SOLUTIONS TO SOME PROBLEMS IN MATHEMATICAL PHYSICS

Thesis by

Vojkan Jakšić

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Abstract

In Part I, we study the adiabatic limit for Hamiltonians with certain complex-analytic dependence on the time variable. We show that the transition probability from a spectral band that is separated by gaps is exponentially small in the adiabatic parameter. We find sufficient conditions for the Landau-Zener formula, and its generalization to nondiscrete spectrum, to bound the transition probability.

Part II is concerned with eigenvalue asymptotics of a Neumann Laplacian $-\Delta_N^\Omega$ in unbounded regions Ω of $\mathbf{R}^2$ with cusps at infinity (a typical example is $\Omega = \{ (x, y) \in \mathbf{R}^2 : x > 1, |y| < e^{-x^2} \}$). We prove that $N_E(-\Delta_N^\Omega) \sim N_E(H_V) + E/2 \operatorname{Vol}(\Omega)$, where H_V is the canonical, one-dimensional Schrödinger operator associated with the problem. We also establish a similar formula for manifolds with cusps and derive the eigenvalue asymptotics of a Dirichlet Laplacian $-\Delta_D^\Omega$ for a class of cusp-type regions of infinite volume.

In Part III we study the spectral properties of random discrete Schrödinger operators H_ω of the form $-\Delta + \xi_n(\omega)(1 + |n|^\alpha)$, $\alpha > 0$, acting on $l^2(Z^d)$, where $\xi_n(\omega)$ are independent random variables uniformly distributed on $[0, 1]$. We show, for typical ω, that H_ω has a discrete spectrum iff $\alpha > d$, and we calculate its eigenvalue asymptotics. If $d/k \geq \alpha > d/(k + 1)$ for positive integer k, we prove that for typical ω and non-random strictly decreasing sequence a_k, $\sigma_{\text{ess}}(H_\omega) = [a_k, \infty)$, $\sigma_{\text{ac}}(H_\omega) = \emptyset$. The large k asymptotic of sequence a_k is studied. We also investigate the continuous analog of the above model.

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Part III: Spectral Properties of Random Schrödinger Operators with Unbounded Potentials

Introduction

This thesis consists of three parts—three different research topics which I have been investigating during my residence as a graduate student at Caltech. Since every part has its separate introduction, we give here just a brief overview.

The first part is concerned with the time evolution of slowly changing quantum-mechanical systems. It is based on joint work with Jan Segert [JS1], [JS2].

The second part deals with the spectral properties of Neumann Laplacian in unbounded regions of $\mathbf{R}^2$. It is based on joint work with B. Simon and S. Molchanov [JMS].

The third part is concerned with the spectral properties of random discrete Schrödinger operators with unbounded, nonhomogeneous potential. It is based on joint work with A. Gordon, S. Molchanov and B. Simon.

There are a number of research results that were originally planned to become a part of this thesis, but have not been incorporated for the simple reason of lack of time. This mainly concerns Part I, regarding the application of techniques developed there to quantum Hall systems—which will be discussed in [J], and Part III, since [GJMS] will contain considerably more results than were presented here. For better or for worse, the projects started with this thesis do not end with it, but will probably occupy me for some time to come.

Part I

Exponential Approach to the Adiabatic Limit and the Landau-Zener Formula

Chapter 1: Introduction

We consider the evolution generated by a time-dependent Hamiltonian $H(t)$ in the adiabatic limit. We recall that this is the limit where the time dependence becomes slow, $H(t/\tau)$ as τ tends to infinity. Consider a state that lies in some spectral subspace of $H(t_0)$, and let the system evolve. By transition probability we mean the probability that the system is measured at some later time to lie outside the initial spectral subspace. The spectral subspaces of interest are usually separated by gaps from the remainder of the spectrum for all values of t in some interval. The adiabatic theorem states that the transition probability across a spectral gap goes to zero as τ goes to infinity. The rate of vanishing of the transition probability depends on the smoothness of the time dependence. If the time dependence is k times differentiable (in a sense to be specified), then the transition probability is $O(1/\tau^k)$. This has been proven under very general conditions in [KAT1], [NEN], [ASY].

