{\nu_m^0}). \tag{5.7}$$

A natural Ansatz for the solution of an energy E, $\nu_1^1 \le E < \nu_1^0$, is

$$\begin{aligned} \Psi_{s/a}(x,y) &= \sum_{n=1}^{\infty} b_n^{s/a} e^{-q_n(x-a)}\chi_n(y) \qquad\qquad \text{for} \quad x \ge a \\ \Psi_{s/a}(x,y) &= \sum_{n=1}^{\infty} a_n^{s/a} \left\{ \begin{array}{c} \frac{\cosh p_n x}{\cosh p_n a} \\ \\ \frac{\sinh p_n x}{\sinh p_n a} \end{array} \right\} \phi_n(y) \qquad \text{for} \quad 0 \le x < a \end{aligned} \tag{5.8}$$

where the subscripts and superscripts (we will omit them for the most part) s, a distinguish the symmetric and antisymmetric case, respectively. The longitudinal momenta are defined by

$$q_n := \sqrt{\nu_n^0 - E}\,, \qquad p_n := \sqrt{\nu_n^1 - E}\,.$$

As an element of the domain (2.1), the function Ψ should be continuous together with its normal derivative at the segment dividing the two regions, $x = a$. Using the orthonormality of $\{\chi_n\}$ we get from the requirement of continuity

$$b_m = \sum_{n=1}^{\infty} a_n(\chi_m, \phi_n)\,. \tag{5.9}$$

In the same way, the normal-derivative continuity at $x = a$ yields

$$b_m q_m + \sum_{n=1}^{\infty} a_n p_n \left\{ \begin{array}{c} \tanh \\ \coth \end{array} \right\} (p_n a)(\chi_m, \phi_n) = 0\,. \tag{5.10}$$

Substituting from (5.9) to (5.10), we can write the equation as

$$\boldsymbol{Ca = 0}\,, \tag{5.11}$$

where

$$C_{mn} := \left(q_m + p_n \left\{ \begin{array}{c} \tanh \\ \coth \end{array} \right\} (p_n a) \right) (\chi_m, \phi_n) \tag{5.12}$$

with the overlap integrals given by (5.7).

It is straightforward to compute the norms of the function (5.8); since $n^{-1}q_n$ an $n^{-1}p_n$ tend to $\frac{\pi}{d}$ as $n \to \infty$ (see (2.10)), the square integrability of Ψ requires the sequences $\{a_n\}$ and $\{b_n\}$ to belong to the space $\ell^2(n^{-1})$.

To make sure that the equation (5.11) makes sense, it is enough to notice that if Ψ is an eigenvector of H_α, it must belong to the domain of any integer power of this operator. It is easy to check that

$$\forall i \in \mathbb{N}\setminus\{0\}: \quad \Psi \in D(H_\alpha^i) \Leftrightarrow \{a_n\}, \{b_n\} \in \ell^2(n^{4i-1})\,; \tag{5.13}$$

hence the sought sequences should belong to $\ell^2(n^r)$ for all $r \geq -1$, *i.e.* both sequences have a faster than powerlike decay. This fact also justifies *a posteriori* the interchange of summation and differentiation we have made in the matching procedure.

Next one has to check that the equation (5.11) can be solved by a sequence of truncations. The idea of [20], Sec. IV.1, consists in making use of the diagonal operator S_r on $\ell^2(n^{-1})$, $(S_r a)_n := n^{-r} a_n$. Instead of C the authors consider the operator $C^{(p,r)} := S_p C S_r$ with arbitrary non-negative p, r. If C has zero eigenvalue with a fast decaying eigenvector, the same is true for $C^{(p,r)}$, which is Hilbert-Schmidt for p, r large enough, and its eigenvalues can therefore be obtained from a sequence of truncated operators.

Remark V.1 (an alternative method) We can use the orthonormality of $\{\phi_n\}$ instead of $\{\chi_n\}$ and express $\{a_n\}$ in analogy to (5.9), and then substitute it into (5.10). We find that the coefficient sequence $\{b_n\}$ is then determined by the following equation:

$$\boldsymbol{b} + \boldsymbol{K}\boldsymbol{b} = \boldsymbol{0}\,, \tag{5.14}$$

where

$$K_{mn} := \frac{1}{q_m} \sum_{k=1}^{\infty} (\chi_m, \phi_k)\, p_k \left\{ \begin{array}{c} \tanh \\ \coth \end{array} \right\} (p_k a)\, (\phi_k, \phi_n)\,. \tag{5.15}$$

As was mentioned in Sec IV.2 of [20], even if the two approaches (5.11), (5.14) are equivalent, the analysis of their numerical results can give a good idea about the numerical stability of the solution. It is due to the fact that the sequences coming from (5.11) were approaching the limiting values from above, while those obtained from (5.14) were increasing. We do not elaborate on this investigation here.

Now passing to the natural non-dimensional quantities, one can solve the equation (5.11) by standard numerical methods (*cf.* [36]).

V.2.2 The Asymmetric Case

Let us pass now to the case, when the widths of the ducts are nonequal, $\nu \neq 1$. Becauase of the mirror symmetry with respect to the y-axis, we shall consider right-halfplane part of Ω only with the Neumann and Dirichlet condition on the segment $[-d_2, d_1]$ of the y-axis.

This case differs from the previous just in the choice of transverse base. Now we can take

$$\chi_n(y) := \chi_n(y; \alpha_0) \qquad \text{if} \quad x \geq a \tag{5.16}$$

$$\phi_n(y) := \chi_n(y; \alpha_1) \qquad \text{if} \quad 0 \leq x < a, \tag{5.17}$$

where $\chi_n(\cdot, \alpha_s)$ are of the form (2.6) with the norms N_n^s given by (2.7). The corresponding eigenvalues ν_n^0, ν_n^1 are then determined by (see (2.4))

$$\begin{aligned} -\alpha_0 &= k\,(\cot kd_1 + \cot kd_2) \qquad \text{if} \quad x \geq a \\ -\alpha_1 &= k\,(\cot kd_1 + \cot kd_2) \qquad \text{if} \quad 0 \leq x < a\,. \end{aligned}$$

The overlap integrals are now given by

$$(\chi_m, \phi_n) = \frac{N_m^0 N_n^1}{\nu_m^0 - \nu_n^1} \left(\sqrt{\nu_n^1} \sin\sqrt{\nu_m^0} d_1 \sin\sqrt{\nu_m^0} d_2 \sin\sqrt{\nu_n^1} D \right. \\ \left. -\sqrt{\nu_m^0} \sin\sqrt{\nu_n^1} d_1 \sin\sqrt{\nu_n^1} d_2 \sin\sqrt{\nu_m^0} D\right) . \tag{5.18}$$

The other results do not change and one can again solve the equation (5.11) (or (5.14), respectively). By a straightforward modification of the above argument, one can also check that the coefficient sequences have a faster than powerlike decay and the equation can be solved by a sequence of truncations.

V.3 Scattering

The scattering can be treated in an analogous way. The incident wave is supposed to be of the form $e^{-ik_r x}\chi_r(y)$, where we have introduced $k_r := \sqrt{k^2 - \nu_r^0}$. We denote by r_{rn}, t_{rn}, respectively, the corresponding reflection and transmission amplitudes to the n-th transverse mode. Due to the mirror symmetry , we can again separate the symmetric and antisymmetric situation w.r.t. $x = 0$ ant to write

$$r_{rn} = \frac{1}{2}(\rho_{rn}^s + \rho_{rn}^a) , \qquad t_{rn} = \frac{1}{2}(\rho_{rn}^s - \rho_{rn}^a) , \tag{5.19}$$

where ρ_{rn}^σ, $\sigma = s, a$, are the reflection amplitudes in the halfwaveguide with the Neumann and Dirichlet condition at $x = 0$, respectively.

We use the following Ansatz

$$\begin{aligned} \Psi_{s/a}(x, y) &= \sum_{n=1}^{\infty} \left(\delta_{rn} e^{-ik_n(x-a)} + \rho_{rn}^{s/a} e^{ik_n(x-a)}\right) \chi_n(y) \qquad \text{for} \quad x \geq a \\ \Psi_{s/a}(x, y) &= \sum_{n=1}^{\infty} a_n^{s/a} \left\{ \begin{array}{c} \frac{\cos p_n x}{\cos p_n a} \\ \\ \frac{\sin p_n x}{\sin p_n a} \end{array} \right\} \phi_n(y) \qquad \text{for} \quad 0 \leq x < a \end{aligned} \tag{5.20}$$

for the energy k^2 of the incident wave in the r-th mode. The longitudinal momentum is $p_n := \sqrt{k^2 - \nu_n^1}$. Matching these functions smoothly at $x = a$ we arrive in the same way as above at the equation

$$\boldsymbol{Ca} = \boldsymbol{f} , \tag{5.21}$$

where

$$C_{mn} := \left(ik_m + p_n \left\{ \begin{array}{c} \tan \\ -\cot \end{array} \right\} (p_n a)\right) (\chi_m, \phi_n) \tag{5.22}$$

$$f_m := 2ik_m \delta_{rm} \tag{5.23}$$

where the index r corresponds to the incident wave and the overlap integrals are given again by (5.18). The reflection amplitudes are given then by

$$\rho_{rm} = -\delta_{rm} + \sum_{n=1}^{\infty} a_n(\chi_m, \phi_n)\,; \tag{5.24}$$

they determine the full S-matrix via (5.19).

V.3.1 Physically Interesting Quantities

The knowledge of the reflection and transmission coefficients makes it possible to express quantities of a direct physical interest, in the first place the conductivity which is given by the Landauer formula (measured in the standard units $2e^2/h$)

$$G(k) = \sum_{m,n=1}^{[k]} \frac{k_n}{k_m} |t_{mn}(k)|^2\,, \tag{5.25}$$

where $t_{mn}(k)$ are the coefficients (5.19). The summation runs over all open channels.

Another physically interesting quantity is the probability flow distribution associated with the generalized eigenvector $\Psi = \Psi_s + \Psi_a$. Putting $\hbar/2m = 1$, we may write (*cf.* [22], Kap. 3.3)

$$\vec{j}(\vec{x}) = 2\,\mathrm{Im}\left(\bar{\Psi}(\vec{x})\nabla\Psi(\vec{x})\right). \tag{5.26}$$

V.4 The Results

Let us now mention of the results of the mode-matching computation. Some of them are illustrated on figures in Appendix A.

Since it is advantageous to solve the equations (5.11) and (5.21) in the natural non-dimensional quantities, the figures are presented in them as well. In order to avoid any obscurities we summarize the redefined quantities in Table V.1.

Table V.1: Passing to the non-dimensional quantities

dimensional quantity	=	conversion factor	×	non-dimensional quantity
α_s	=	$1/d$	×	α_s
ν_n^s	=	$(\pi/d)^2$	×	ν_n^s
E	=	$(\pi/d)^2$	×	E
k	=	(π/d)	×	k

V.4.1 Bound States

Eigenvalues

Figures 1–2 show the bound-state energies as functions of the "window" width a for $\alpha_1 = 0$. There are plotted several curves of distinctive structures; each of them corresponds to a fix *barrier function*, α_0 (*cf.* Table A.1).

In accordance with the general results of Section V.1 the energies decrease monotonously with the increasing "window" and one can sandwich them between the estimates (5.2). Next we can deduce that for a fixed a the energies increase with respect to α_0 and ν; recall that their number increases as a function of α_0 but it decreases as the waveguide becomes more asymmetric. These facts are clear from (5.2), (5.3) and Proposition II.1.

Now we would like to confront our results for large α_0 with the energies computed in [20] which corresponds formally to $\alpha_0 = \infty$. Comparing Figure 1 with Fig. 2 of [20] we see that our result for $\alpha_0 = 100000$ is almost identical with the latter.

Threshold Behaviour

For simplicity, let us assume that $\alpha_1 = 0$. As a consequence of Section IV.2 we get for the ground-state energy in the case of small α_0 the asymptotic formula (*cf.* (4.21) or (4.22))

$$E(a) = \nu_1^0 - ca^2 + \mathcal{O}(a^3) \ , \qquad c := \frac{\alpha_0^2}{(\pi d)^2} \ |\chi_1(0)|^4 \tag{5.27}$$

(we still use the non-dimensional quantities), while due to the results of Section IV.3 (*cf.* Remarks IV.2 2.) we may suppose that $E(a)$ converges to the order $\mathcal{O}(a^4)$ as $\alpha_0 \to \infty$. (This would also coincide with the result of [20].) Nevertheless, since $\chi_n(0)$ is a function of α_0, the asymptotic formula (4.34) does not give a satisfactory idea of the general rate at which the first eigenvalue emerges from the continuum.

In view of the above analysis we may assume that $E(a) = \nu_1^0 - ca^\beta$ for sufficiently small a and we look for the dependence of the coefficients β and c on α_0 numerically.

Indeed, redrawing the first eigenvalue curves of Figures 1–2 in the logarithmic scale, we find that the asymptotic behaviour is powerlike. The resulting functional dependences of the coefficients are illustrated on Figure 3 for the symmetric case. The expected limit cases $\beta = 2, 4$ for $\alpha_0 \to 0, \infty$, respectively, are thus clearly confirmed by the first graph and the behaviour of c for small α_0 coincides with that of (5.27).

Since the convergence of our method for small a is rather slow, we should use cut-off dimensions of large order. The authors of [20] use order 10^3 but due to lack of an efficient computer we use order 10^1 only. Furthermore, to find then the values of the coefficients we use the *method of least squares* but then there is a problem which points should be still included in the procedure (*i.e.*, which points still have a powerlike behaviour). We choose the best correlated points. In consequence, the first graph is slightly shifted down and exhibits numerical instability at small α_0.

Eigenfunctions

The evolution of the ground-state wavefunction with respect to α_0 is illustrated on Figure 4. One can again compare our result for $\alpha_0 = 100000$ with Fig. 3 in [20].

Figure 5 shows the analogous evolution of the first excited state in the unsymmetric case.

V.4.2 Scattering

Conductivity

An example of the conductivity for the particle coming from the right and leaving to the left as a function of the momentum k and the width d_2 is shown on Figure 6. We see that the perturbation, $\alpha_1 - \alpha_0$, deforms the ideal steplike shape. The deep resonances are clearly visible. We reproduce Fig. 5a of [20] provided $\alpha_0 = 100000$.

Figure 7 shows the same dependence for large a; as a result we have many more resonances.

Probability Flow

The examples of the quantum probability flows are shown on Figures 8–9. The flow patterns change with the momentum of the incident particle and the value of α_0. They exhibit conspicuous vortices at the resonance energies which represent the "trapped part" of the wavefunction.

An interesting phenomenon is illustrated on Figure 8 a: for $\alpha_0 = 100000$ there is a double vortex (corresponding to the sharp stopping resonance of Figure 6), right-handed in the upper duct, while for $\alpha_0 = 50$ we get a left-handed vortex. The conductivity is small in these situations so the waveguide system is closed for the particle transport. As α_0 decreases the conductivity grows and the system opens for the transport (*cf.* Figures 8 b–c).

Another interesting situation is demonstrated on Figure 9: for $\alpha_0 = 2$ we get suddenly a system of several vortices.

In [20] a remark was made that the vortices which emerge in resonance situations lead to the appearence of a magnetic dipole moment, which might be in principle measured experimentally; this idea was elaborated recently using a different geometry in [18].

Chapter VI

Aharonov-Bohm Cylinder

Let us show now how the preceding can be modified for a different geometry: we consider a nonrelativistic quantum particle living on the surface of an infinite straight cylinder of a radius R, which is placed into a homogeneous magnetic field $\vec{B}$ parallel to the cylinder axis. We assume that the motion is further restricted by a δ-barrier imposed on a line parallel to the axis.

VI.1 Preliminaries

VI.1.1 "Unfolding" the Cylinder

Figure VI.1 shows how the coordinate system is chosen. Now we can identify our configuration space with the set

$$\tilde{\Omega} := \{(x, y, z) \in \mathbb{R}^3 |\ y^2 + z^2 = R^2\}\,. \tag{6.1}$$

If we choose the gauge conditions so that the electromagnetic potentials fulfil $\varphi(\vec{x}) \equiv 0$ and $\vec{A}(\vec{x}) = \frac{1}{2}\vec{B} \times \vec{x}$, the particle Hamiltonian acquires the form (*cf.* [22], Kap. 8.2)

$$\tilde{H}_\alpha := (-i\nabla + \vec{A})^2 = -\Delta - i\frac{B}{2}(y\partial_z - z\partial_y) + \frac{B^2R^2}{4}\,. \tag{6.2}$$

(We have put $\hbar = 1$, $e = -1$ (charge), $m = \frac{1}{2}$ (mass).) The subscript α indicates the real function which gives the shape of the barrier as in the "waveguide situation". The Hamiltonian acts on $L^2(\tilde{\Omega})$ but it would be cumbersome to specify the δ-interaction by means of the Cartesian coordinates.

In view of the above stated conditions we have $A = \frac{1}{2}BR = \frac{\phi}{2\pi R}$, where ϕ is the magnetic flux through the cylinder.

A convenient way to study (6.2) is to introduce the unitary transformation (*cf.* [5], Příklad 5.5.3) $U : L^2(\tilde{\Omega}) \to L^2(\mathbb{R} \times [0, 2\pi R], dudv)$

$$(U\psi)(u, v) := \psi(u, R\cos\frac{v}{R}, R\sin\frac{v}{R})\,, \tag{6.3}$$

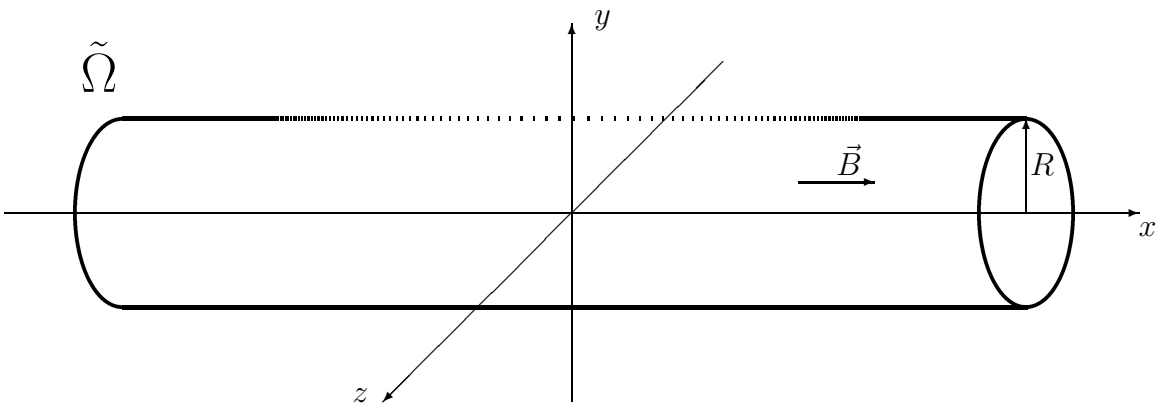

Figure VI.1: Cylindrical strip with a δ-barrier in axial magnetic field

which "straightens" the cylinder surface. More precisely, the configuration space $\tilde{\Omega}$ is in this way mapped onto the strip $\Omega := \mathbb{R} \times [0, 2\pi R]$ (*cf.* Figure VI.2), and the operator $\tilde{H}_\alpha$ is then unitarily equivalent to

$$H_\alpha := U \tilde{H}_\alpha U^{-1} = -\partial_u^2 + (-i\partial_v + A)^2 \,, \tag{6.4}$$

which acts on

$$D(H_\alpha) := \left\{ \psi \in W_2^2(\Omega) \,|\, \forall u \in \mathbb{R} : \begin{array}{l} \psi(u,0+) = \psi(u,2\pi R-) =: \psi(u,0) \\ \psi_v(u,0+) - \psi_v(u,2\pi R-) = \alpha(u)\psi(u,0) \end{array} \right\} . \tag{6.5}$$

Remark VI.1 We abuse notation and denote by the same *vector* symbol both a vector in $\mathbb{R}^3$, and a vector in $\mathbb{R}^2$. Hereafter, we shall be interested in the strip case only, however, we would like to stress the difference caused by the choice of the diverse coordinate systems only (*e.g.* a modulus is the same):

	$\mathbb{R}^3$	$\mathbb{R}^2$
$\vec{B} =$	$B\,(0,0,1)$	$B\,(1,0)$
$\vec{A} =$	$\frac{1}{2}B\,(0,-z,y)$	$\frac{1}{2}B\,(0,R)\,.$

Next we define the associated quadratic form q_α on $D(q_\alpha) := W_2^1(\Omega)$

$$\begin{aligned} q_\alpha[\psi] \;:=\; & \int_\Omega |\nabla\psi|^2(u,v)dudv + \int_{\mathbb{R}} \alpha(u)|\psi(u,0)|^2 du \\ & -i2A\int_\Omega (\bar{\psi}\partial_v\psi)(u,v)dudv + A^2\int_\Omega |\psi|^2(u,v)dudv \,. \end{aligned} \tag{6.6}$$

VI.1.2 The Unperturbed System

Now we shall look into the case $\alpha(u) = \alpha = const.$ when we can solve the Schrödinger equation by separation of variables again. Since our system is a little more complicated because of the presence of the magnetic field, we have to divide the transverse

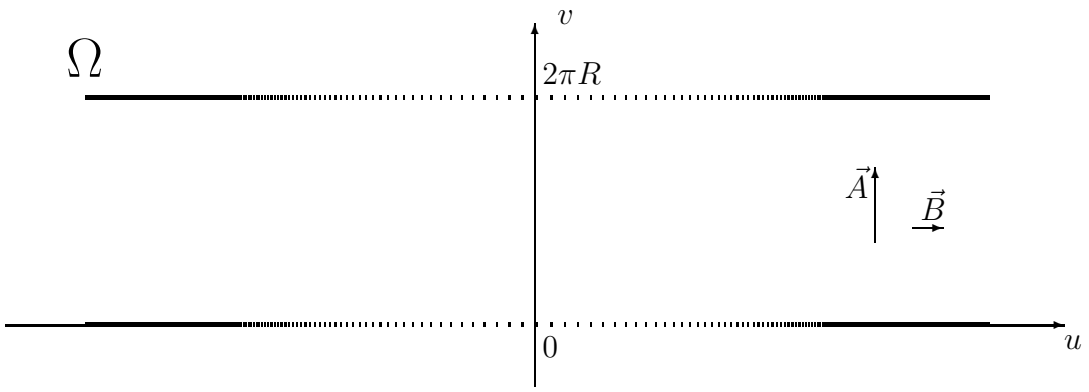

Figure VI.2: "Straightened" cylinder

solutions into several cases ($\{\nu_n\}_{n=1}^{\infty}$ and $\{\chi_n\}_{n=1}^{\infty}$ denote the sets of arranged transverse eigenvalues and corresponding eigenfunctions, respectively).

1. $\underline{\alpha = 0}$:

$$\forall \ell \in \mathbb{Z}: \qquad \tilde{\chi}_\ell(v) = \frac{1}{\sqrt{2\pi R}}\, e^{i\frac{\ell}{R}v}\,. \tag{6.7}$$

The tilde denotes the eigenfunctions of the corresponding eigenvalues $(\frac{\ell}{R}+A)^2$. To get $\{\nu_n\}$ one has to arrange them into a nondecreasing sequence. The corresponding eigenfunctions will be then denoted as $\{\chi_n\}$.

2. $\underline{0 \neq \alpha > \alpha_m := -\frac{2\sin^2 \pi RA}{\pi R}}$ and $\underline{2RA \notin \mathbb{N}}$:

$$\forall n \in \mathbb{N}\backslash\{0\}: \qquad \chi_n(v) = N_n e^{-iAv}\left(e^{i\sqrt{\nu_n}v} - \frac{e^{i2\pi RA} - e^{i2\pi R\sqrt{\nu_n}}}{e^{i2\pi RA} - e^{-i2\pi R\sqrt{\nu_n}}} e^{-i\sqrt{\nu_n}v}\right), \tag{6.8}$$

where N_n denotes the normalization factor chosen in such a way that χ_n would be a unit vector in $L^2(0, 2\pi R)$

$$|N_n|^2 := \frac{\sqrt{\nu_n}\ [1-\cos 2\pi R(\sqrt{\nu_n}+A)]}{4\pi R\sqrt{\nu_n}(1-\cos 2\pi RA\cos 2\pi R\sqrt{\nu_n})+2\sin 2\pi R\sqrt{\nu_n}(\cos 2\pi RA-\cos 2\pi R\sqrt{\nu_n})} \tag{6.9}$$

and the increasing sequence $\{\nu_n\}$ arises from the spectral condition

$$-\alpha = 2k\left(\cot 2\pi Rk - \frac{\cos 2\pi RA}{\sin 2\pi Rk}\right). \tag{6.10}$$

In analogy to (2.10) we have $\forall n \in \mathbb{N}\backslash\{0\}: \sqrt{\nu_n} \in \frac{1}{2R}(n-1, n)$.

3. $\underline{0 \neq \alpha > \alpha_m}$ and $\underline{2RA \ \text{ is } \ \textit{even}}$:

The transverse eigenfunctions are of the form (6.8), while the spectral condition (6.10) passes to

$$\alpha = 2k\tan \pi Rk\,. \tag{6.11}$$

Moreover, for $k = \frac{n}{R},\ n \in \mathbb{N}\backslash\{0\}$ we always get the trivial solutions

$$\chi_n^{triv}(v) = \frac{1}{\sqrt{\pi R}}\, e^{-iAv}\sin kv\,, \tag{6.12}$$

which are independent of α. The roots $\{\tilde{\nu}_n\}$ of (6.11) satisfy the estimates $\sqrt{\tilde{\nu}_1} \in \frac{1}{2R}(0,1)$ and $\sqrt{\tilde{\nu}_n} \in \frac{1}{2R}(2n-3, 2n-1)$ for $n \in \mathbb{N}\setminus\{0,1\}$.

4. $\underline{0 \neq \alpha > \alpha_m}$ and $\underline{2RA \text{ is } \textit{odd}}$:

As in the two preceding cases the transverse eigenfunctions are still (6.8) but the spectral condition (6.10) passes now to

$$-\alpha = 2k \cot \pi R k \,. \tag{6.13}$$

The wave functions of the trivial solutions, $k = \frac{1}{2R}(2n+1),\ n \in \mathbb{N}$ are (6.12) again and the nontrivial roots of (6.13) satisfy $\forall n \in \mathbb{N}\setminus\{0\} : \sqrt{\tilde{\nu}_n} \in \frac{1}{2R}(2n-2, 2n)$.

5. $\underline{\alpha < \alpha_m}$:

Now the lowest eigenvalue of the transverse operator is negative, $\nu_1 := -\kappa^2$, and satisfies

$$-\alpha = 2\kappa \left(\coth 2\pi R\kappa - \frac{\cos 2\pi RA}{\sinh 2\pi R\kappa} \right). \tag{6.14}$$

Replacing $\sqrt{\nu_1}$ by $-i\kappa$ in (6.8) we get the corresponding eigenfunction.

6. $\underline{\alpha = \alpha_m \neq 0}$:

In this extreme case there is a zero eigenvalue $\nu_1 := 0$ with

$$\chi_1(v) = \sqrt{\frac{3}{(2\pi R)^3(2+\cos 2\pi RA)}}\, e^{-iAv} \left[2\pi R - (1 - e^{i2\pi RA})\, v \right]. \tag{6.15}$$

Another possibility how to obtain the formula (up to a factor of modulus one) is to regard the limit $\lim_{\nu_1 \to 0} \chi_1(v)$, where χ_1 is given by (6.8).

Remark VI.2 The essential prerequisite for the further investigation of the bound states is the requirement $\chi_1(0) \neq 0$. Only in this case we will be able to proceed as in Chap. IV. If $\alpha = 0$, the eigenfunctions are always positive (see (6.7)) and $\chi_1(0) \neq 0$ for $\alpha \leq \alpha_m$ as well. Otherwise, one can easily find out that $\chi_n(0) = 0$ if and only if $2R\sqrt{\nu_n} \in \mathbb{N}$, which corresponds to the trivial solutions (6.12) of the cases 3 and 4. Nevertheless, only if $\alpha > 0$ and $2RA$ is *odd* the first eigenvalue ν_1 belongs to this class of solutions.

We recall that an analogous situation arose in the precedent case of the double waveguide as well, provided the widths of the ducts were rationally related (*cf.* Remarks II.2 1.).

In analogy to Proposition II.1 we have

Proposition VI.1 *Suppose that* $2RA$ *is not* odd *or* $\alpha \leq 0$. *Then the function* $\nu_1 = \nu_1(\alpha)$ *is strictly increasing and continuous.*

Proof: If $2RA$ is not *odd* one can write

$$\nu_1(\alpha) = \begin{cases} k^2 & \text{if} \quad 0 \neq \alpha > \alpha_m \\ \left(\min\limits_{\ell \in \mathbb{Z}} |\frac{\ell}{R} + A| \right)^2 & \text{if} \quad \alpha = 0 \\ 0 & \text{if} \quad 0 \neq \alpha = \alpha_m \\ -k^2 & \text{if} \quad \alpha < \alpha_m \end{cases} \tag{6.16}$$

where k is determined by the equation $F(\alpha, k) = 0$ with

$$F(\alpha,k) := \begin{cases} \alpha + 2k\left(\cot dk - \frac{\cos dA}{\sin dk}\right) & \text{for } k \in \frac{1}{2R}(0,1) \quad \text{if} \quad 0 \neq \alpha > \alpha_m \\ \\ \alpha + 2k\left(\coth dk - \frac{\cos dA}{\sinh dk}\right) & \text{for } k \in (0,\infty) \quad \text{if} \quad \alpha < \alpha_m \end{cases}$$

($d := 2\pi R$). A straightforward computation yields

$$\frac{\partial F}{\partial \alpha} = 1 \qquad \text{and} \qquad \frac{\partial F}{\partial k} = \begin{cases} -2k\chi_1(0)^{-2} < 0 & \text{if} \quad 0 \neq \alpha > \alpha_m \\ \\ 2k\chi_1(0)^{-2} > 0 & \text{if} \quad \alpha < \alpha_m \,. \end{cases}$$

The continuity follows by means of the implicit-function theorem and the observation that $F(0,k) = 0$ has a solution for $k \in \frac{1}{2R}(0,1)$ coincides with the one for $\alpha = 0$ and

$$\lim_{\substack{k\to 0 \\ \alpha\to\alpha_m\pm}} F(\alpha,k) = 0\,.$$

The monotonous behaviour is then clear from the explicit expression of the first derivative (2.11) and (6.16).

After the restriction $\alpha \leq 0$ everything stays valid for *odd* $2RA$ as well (*cf.* Remark VI.2). ∎

The unperturbed Green's function is the same as in the case of double waveguide (*cf.* (2.9)); one has only to substitute the present transverse eigenfunctions and eigenvalues.

VI.2 Bound States

VI.2.1 Existence

In this section we give a proof of the existence of a bound state as in Theorem IV.1. As was already mentioned in Remark VI.2 the main difference consists in a further requirement imposed on the vector potential $\vec{A}$.

Denote by α_0 a constant function $\mathbb{R} \to \mathbb{R}$ which presents here the unperturbed system discussed above. Then we have

Theorem VI.1 *Assume*

(i) $\alpha - \alpha_0 \in L^1(\mathbb{R})$

(ii) $\alpha(u) - \alpha_0 = \mathcal{O}(|u|^{-1-\varepsilon})$ *for some* $\varepsilon > 0$ *as* $|u| \to \infty$

(iii) $2RA$ *is not* odd *provided* $\alpha_0 > 0$.

If $\int_{\mathbb{R}}(\alpha(u) - \alpha_0)du < 0$, *then* H_α *has at least one isolated eigenvalue below its essential spectrum,* $\sigma_{ess}(H_\alpha) = [\nu_1(\alpha_0), \infty)$.

PROOF: **(a)** To localize the essential spectrum of H_α we can employ the bracketing procedure introduced in the first part of the proof of Theorem IV.1. After the mimicking one finds that $\sigma_{ess}(H_\alpha) = [\nu_1(\alpha_0), \infty)$.

(b) Now one has to find a trial function $\Psi \in D(q_\alpha)$ such that the quadratic form (4.3) is negative. Putting $\Psi(u,v) := \varphi_\sigma(u)\chi_1(v;\alpha_0)$, where φ_σ is defined by a scaling (4.4), we arrive after a straightforward computation at (4.5) and then at (4.6) what proves the claim of the theorem.

The computation is simple in the case $\alpha_0 = 0$ but it is much more laborious (even though straightforward) in the other situations. ∎

VI.2.2 Weak Coupling and Scaling Behaviour

The process would be completely the same as in the "waveguide situation". One has only to add the requirement (iii) of Theorem VI.1 to *(a1), (a2)* (or *(a2')*) and take the "cylindrical" transverse eigenfunctions and eigenvalues. After the formal repeating process one arrives at the same results contained in Sections IV.2 and IV.3.

VI.2.3 Numerical Solution

Substituting the now forms of transverse eigenfunctions and eigenvalues one can straight adopt the results of Chapter V. Due to the different eigenfunctions one has to take the corresponding overlap integrals

$$\begin{aligned}(\chi_m, \phi_n) \;&=\; \frac{8\,\bar{N}_m^0 N_n^1}{(e^{-i2\pi RA} - e^{i2\pi R\sqrt{\nu_m^0}}\,)(e^{i2\pi RA} - e^{-i2\pi R\sqrt{\nu_n^1}}\,)\,(\nu_m^0 - \nu_n^1)}\cdot \\ &\cdot\Big[\sqrt{\nu_m^0}\sin 2\pi R\sqrt{\nu_n^1}\,(\cos 2\pi RA - \cos 2\pi R\sqrt{\nu_m^0}\,) \\ &\quad -\sqrt{\nu_n^1}\sin 2\pi R\sqrt{\nu_m^0}\,(\cos 2\pi RA - \cos 2\pi R\sqrt{\nu_n^1}\,)\Big] \qquad (6.17)\end{aligned}$$

for $\alpha_0 \neq 0 \neq \alpha_1$ $(m, n \in \mathbb{N}\setminus\{0\})$ and

$$(\chi_m, \phi_\ell) = \frac{4\,\bar{N}_m^0\sqrt{\nu_m^0}}{\sqrt{2\pi R}\,\left(\nu_m^0 - (\frac{\ell}{R} + A)^2\right)}\,\left(\sin 2\pi RA + i\cos 2\pi R\sqrt{\nu_m^0}\right) \qquad (6.18)$$

for $\alpha_0 \neq 0$, $\alpha_1 = 0$ $(m \in \mathbb{N}\setminus\{0\},\ \ell \in \mathbb{Z})$. Note, that in the latter case one has to substitute the *arranged* base $\{\phi_n\}_{n=1}^\infty$ (together with the corresponding eigenvalues) into Ansatz (5.8) because of the later cut-off approximation.

Unless $\alpha_1 < 0$ we have to exclude here the possibility $2RA = 2n+1$, $n \in \mathbb{N}$, again (*cf.*, *e.g.*, (5.3)). Next we can restrict our attention only to the situation when $2RA \in [0,1) \cup (1,2)$ because A appears in the overlap integrals (6.17), (6.18) and in the spectral condition (6.10) as an argument of the periodic functions sin, cos; the integrals and the transverse eigenvalues are the only quantities which affect the equations (5.11) and (5.21).

In fact, we can take $2RA$ from $[0,1)$ only because the replacement $2RA \mapsto 2 - 2RA$ in (6.17) and (6.18) (the spectral condition (6.10) does not change at

all) is equivalent to the exchange $A \mapsto -A$ which coincides with the conjugation of Hamiltonian (6.4). It is well known fact that such an operator has the same energies while the corresponding eigenfunctions are given by a simple conjugation.

VI.2.4 Numerical Results

Some of the numerical results are illustrated on Figures 10–14 in Appendix A. We compute with the non-dimensional quantities (see Table VI.1) and use the graphical notation of Table A.1 again. Furthermore, we sometimes use the notation $d := 2\pi R$.

Table VI.1: Passing to the non-dimensional quantities

dimensional quantity	=	conversion factor	×	non-dimensional quantity
α_s	=	$1/2R$	×	α_s
A	=	$1/2R$	×	A
ν_n^s	=	$(1/2R)^2$	×	ν_n^s
E	=	$(1/2R)^2$	×	E
k	=	$(1/2R)$	×	k

Figure 10 illustrates the bound-states energies as functions of the "window" width while Figure 11 shows more natural dependence of the ground-state energy on the vector potential. The thin dotted lines represent the first transverse eigenvalue ν_1^0 (from which the essential spectrum starts) corresponding to each value of α_0; we recall that $\nu_1^0 = \nu_1^0(\alpha_0)$ is an increasing function (*cf.* Proposition VI.1). The evolution of the probability density of a ground-state wavefunction w.r.t. α_0 is illustrated on Figure 12.

Figure 13 shows the conductivity for the particle coming from the right and leaving to the left as a function of the momentum and the vector potential.

The figure appendix is then concluded by the evolution of the quantum probability flow illustrated on Figure 14.

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Appendix A

Figures

A.1 Figure Captions

A.1.1 Double Waveguide

Figure 1 The dependence of bound-state energies on the "window" width a in the symmetric case ($\nu = 1$) for $\alpha_1 = 0$.

Figure 2 The dependence of bound-state energies on the "window" width a in the asymmetric case, $\nu = 1/2\pi$, for $\alpha_1 = 0$.

Figure 3 The coefficients of the threshold formula $E(a) = \nu_1^0 - ca^\beta$ as functions of $\ln \alpha_0$ in the symmetric case for $\alpha_1 = 0$.

Figure 4 The evolution of the ground-state eigenfunction w.r.t. α_0 in the symmetric case for $a/d = 0.15$, $\alpha_1 = 0$.

Figure 5 The evolution of the first excited state w.r.t. α_0 in the asymmetric case, $\nu = 1/\pi$, for $a/d = 2.8$, $\alpha_1 = 0$.

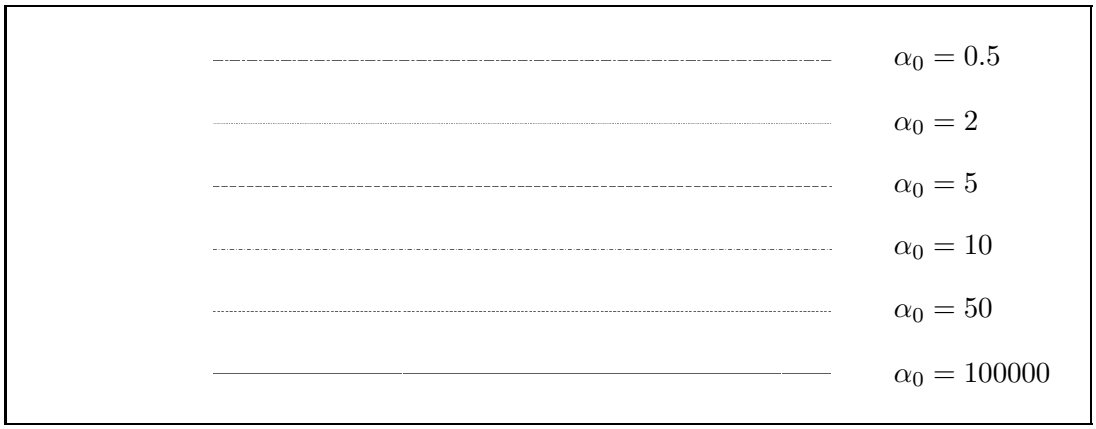
Figure 6 The evolution of the conductivity for the particle coming from the right and leaving to the left as a function of the momentum k and the width d_2 for $d = \pi$, $a = 1$, $\alpha_1 = 0$.

Figure 7 The evolution of the conductivity for the particle coming from the right and leaving to the left as a function of the momentum k and the width d_2 for $d = \pi$, $a = 2\pi$, $\alpha_1 = 0$.

Figure 8 The quantum probability flow for $k = 1.745$, $\alpha_1 = 0$ as a function of α_0.

Figure 9 The quantum probability flow for $k = 1.554$, $\alpha_1 = 0$ as a function of α_0.

Table A.1: Graphical notation for α_0



A.1.2 Aharonov-Bohm Cylinder

Figure 10 Bound-state energies *vs.* the "window" width a for $A = 0.5$, $\alpha_1 = 0.00001$.

Figure 11 Bound-state energies *vs.* the vector potential A for $a/d = 0.5$, $\alpha_1 = 0.00001$.

Figure 12 The evolution of the probability density of the ground-state w.r.t. α_0 for $a/d = 0.2$, $A = 0.2$, $\alpha_1 = 0.00001$.

Figure 13 The evolution of the conductivity for the particle coming from the right and leaving to the left as a function of the momentum k and the vector potential A for $a/d = 1/\pi$, $\alpha_1 = 0.00001$.

Figure 14 The quantum probability flow for $A = 0.5$, $k = 1.705$, $\alpha_1 = 0.00001$ as a function of α_0.

FIGURES

Figure 1

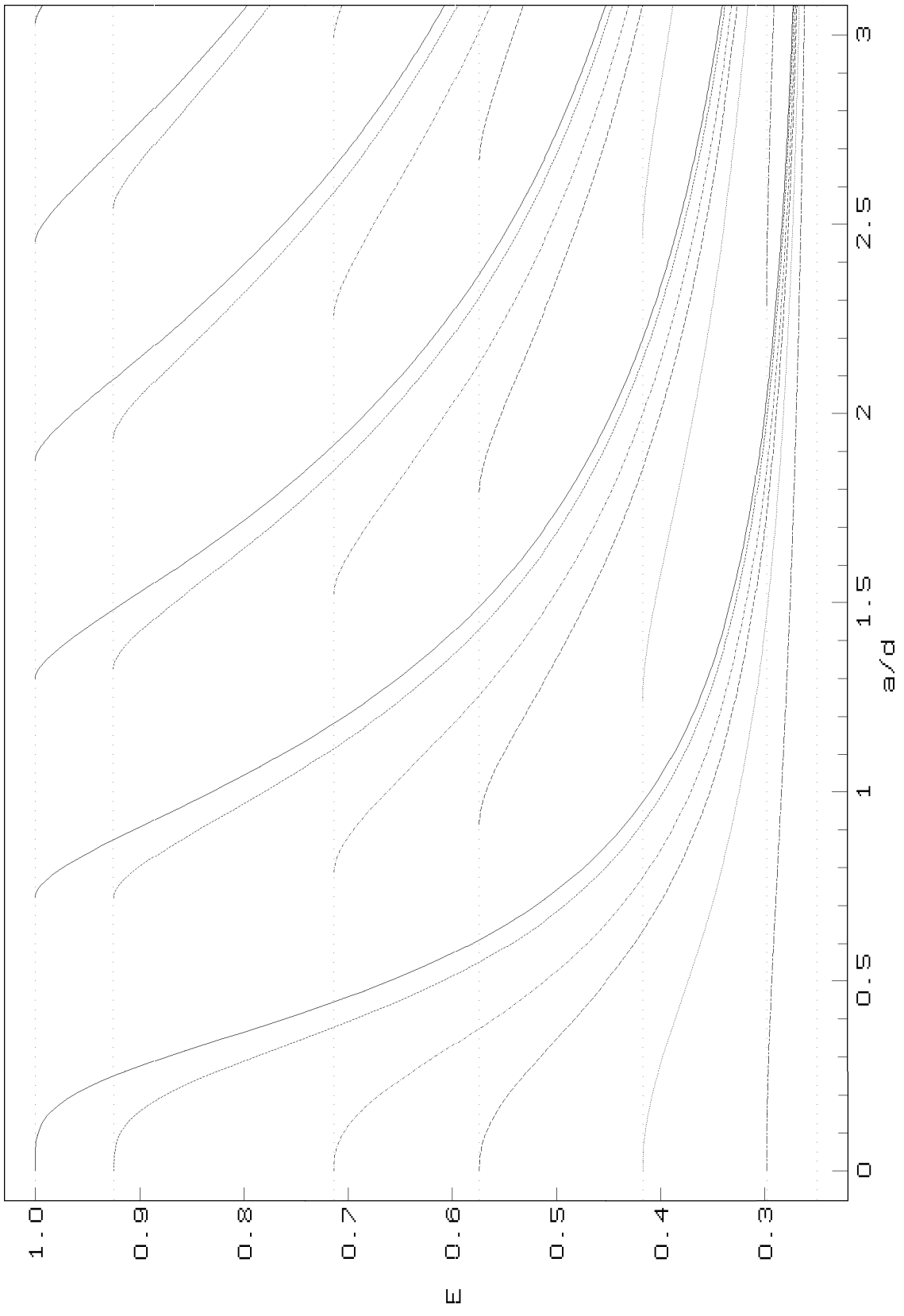


Figure 2

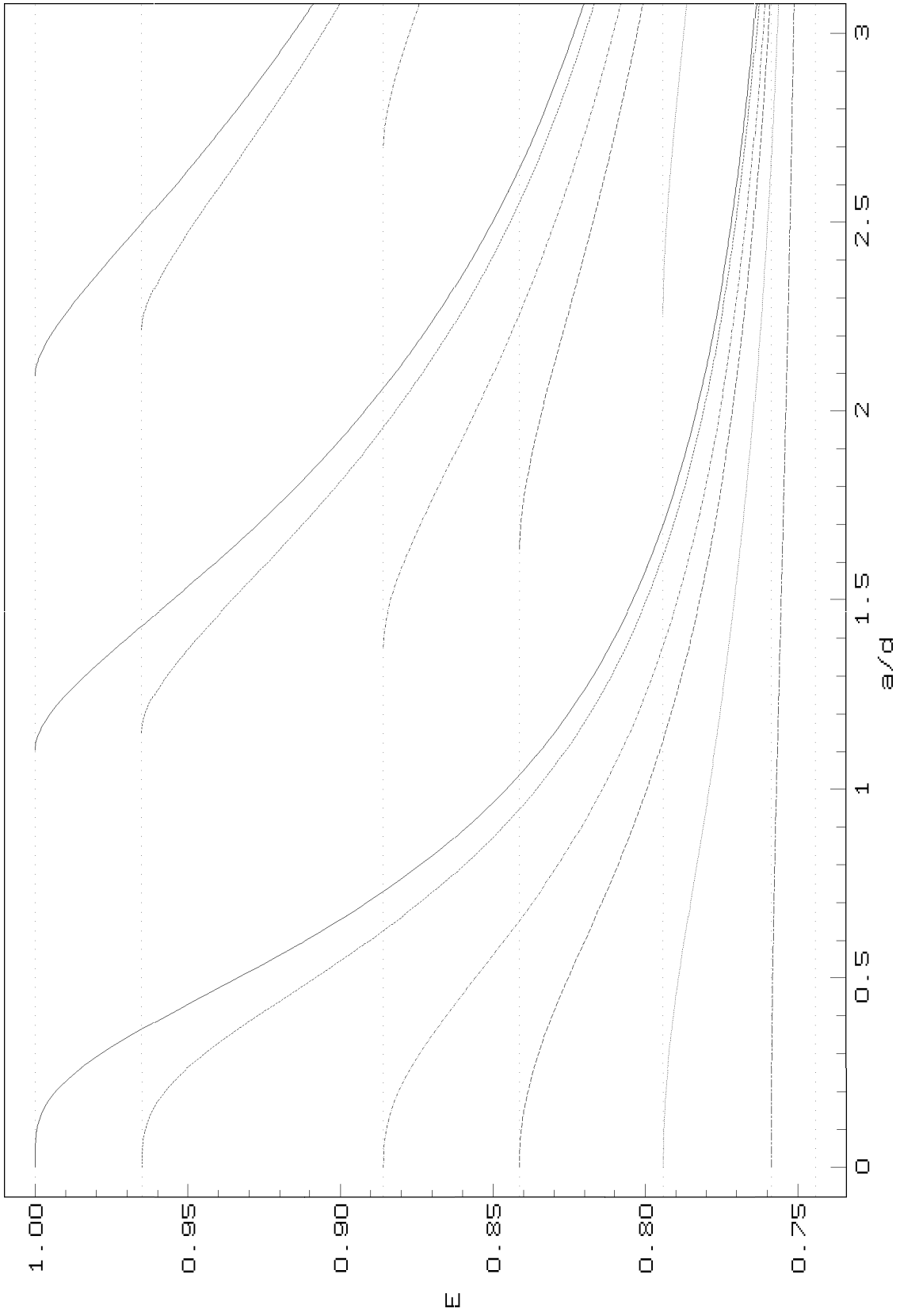
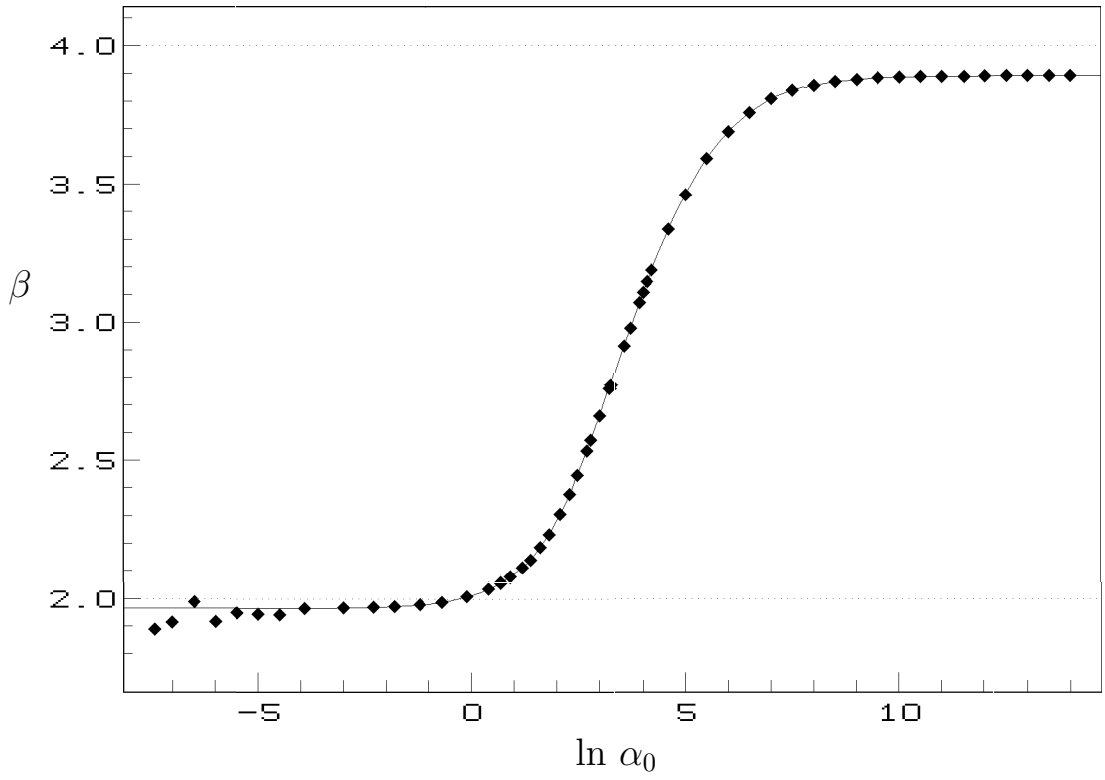


Figure 3



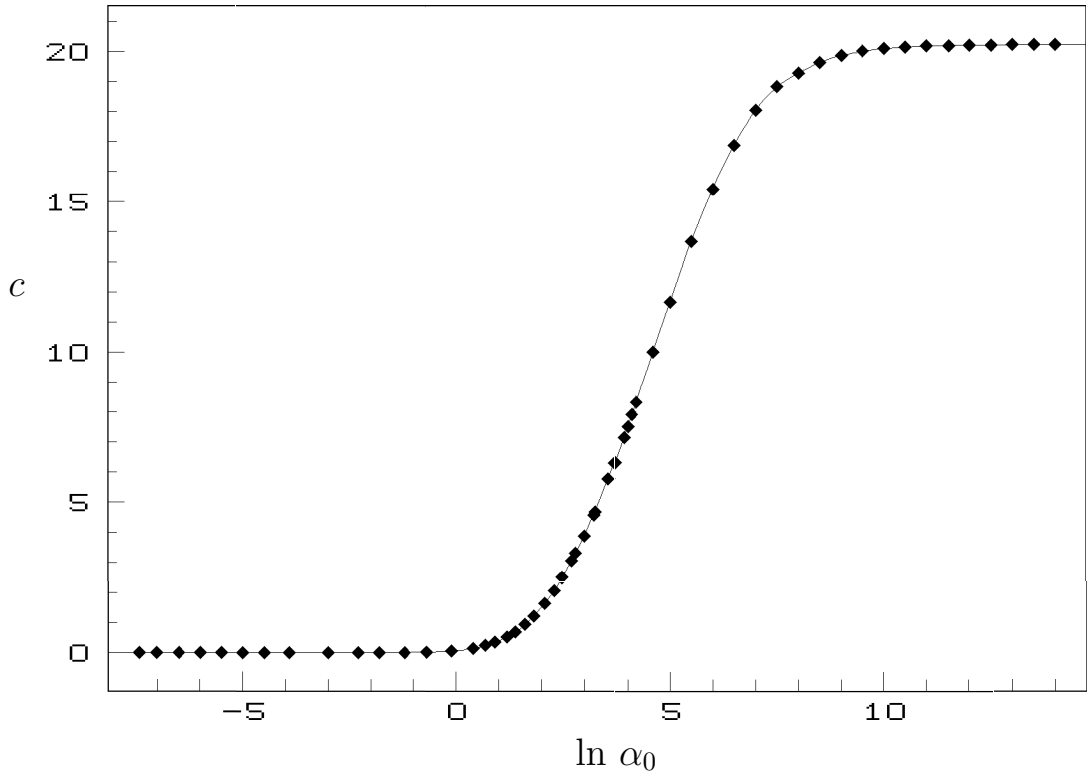


Figure 4 a

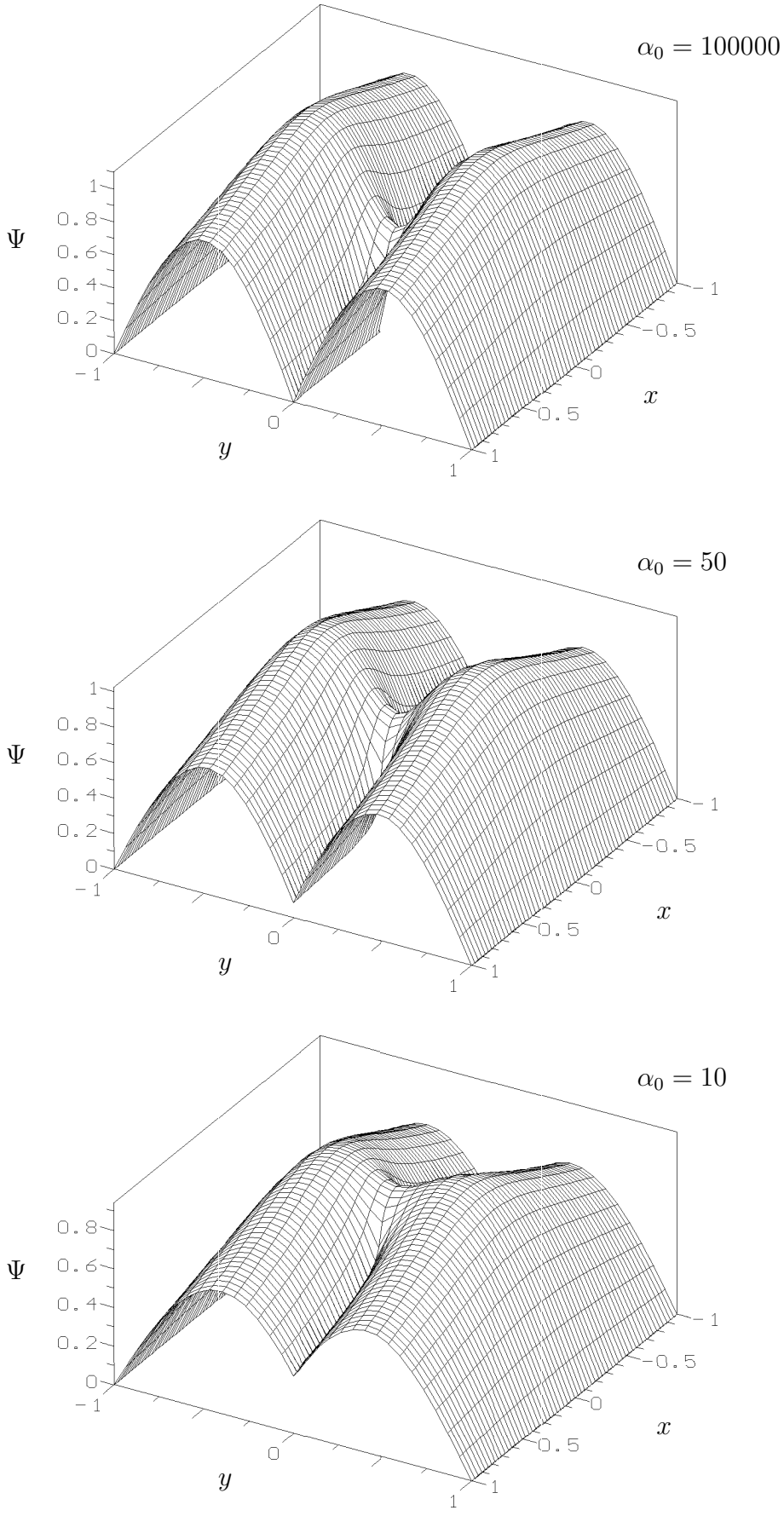

$\alpha_0 = 100000$
Ψ
1
0.8
0.6
0.4
0.2
0
−1
0
1
y
1
0.5
0
−0.5
−1
x
$\alpha_0 = 50$
Ψ
1
0.8
0.6
0.4
0.2
0
−1
0
1
y
1
0.5
0
−0.5
−1
x
$\alpha_0 = 10$
Ψ
0.8
0.6
0.4
0.2
0
−1
0
1
y
1
0.5
0
−0.5
−1
x

Figure 4 b

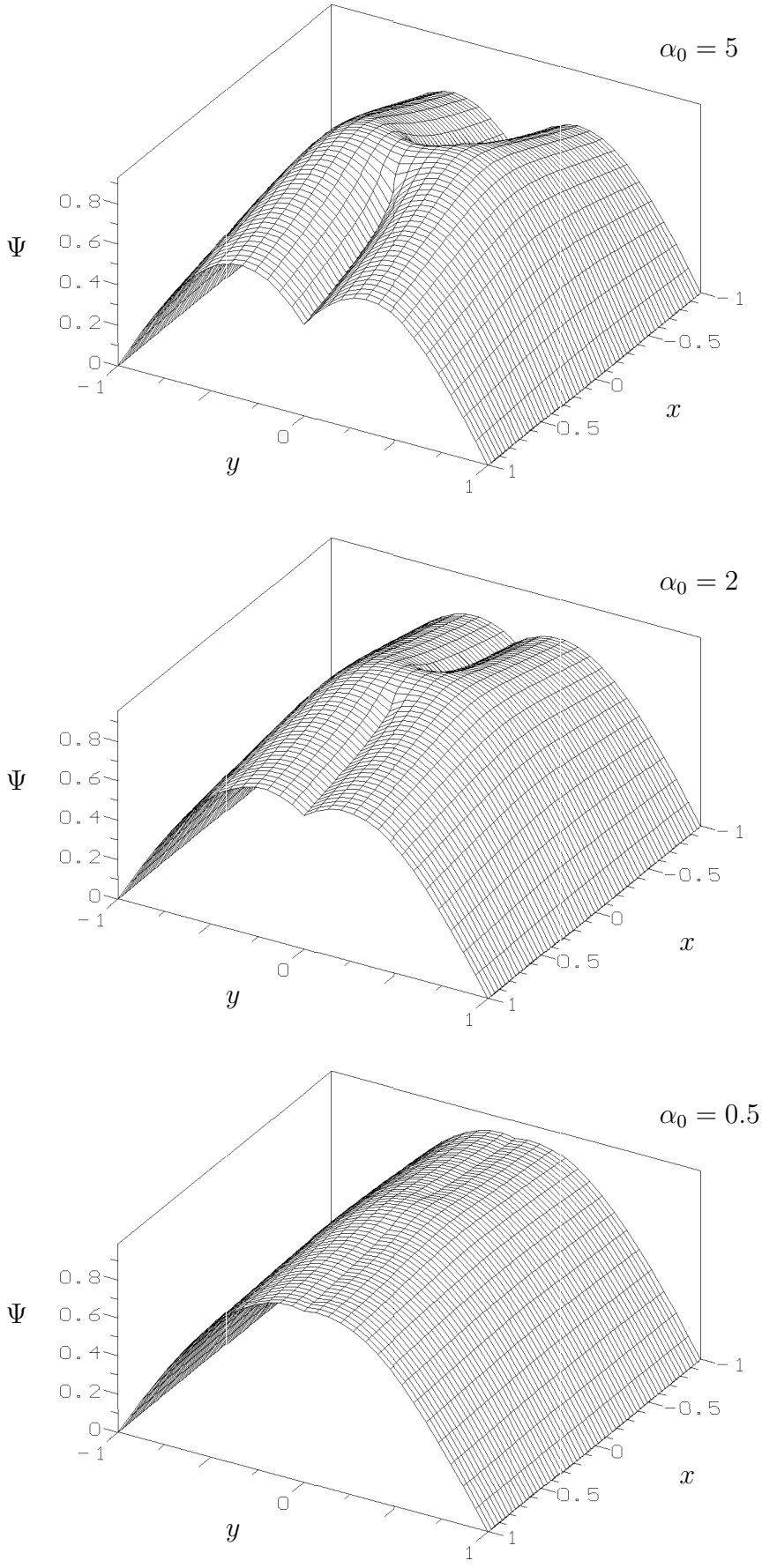


Figure 5

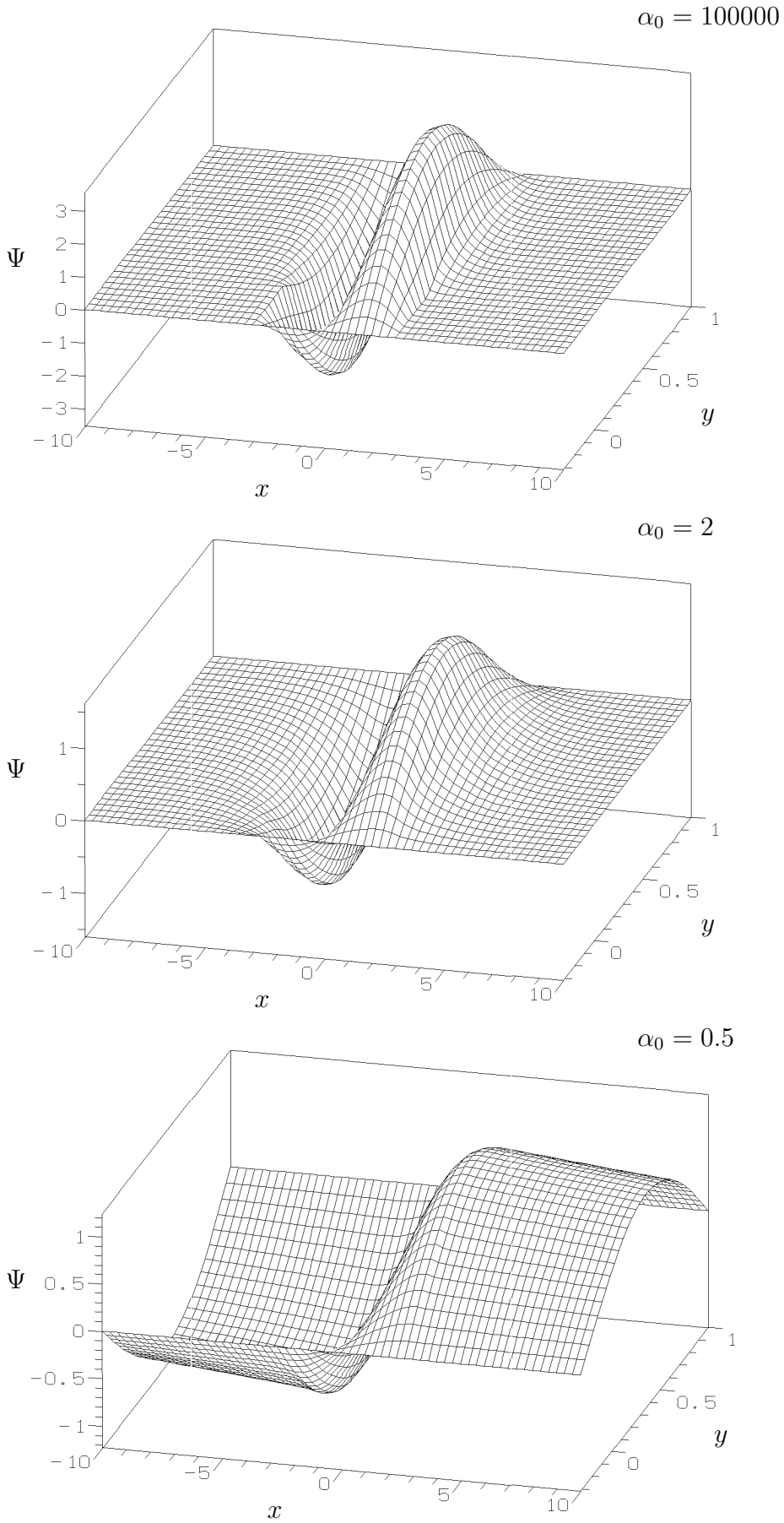
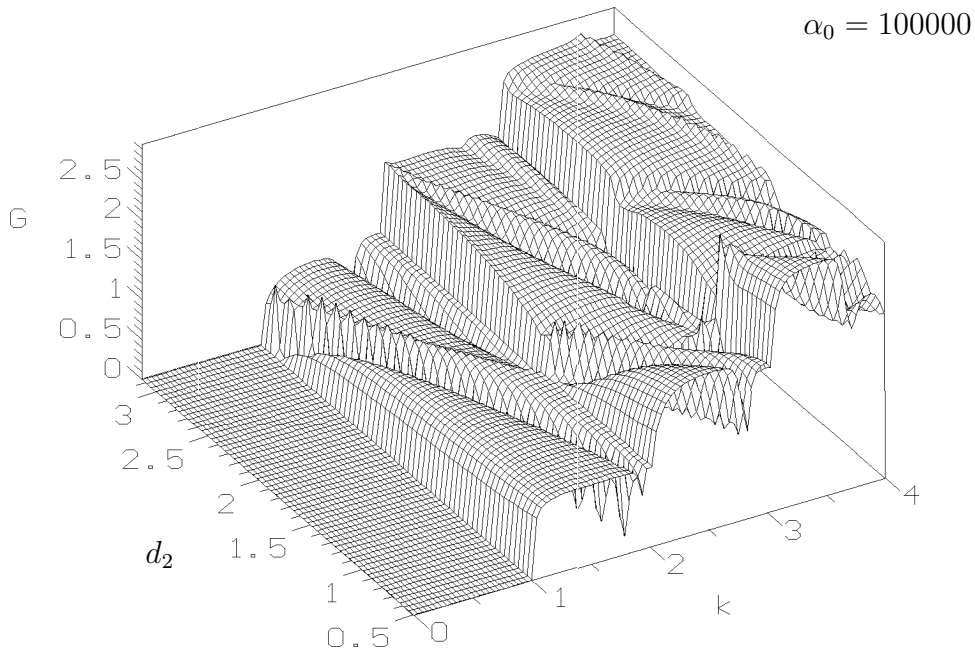

$\alpha_0 = 100000$
Ψ
3
2
1
0
−1
−2
−3
−10
−5
0
5
10
x
1
0.5
0
y
$\alpha_0 = 2$
Ψ
1
0
−1
−10
−5
0
5
10
x
1
0.5
0
y
$\alpha_0 = 0.5$
Ψ
1
0.5
0
−0.5
−1
−10
−5
0
5
10
x
1
0.5
0
y

Figure 6 a


$\alpha_0 = 100000$
G
2.5
2
1.5
1
0.5
0
3
2.5
2
1.5
1
0.5
d_2
0
1
2
3
4
k

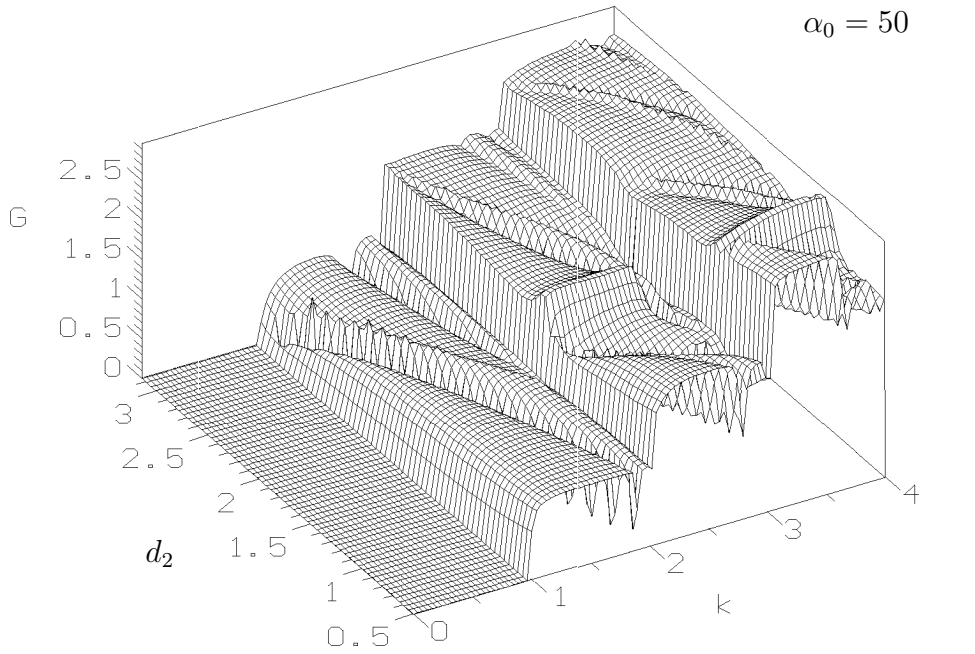
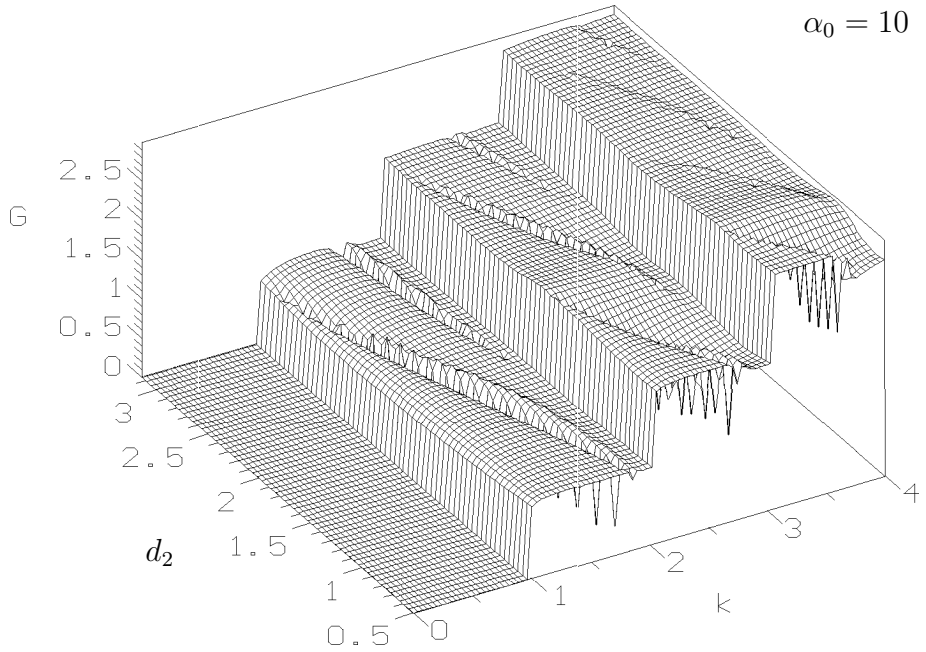

$\alpha_0 = 50$
G
2.5
2
1.5
1
0.5
0
3
2.5
2
1.5
1
0.5
d_2
0
1
2
3
4
k

Figure 6 b


$\alpha_0 = 10$
G
2.5
2
1.5
1
0.5
0
3
2.5
2
1.5
1
0.5
d_2
0
1
2
3
4
k

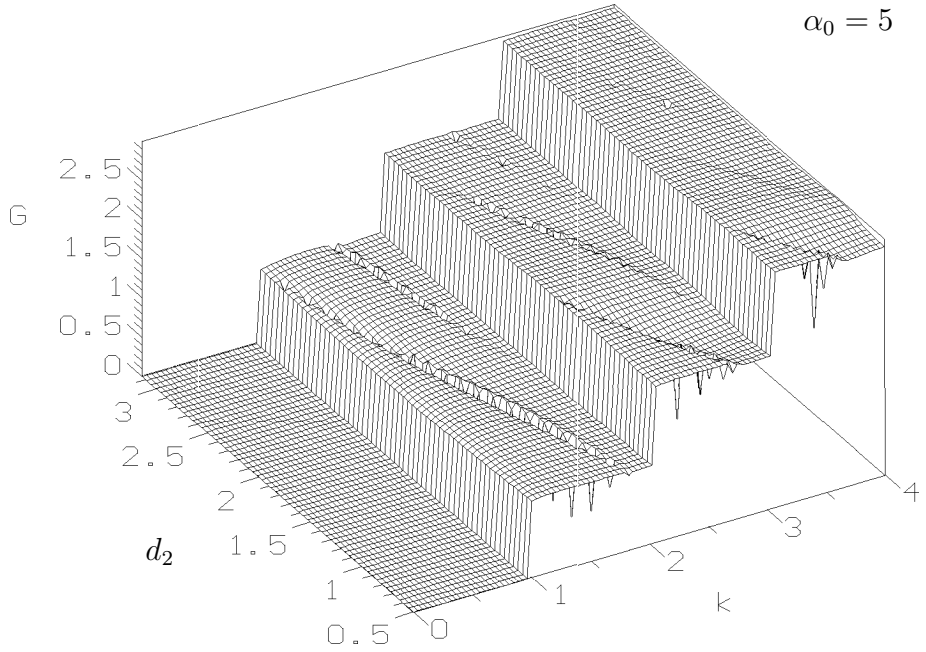
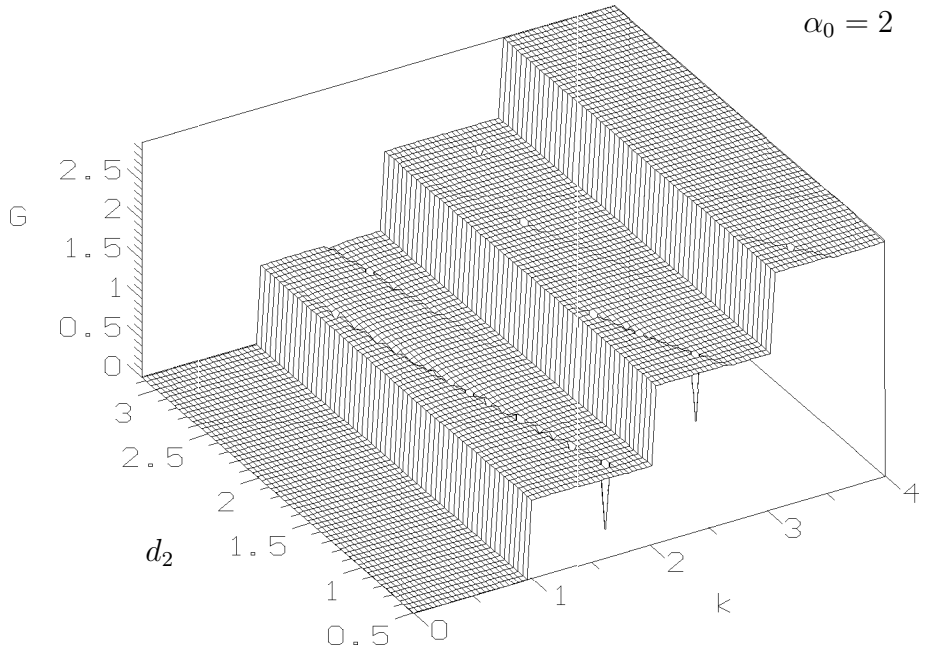

$\alpha_0 = 5$
G
2.5
2
1.5
1
0.5
0
3
2.5
2
1.5
1
0.5
d_2
0
1
2
3
4
k

Figure 6 c


$\alpha_0 = 2$
G
2.5
2
1.5
1
0.5
0
3
2.5
2
1.5
1
0.5
d_2
0
1
2
3
4
k

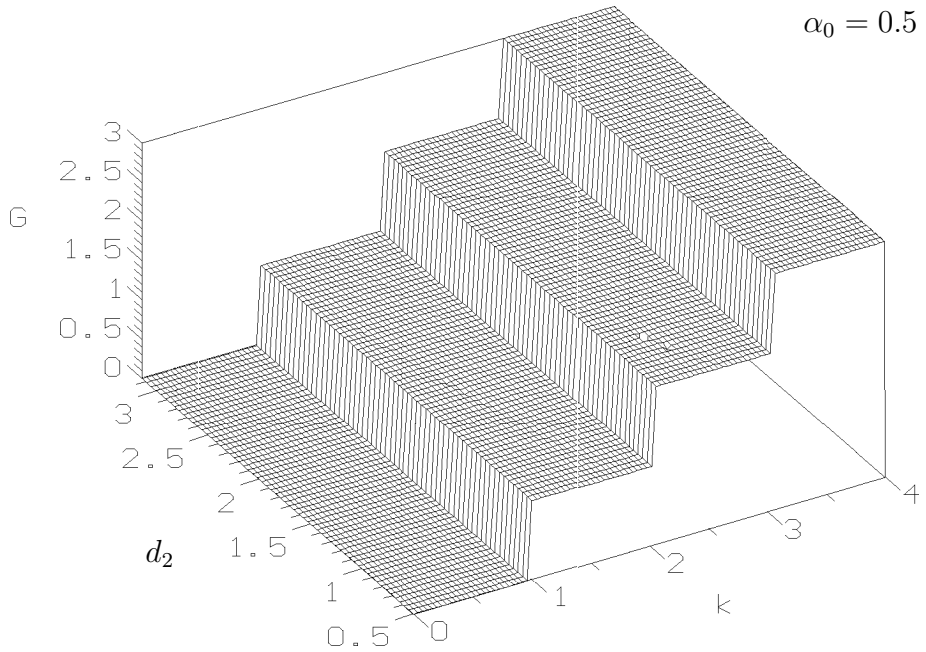
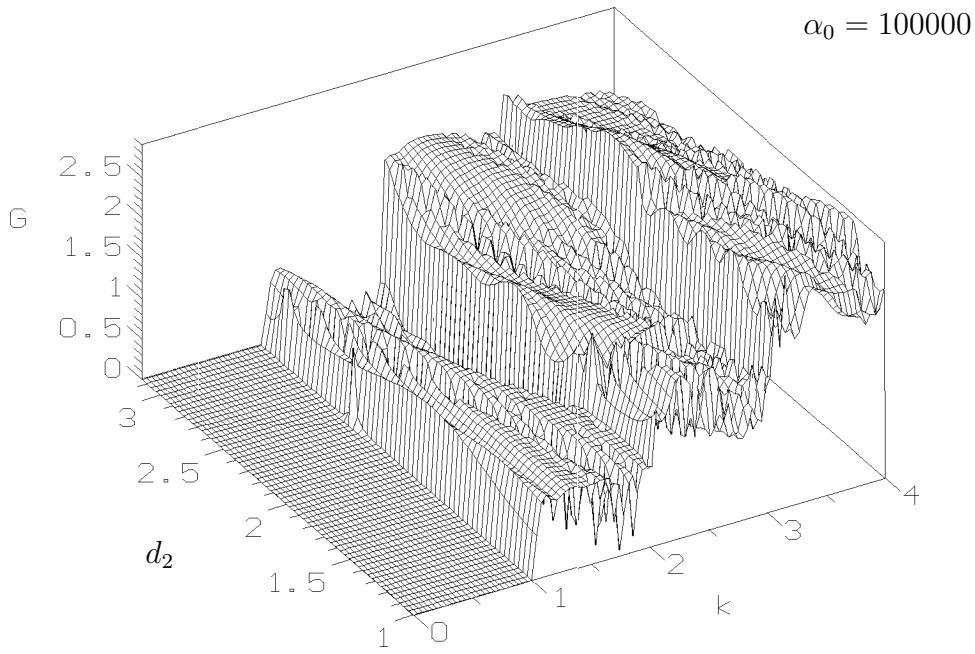

$\alpha_0 = 0.5$
G
3
2.5
2
1.5
1
0.5
0
3
2.5
2
1.5
1
0.5
d_2
0
1
2
3
4
k

Figure 7


$\alpha_0 = 100000$
G
2.5
2
1.5
1
0.5
0
3
2.5
2
1.5
1
d_2
0
1
2
3
4
k

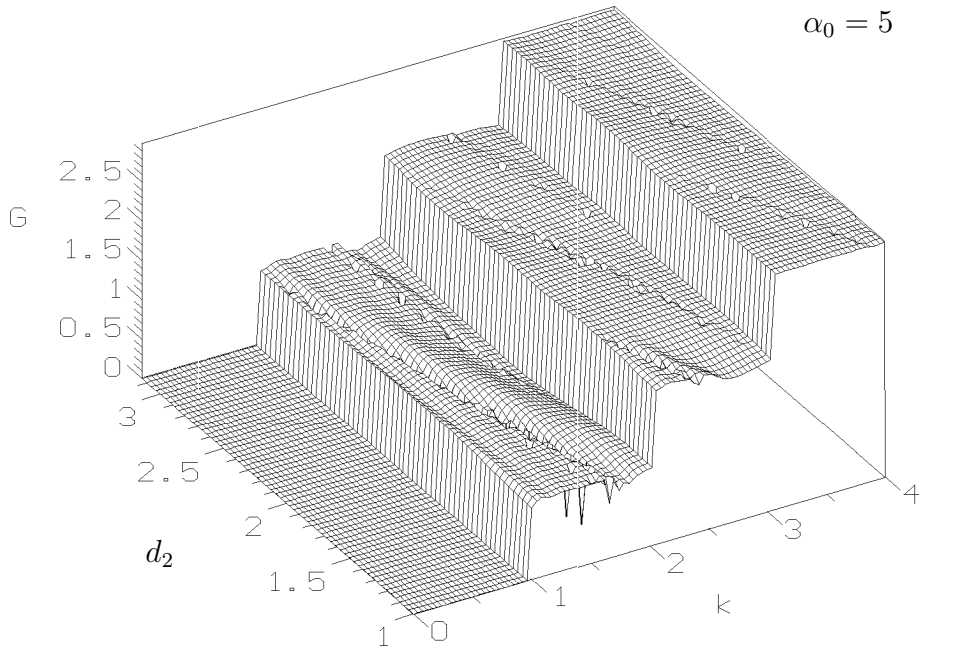
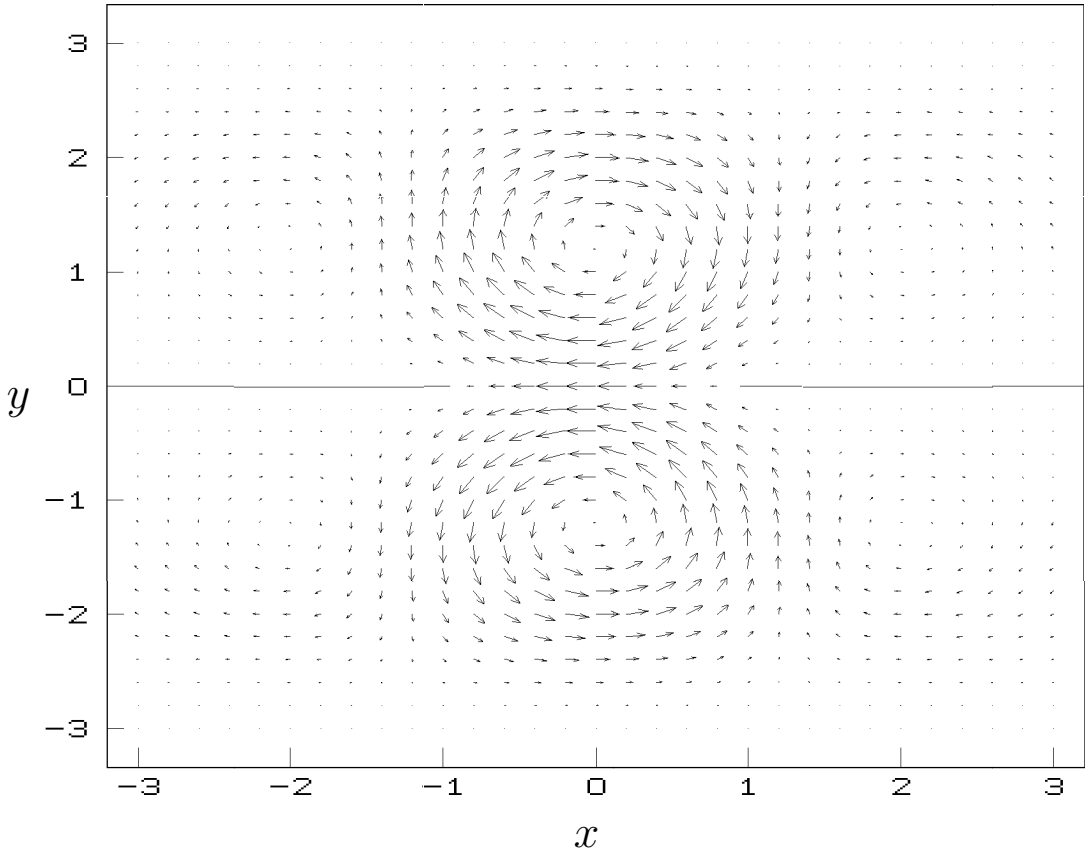

$\alpha_0 = 5$
G
2.5
2
1.5
1
0.5
0
3
2.5
2
1.5
1
d_2
0
1
2
3
4
k

Figure 8 a

$\alpha_0 = 100000$



$\alpha_0 = 50$

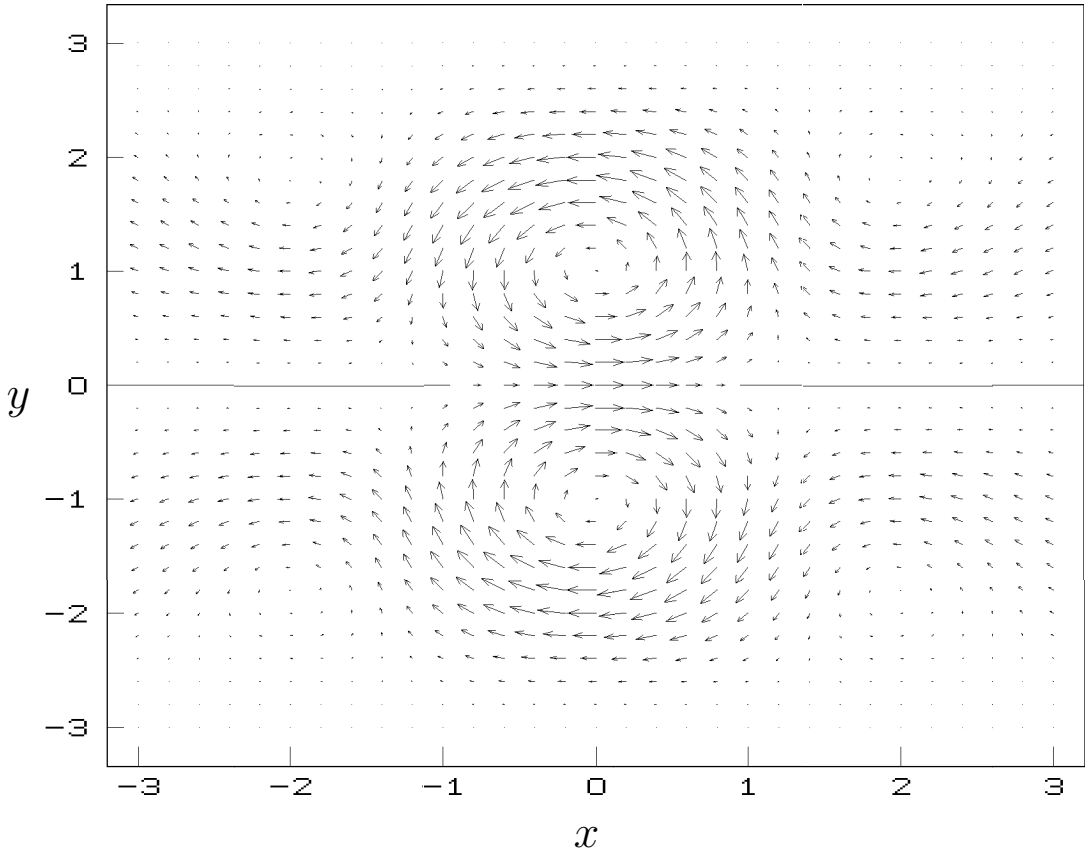
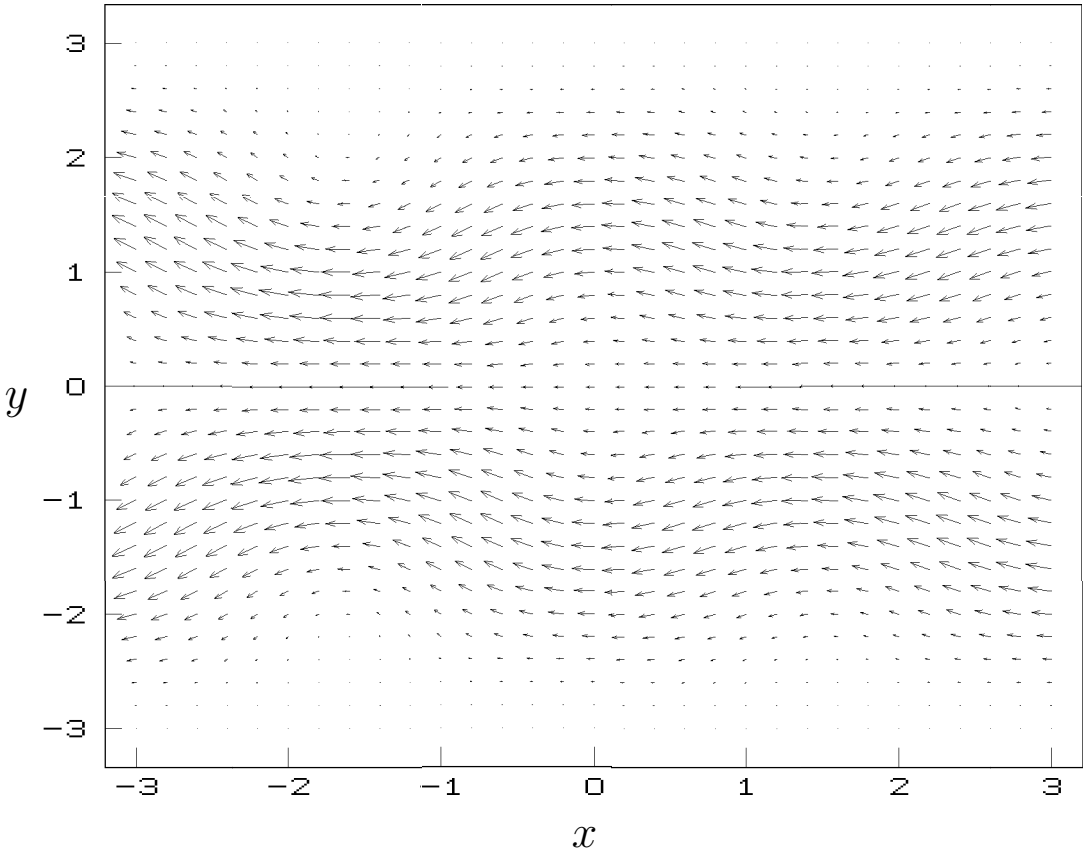


Figure 8 b

$\alpha_0 = 10$



$\alpha_0 = 5$

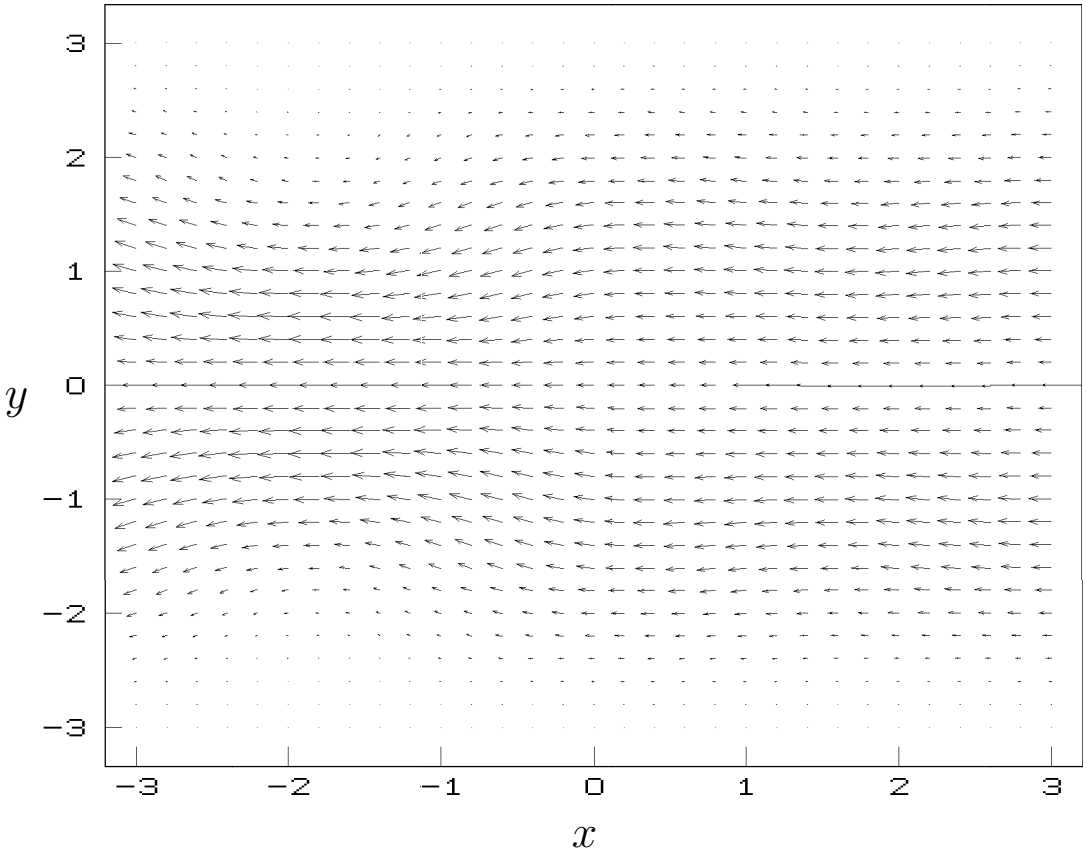
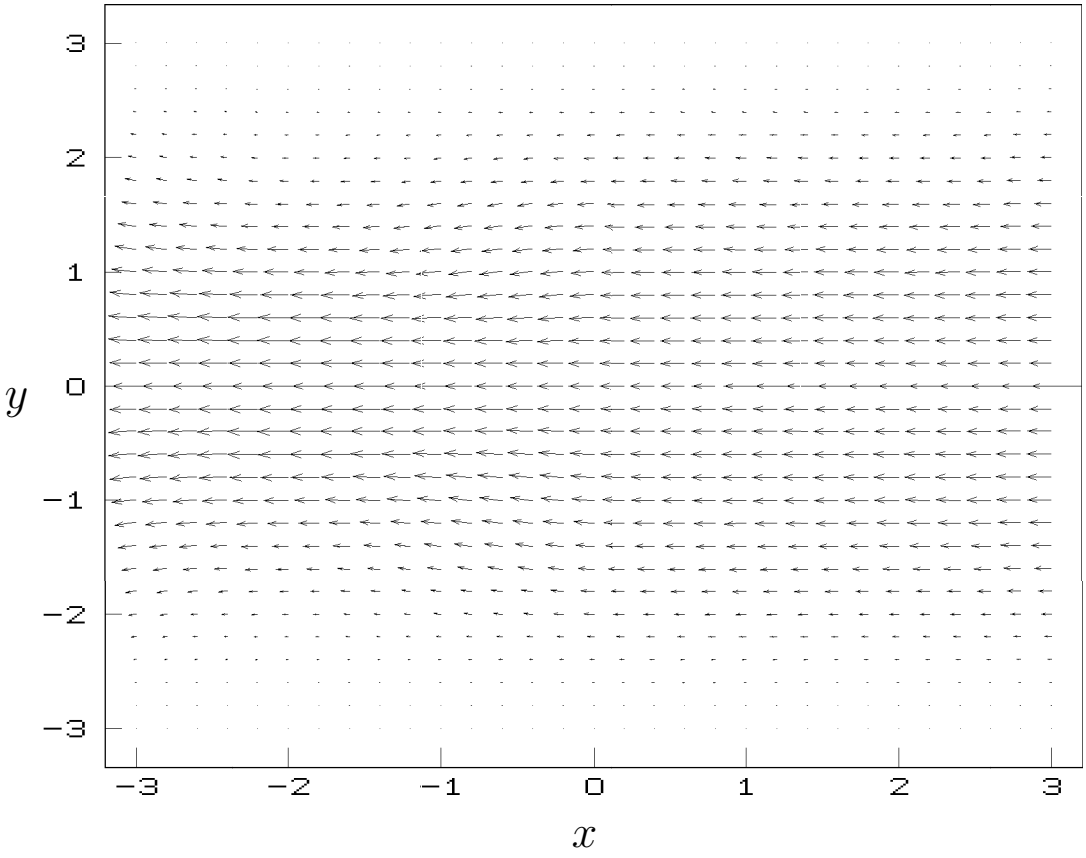


Figure 8 c

$\alpha_0 = 2$



$\alpha_0 = 0.5$

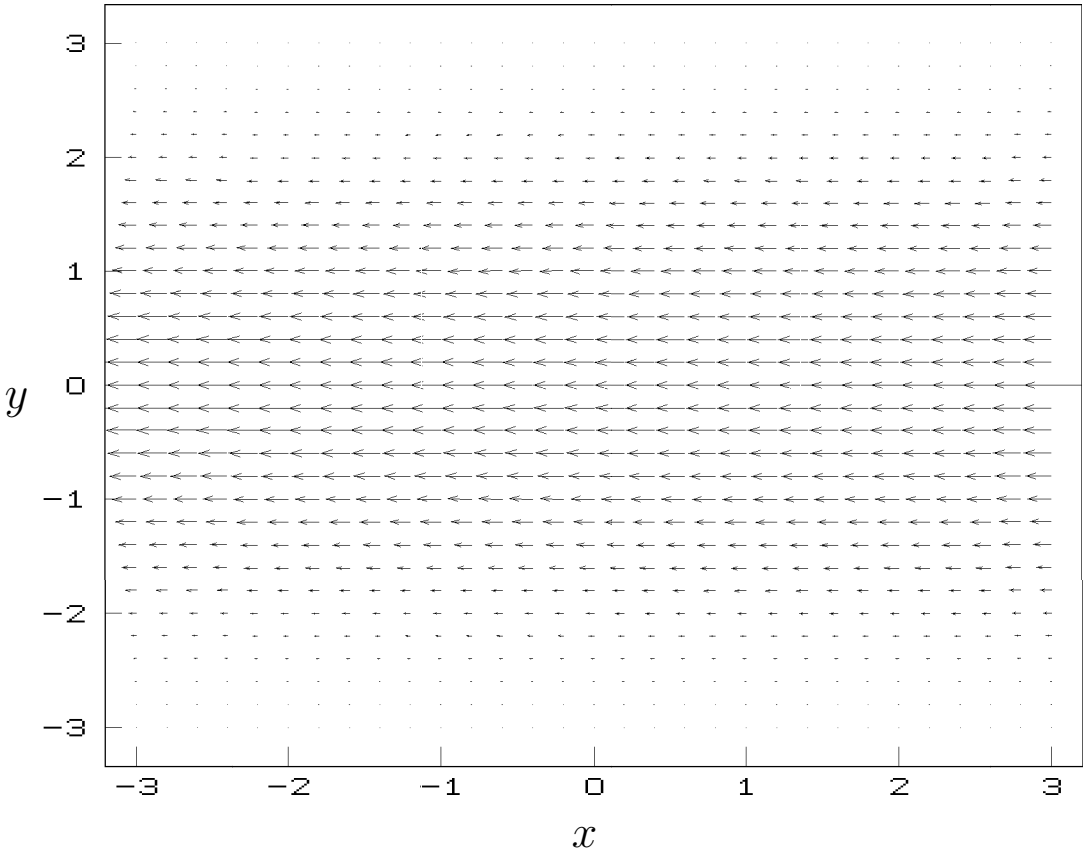
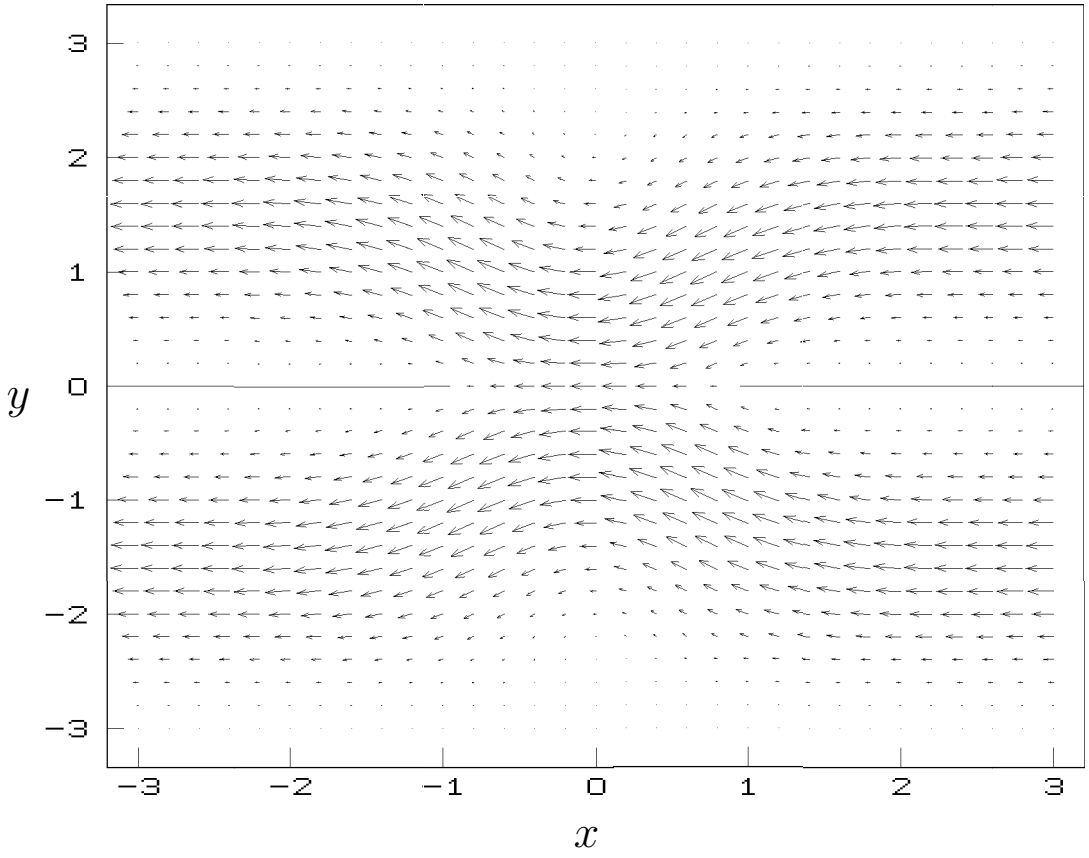


Figure 9 a

$\alpha_0 = 100000$



$\alpha_0 = 5$

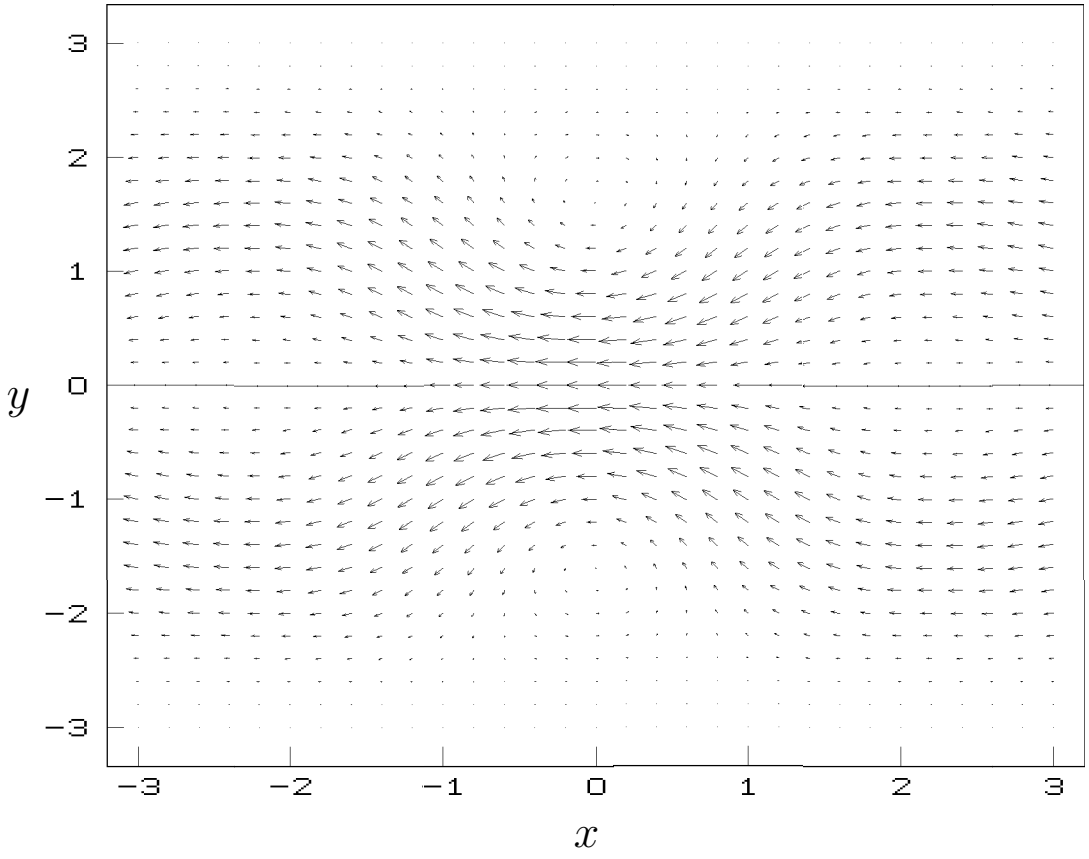
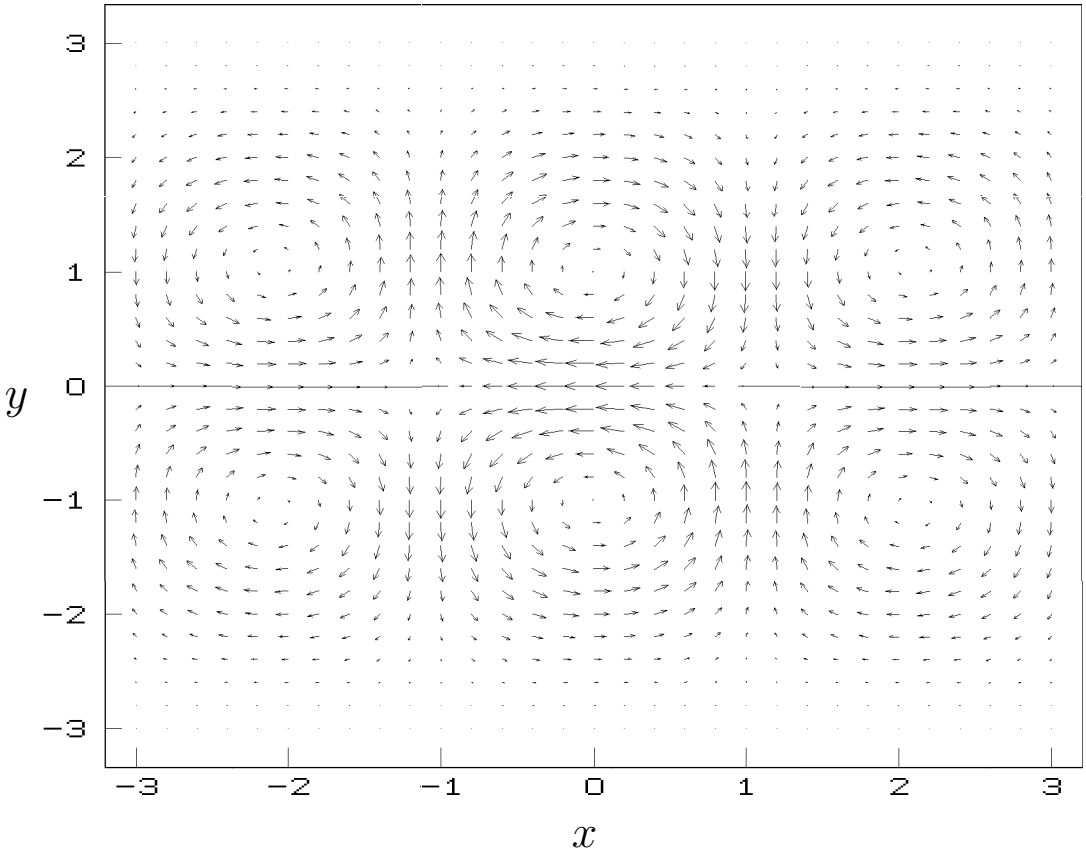


Figure 9 b

$\alpha_0 = 2$



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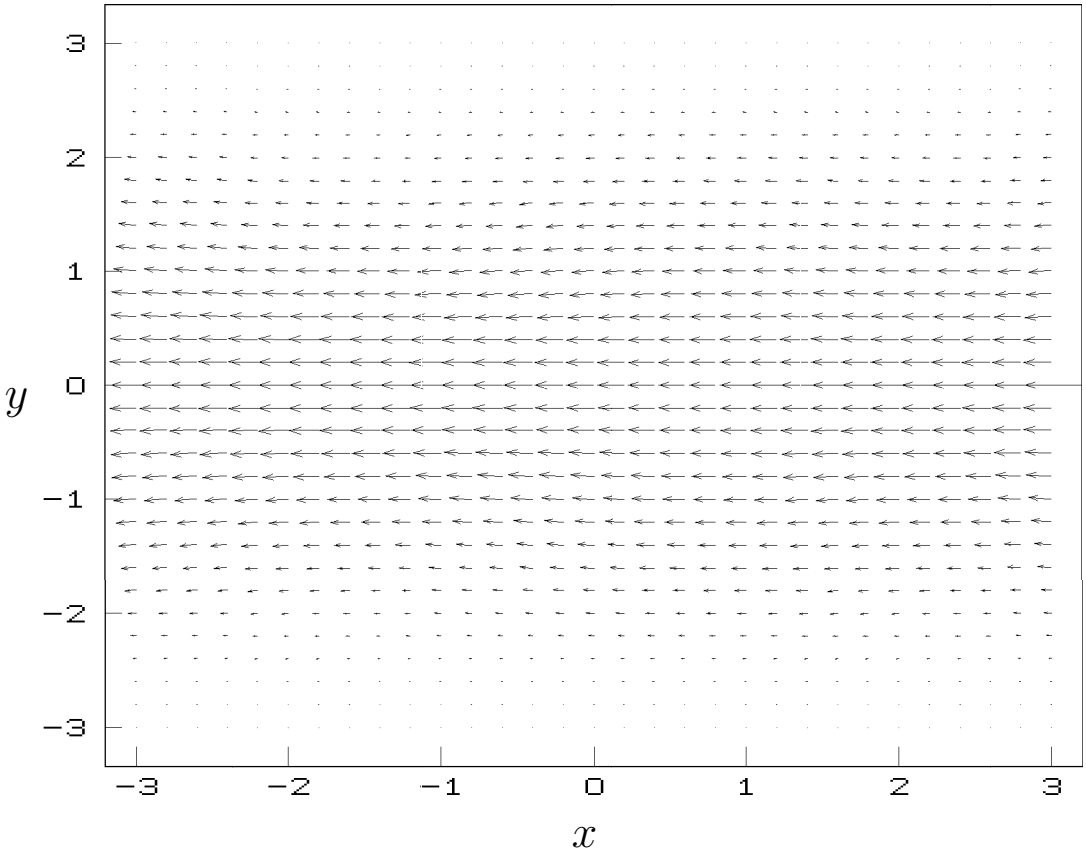


Figure 10

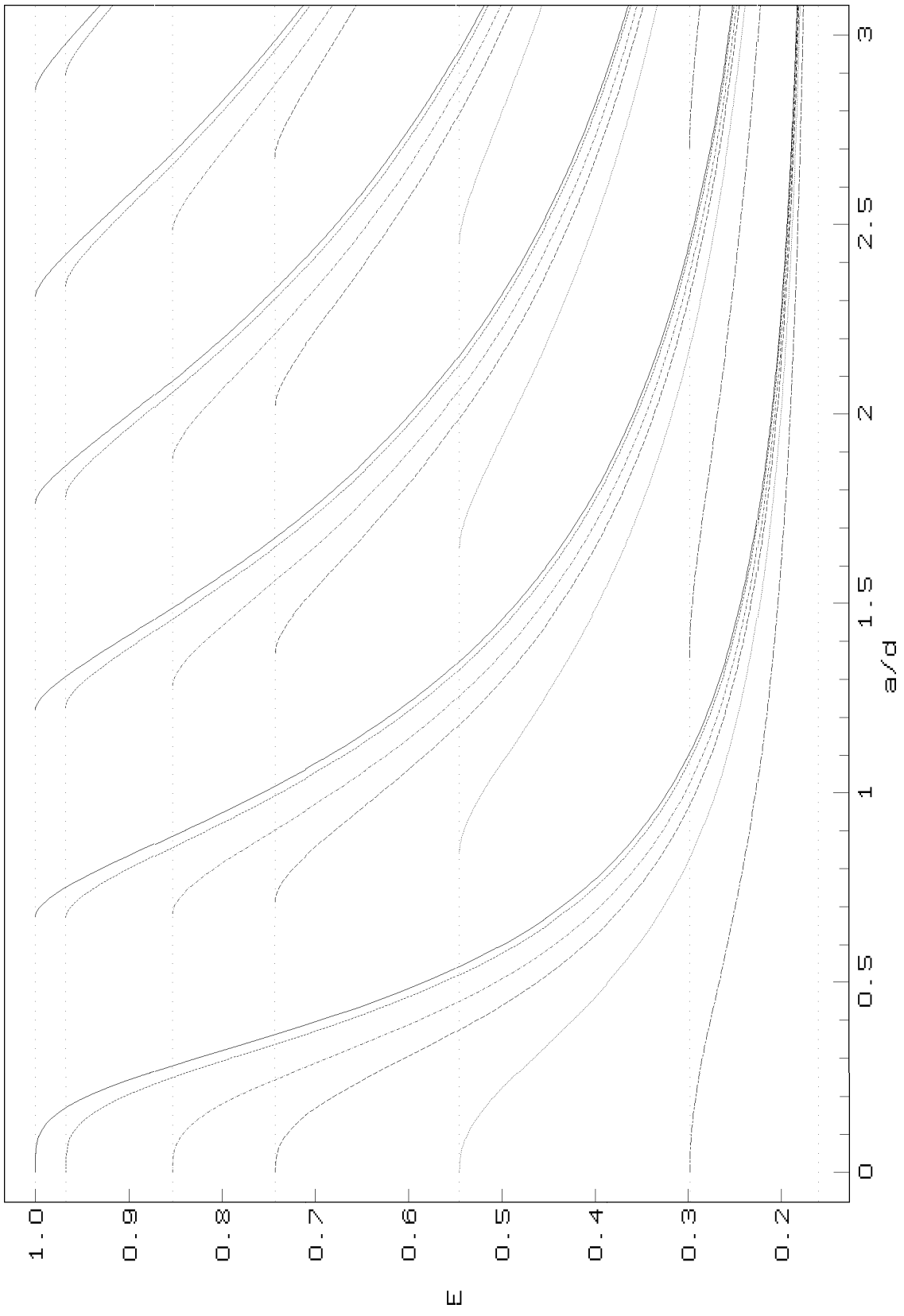


Figure 11

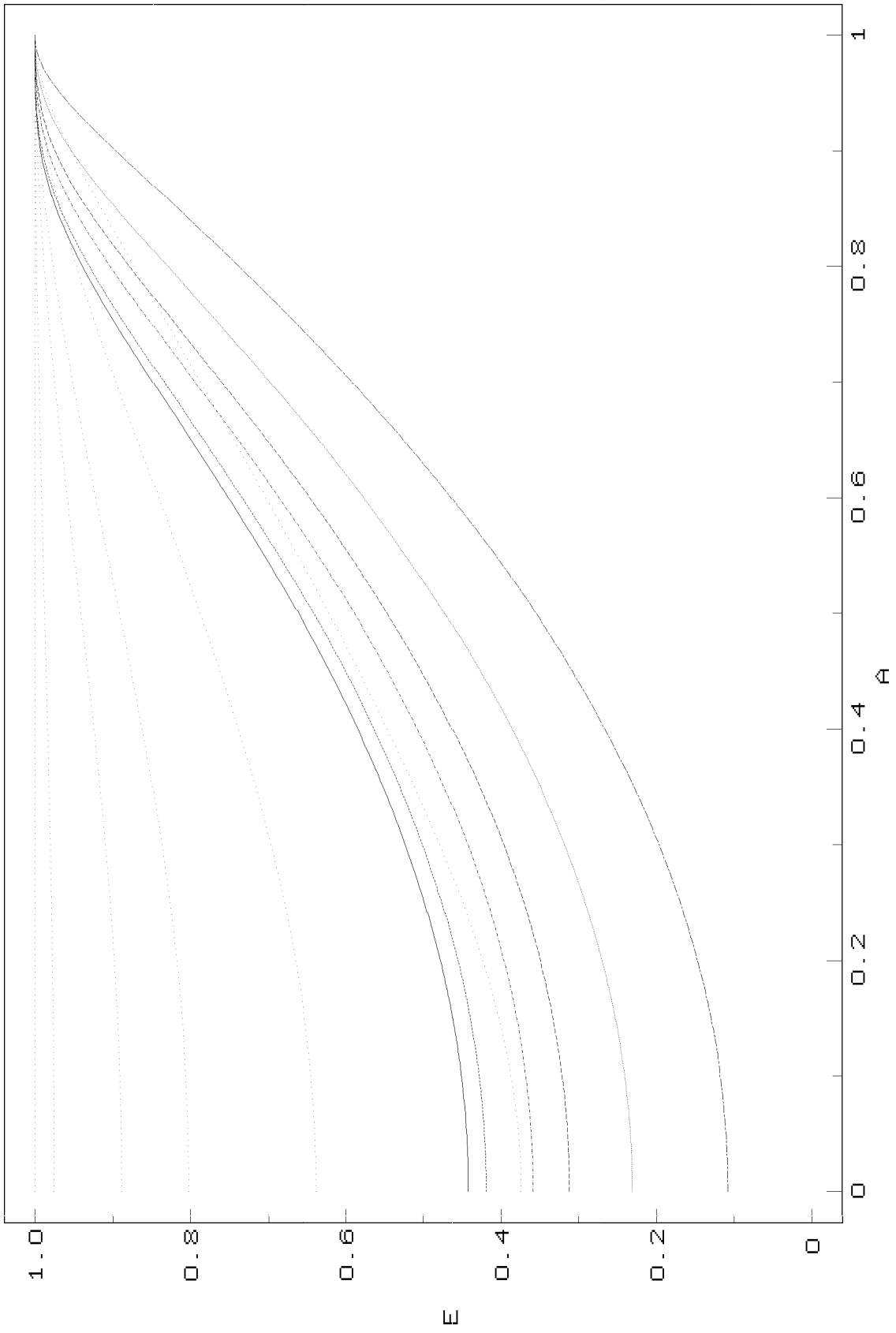


Figure 12

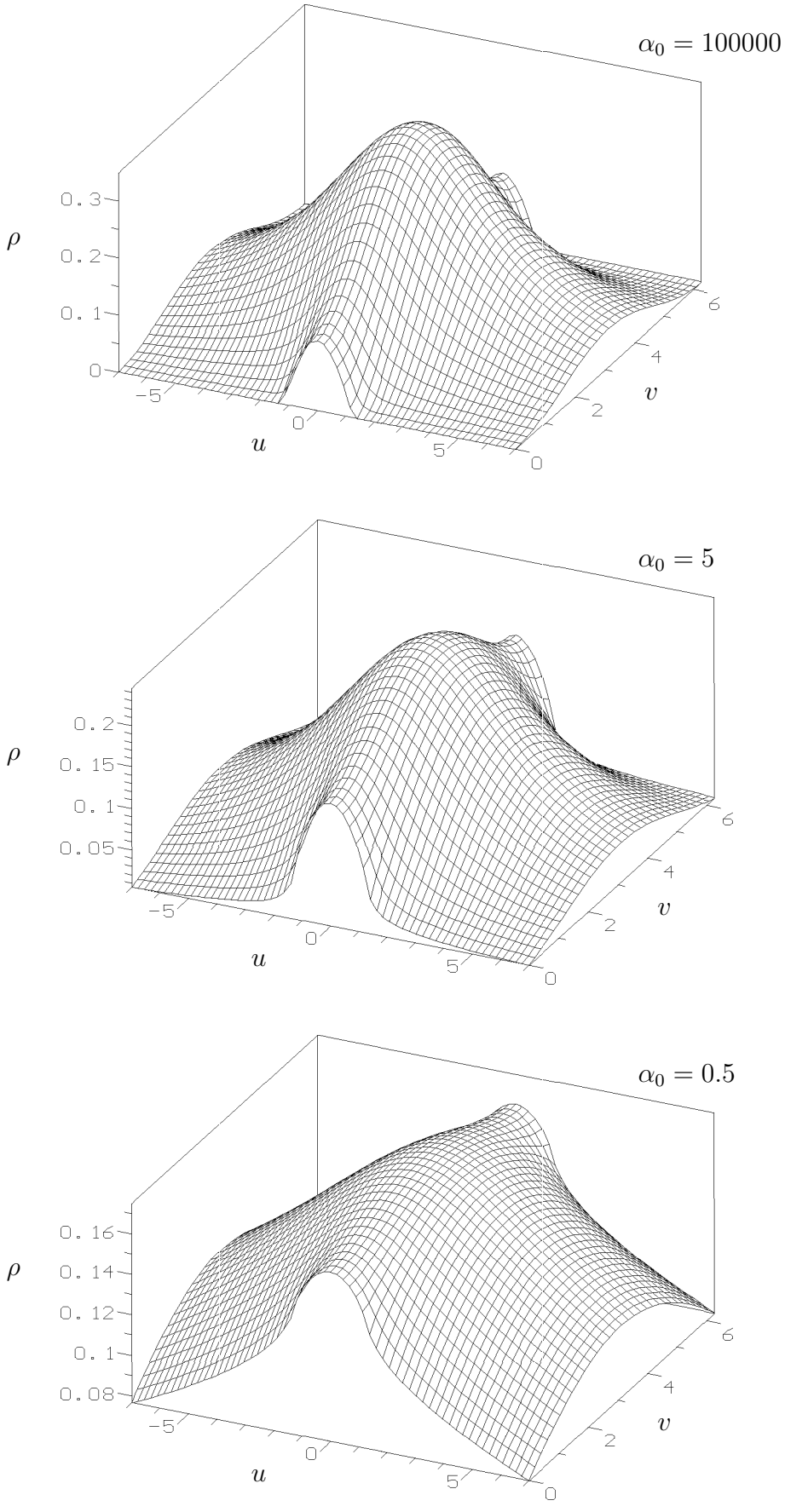
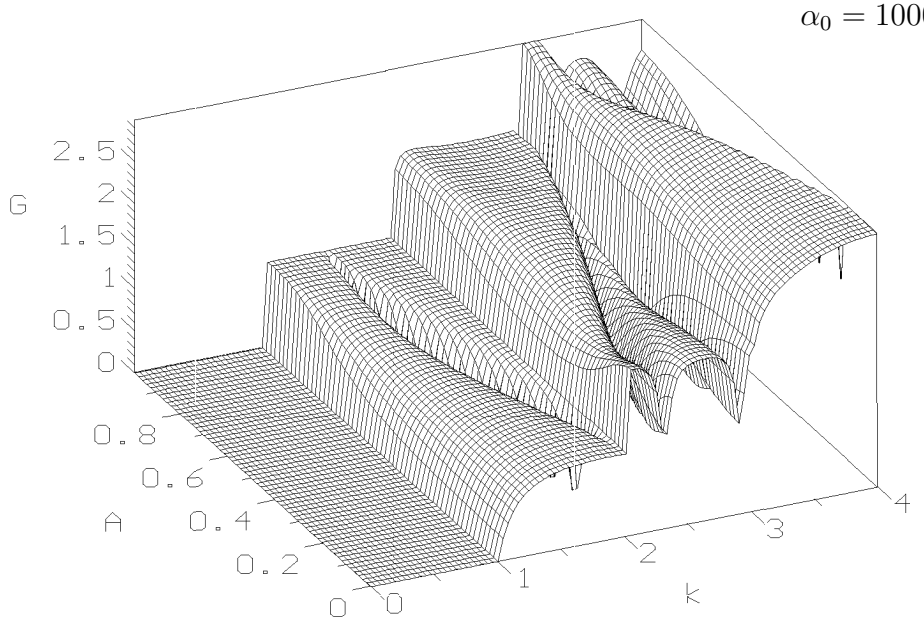

$\alpha_0 = 100000$
ρ
0.3
0.2
0.1
0
u
−5
0
5
v
0
2
4
6
$\alpha_0 = 5$
ρ
0.2
0.15
0.1
0.05
u
−5
0
5
v
0
2
4
6
$\alpha_0 = 0.5$
ρ
0.16
0.14
0.12
0.1
0.08
u
−5
0
5
v
0
2
4
6

Figure 13 a

$\alpha_0 = 100000$



$\alpha_0 = 50$

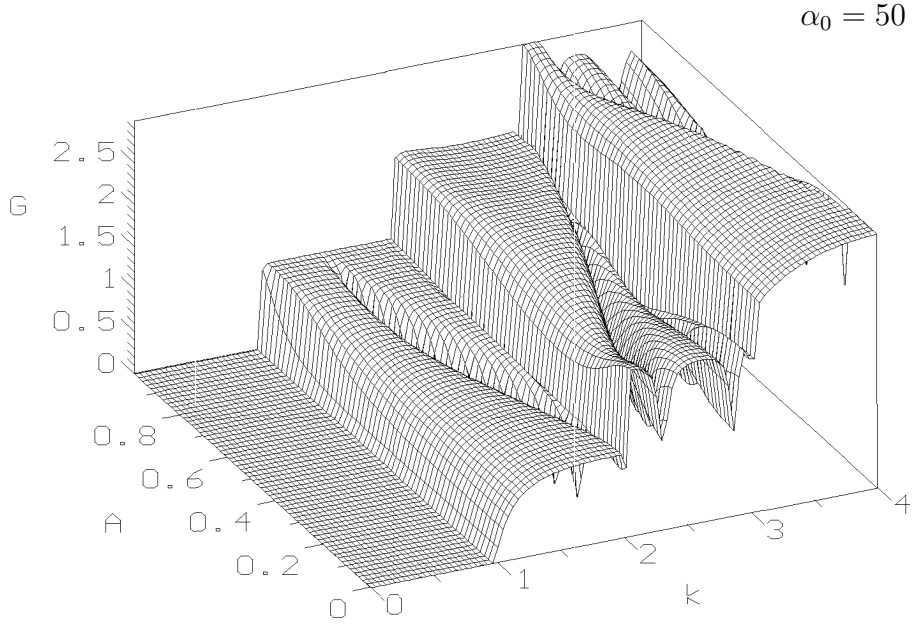
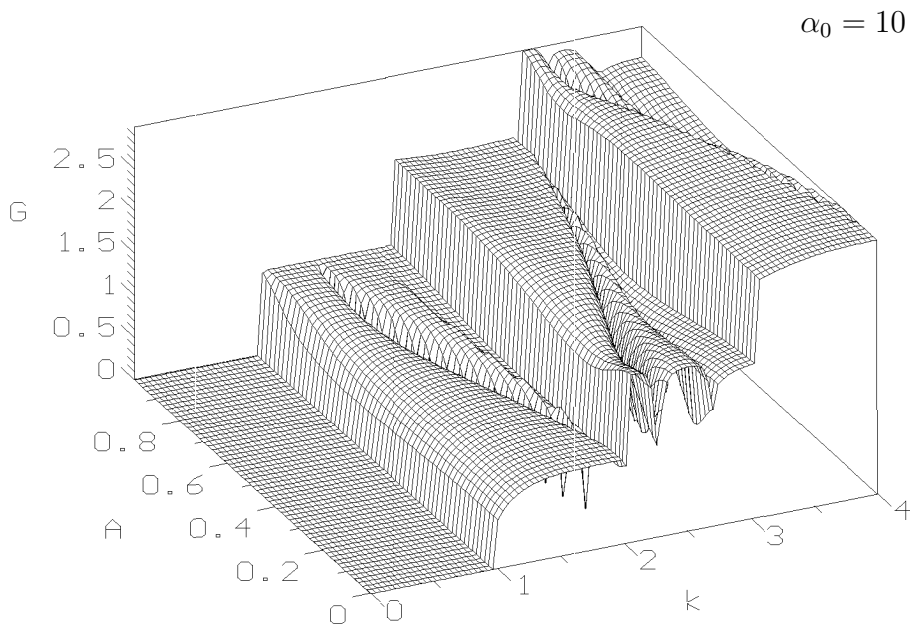


Figure 13 b


$\alpha_0 = 10$
G
2.5
2
1.5
1
0.5
0
0.8
0.6
A
0.4
0.2
0
0
1
2
3
4
k

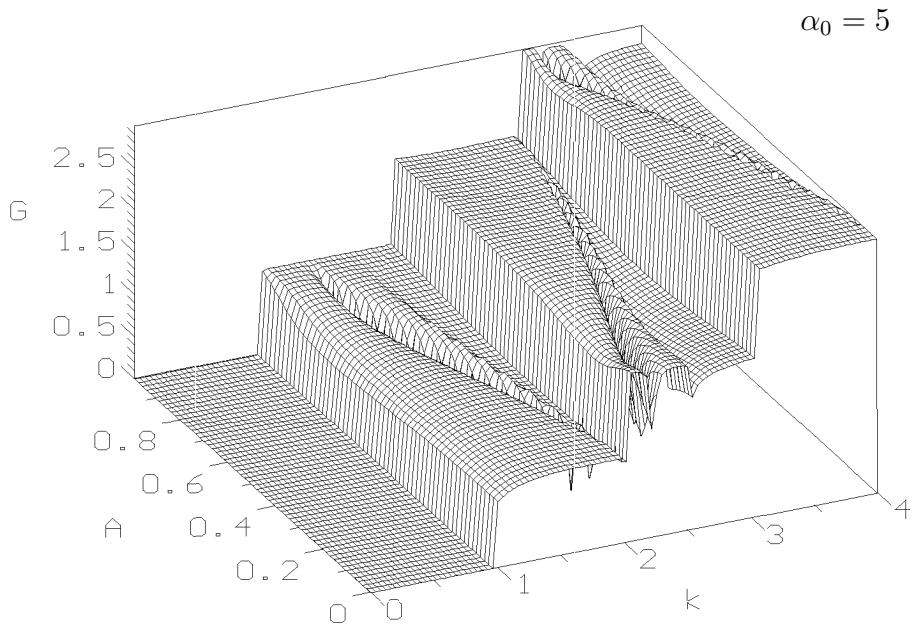
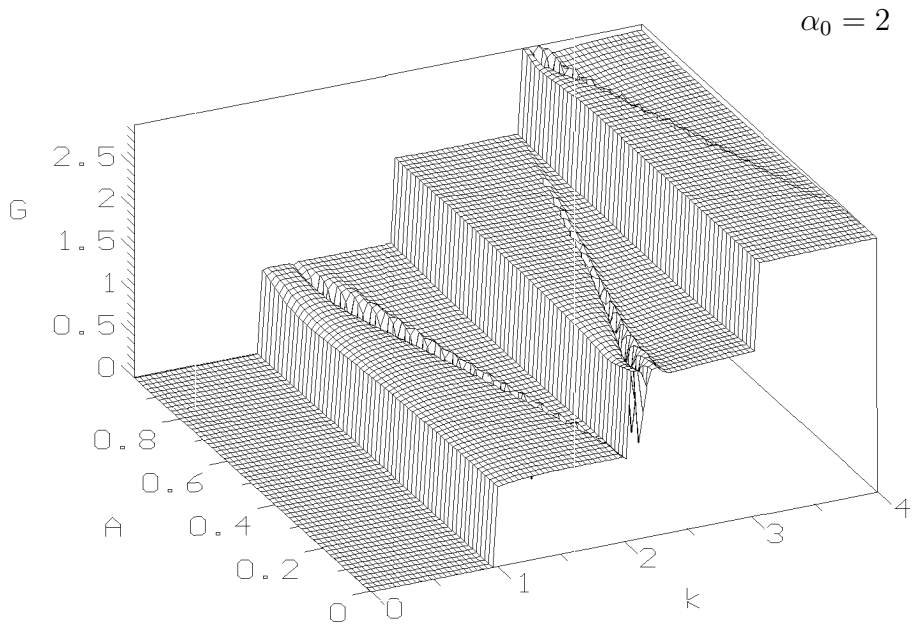

$\alpha_0 = 5$
G
2.5
2
1.5
1
0.5
0
0.8
0.6
A
0.4
0.2
0
0
1
2
3
4
k

Figure 13 c


$\alpha_0 = 2$
G
2.5
2
1.5
1
0.5
0
0.8
0.6
A
0.4
0.2
0
0
1
2
3
4
k

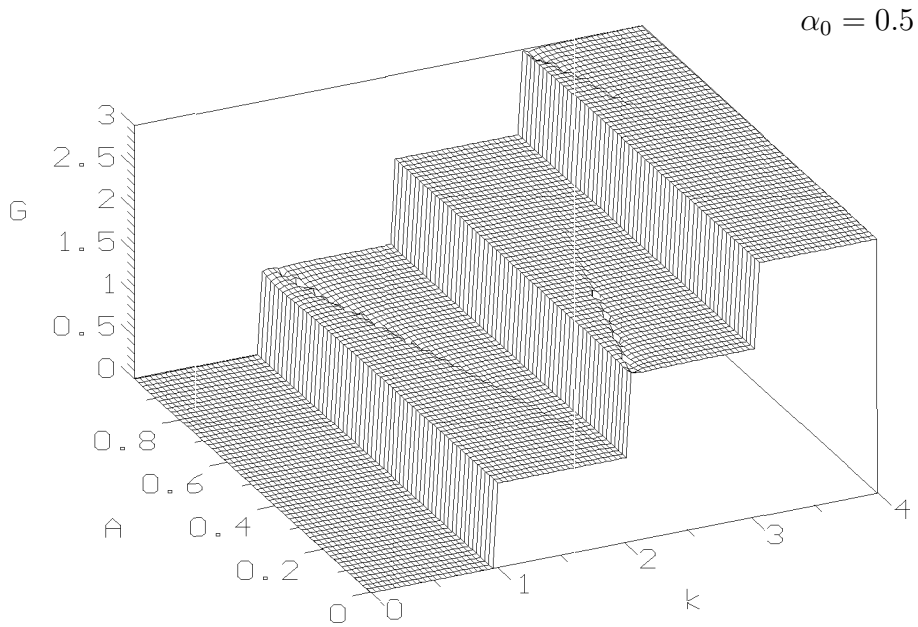
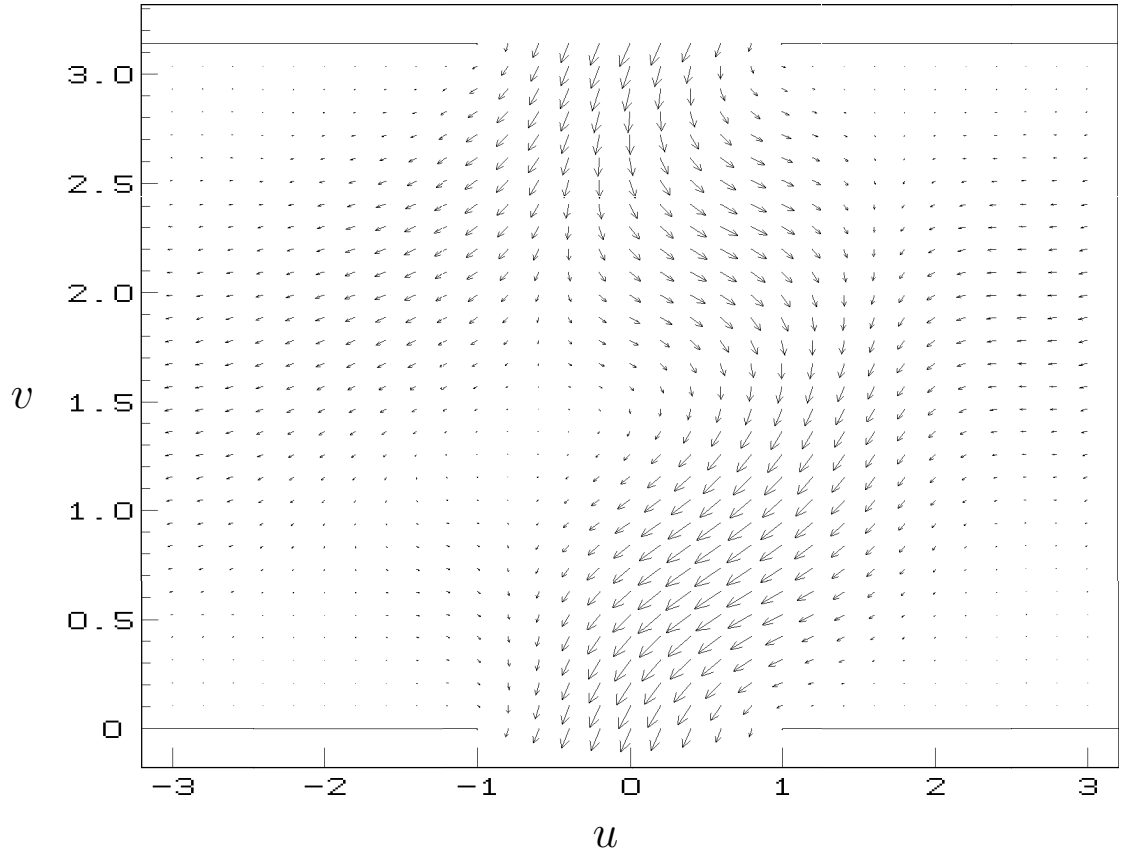

$\alpha_0 = 0.5$
G
3
2.5
2
1.5
1
0.5
0
0.8
0.6
A
0.4
0.2
0
0
1
2
3
4
k

Figure 14 a

$\alpha_0 = 100000$



$\alpha_0 = 50$

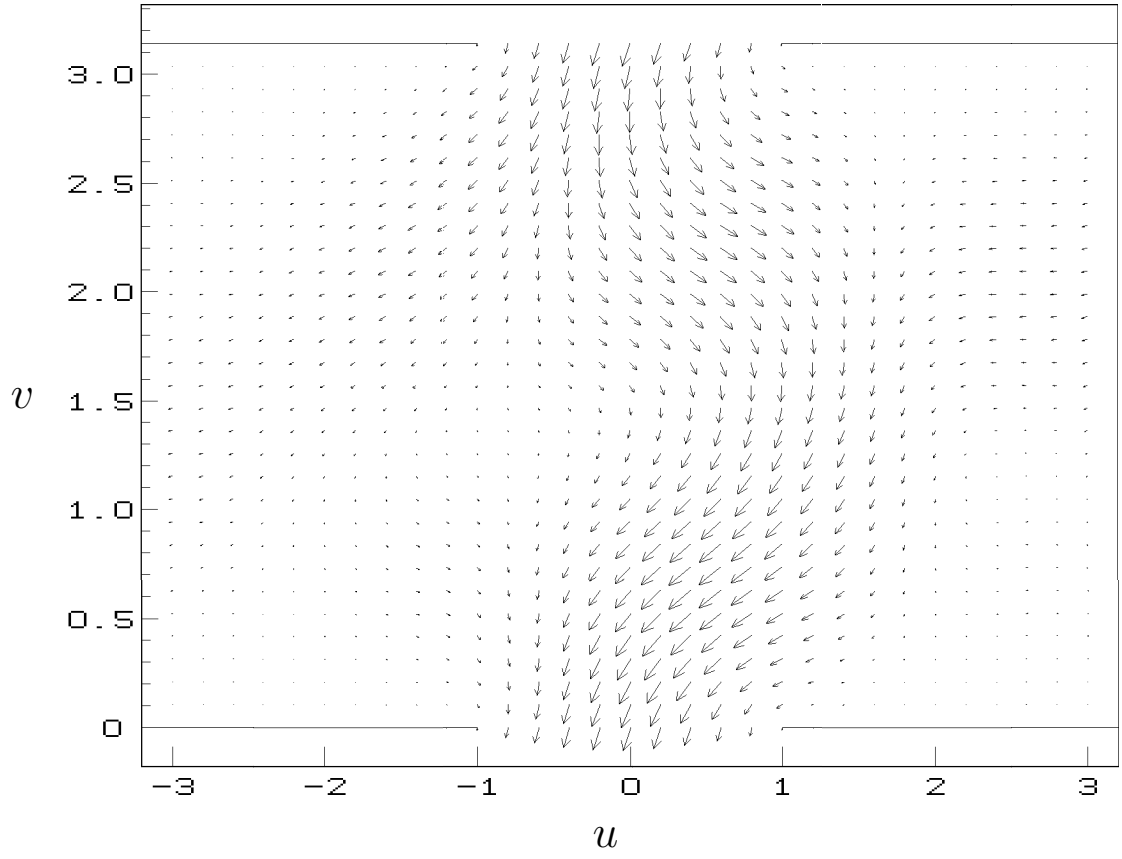
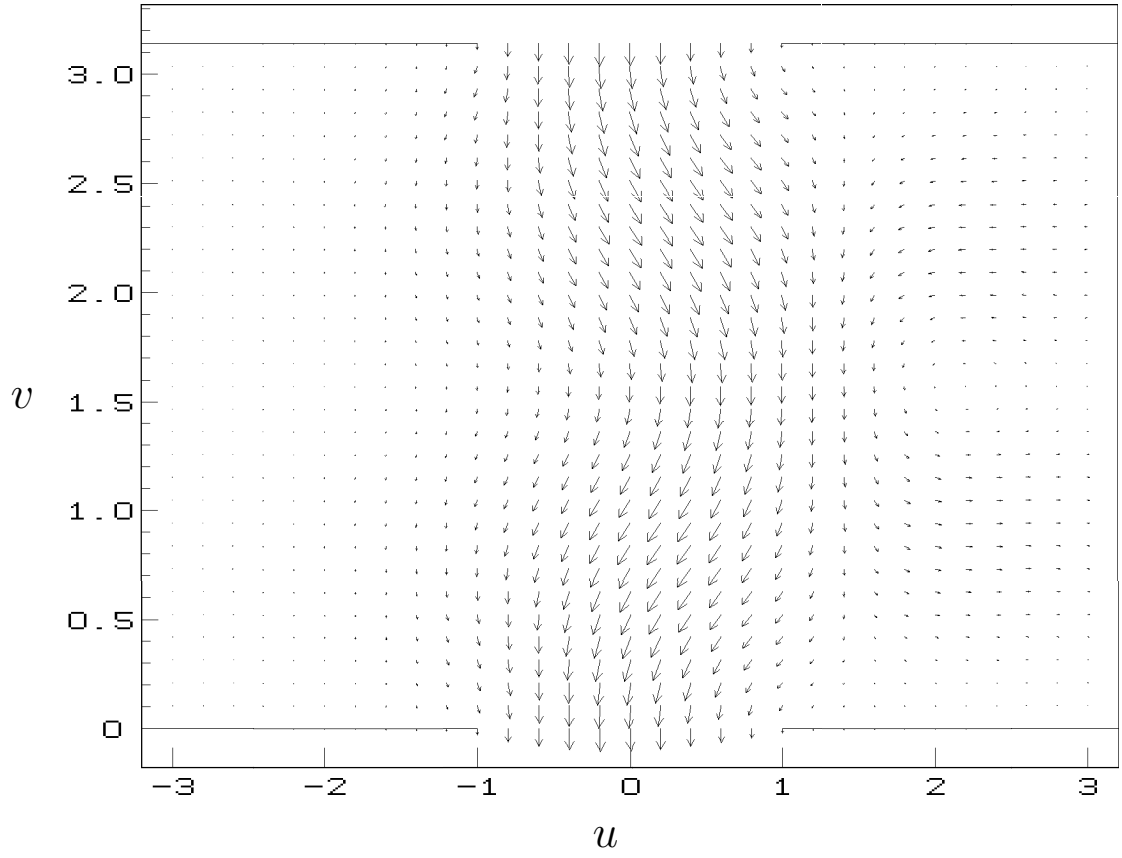


Figure 14 b

$\alpha_0 = 10$



$\alpha_0 = 5$

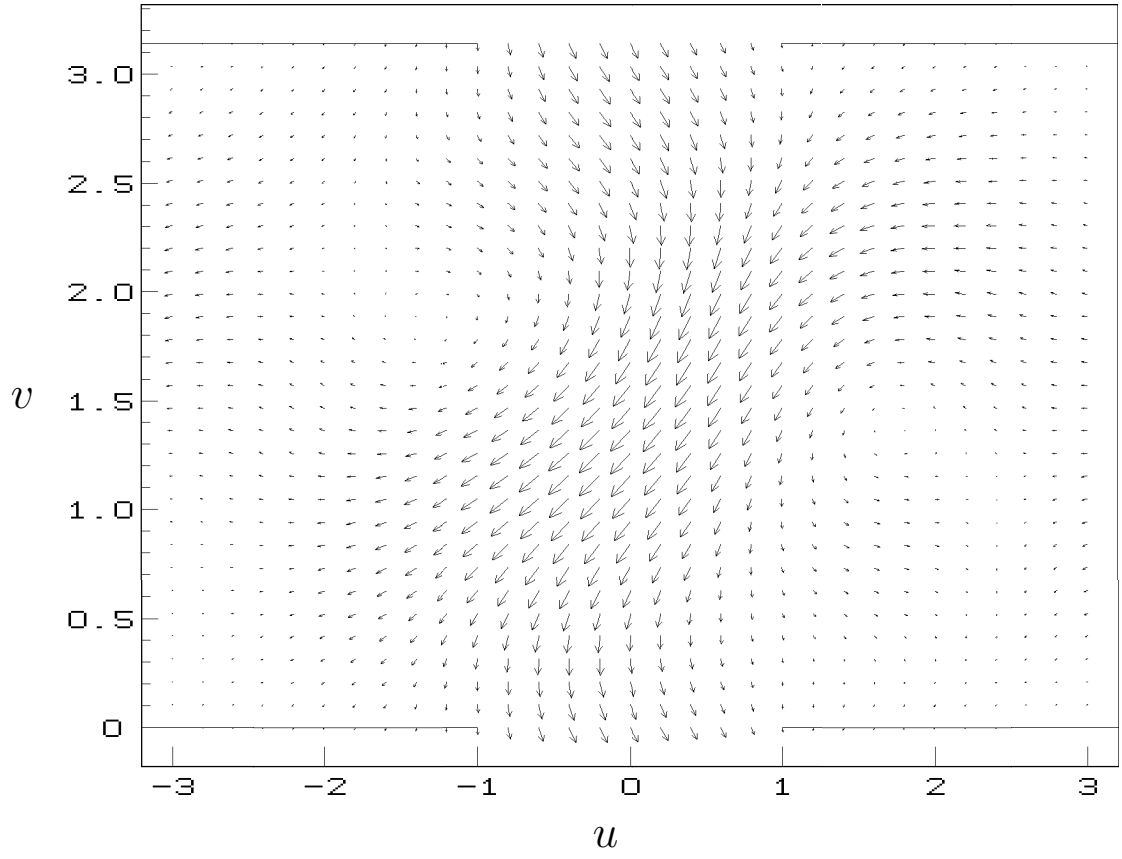
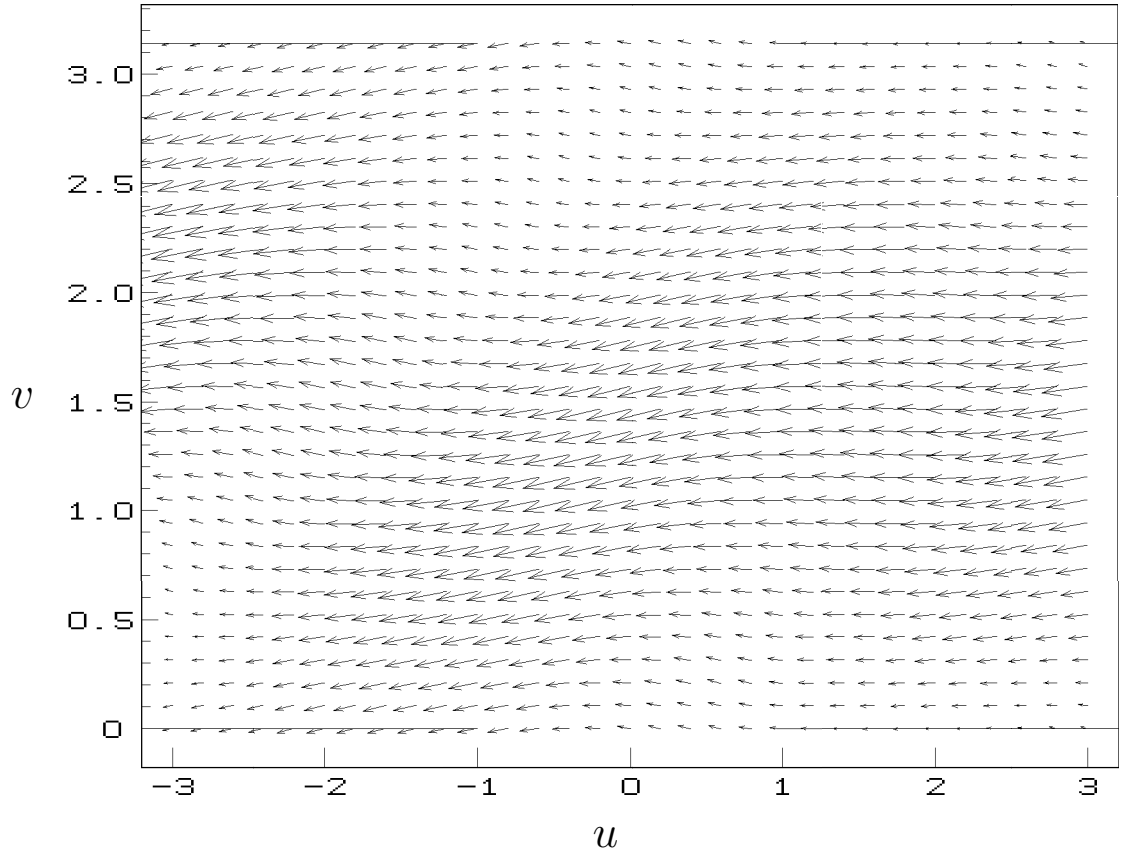
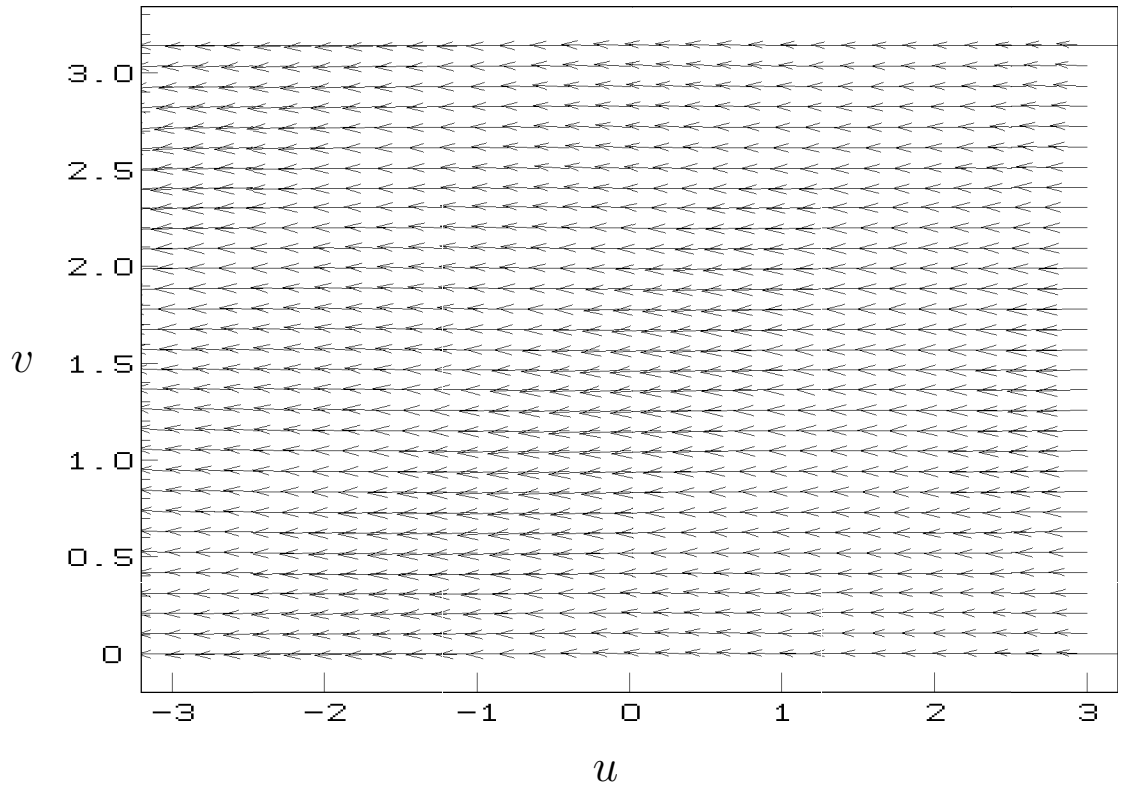


Figure 14 c

$\alpha_0 = 2$



$\alpha_0 = 0.5$