We study time-dependent Hamiltonians for which the transition probability across spectral gaps is $O(\exp(-2\tau L))$ for some $L > 0$. We call this behavior *exponential approach to the adiabatic limit.* It is generally believed that exponential approach to the adiabatic limit is related to some type of analyticity in the complex time plane.

This observation is widely attributed to Landau, arising from his 1932 study [LN] of atomic transitions induced by collisions. Zener [ZEN] showed that a particular two-level system exhibits exponential approach to the adiabatic limit. There is a formula for the exponential rate of approach, often called the *Landau-Zener formula*, or just the *Landau formula.* A partial chronology of related work in the physics and chemistry literature follows. Stueckelberg [ST] independently studied exponential approach by the WKB method, but his paper received relatively little attention, presumably because of its relative length and complexity. The currently common version of the Landau-Zener formula appeared in a paper of Dykhne [DY2] on two-level systems, and is described in more general terms in the book of Landau and Lifshitz [LNLF]. Davis and Pechukas [DVPE] have analyzed in greater detail the two-level system, and Hwang and Pechukas [HWPE] considered the finite-level system. For some applications in physics see [IKN], [GBC], [HX], notably [ZIM] for a discussion of the Zener diode.

The Landau-Zener paradigm is to consider transitions between noncrossing eigenvalues E_i and E_k, in the limit where the system is prepared at time $-\infty$, and measured at time $+\infty$. Suppose that the gap function $E_k(t) - E_i(t)$ has an analytic extension to the complex t-plane, and that there is a point w in the complex t-plane where $E_k(w) - E_i(w) = 0$. The Landau-Zener formula then states that the approach to the adiabatic limit is exponential, with the constant L:

$$L = \mathrm{Im}\left(\int_0^w (E_k(z) - E_i(z))dz\right). \tag{1.1}$$

Zener [ZEN] proved that this formula holds for the simple two-level Hamiltonian

$$H(t) = \begin{pmatrix} t & 1 \\ 1 & t \end{pmatrix}, \tag{1.2}$$

by reducing the problem to a second-order differential equation, the asymptotics of which had been previously analyzed. For two-level systems depending analytically on time, this formula appears to be correct [DVPE].

For more complicated systems, even with a finite number of levels, the applicability of the Landau formula is a difficult question; see e.g. [HWPE]. In 1960, Bates [BAT] argued that the Landau-Zener formula is problematic when applied to the very process for which it was created, namely, atomic collisions:

> *This formula ... has been used in a number of computations and because of its attractive simplicity it is introduced in many textbooks on quantum mechanics. The object of the present note is to point out that it is in fact invalid over much of the energy range for which it seemingly was designed, and certainly has been employed.*

Although our considerations are quite different from Bates', we are also interested in examining the applicability of the Landau formula. We shall prove several theorems about exponential approach to the adiabatic limit. In special cases, particularly for a finite-dimensional Hilbert space, our expression for the exponential rate resembles that of the Landau formula. We now state the simplest case of our results.

An analytic operator-valued function $T(z)$ on the strip $\mathcal{S}(a) = \{z \in \mathbf{C} | -a < \mathrm{Im}(z) < a\}$ is said to belong to $\mathrm{H}^1(a)$ if

$$\sup_{-a<c<a} \int_{-\infty}^{\infty} \|T(x+ic)\| dx < \infty.$$

Suppose that H is a bounded, self-adjoint operator, and let P_i be the spectral projection of H onto a band separated by a gap $g_i > 0$ from the remainder of the spectrum. Let $H(t;\tau) = W(t/\tau)HW^{-1}(t/\tau)$, with $W(t)$ unitary for real t. If the system is prepared to lie in the band P_i at time t_0, the probability that at time t it has made a transition to a state outside the band P_i is denoted by $p_i(t, t_0; \tau)$. We then have

Theorem 5.4. Suppose that the derivative $W'(t)$ is analytically extendible to $\mathcal{S}(a)$, and $W'(\cdot) \in \mathrm{H}^1(a)$. Then there is a finite constant C_a such that

$$\lim_{t\to\infty} \lim_{t_0\to-\infty} p_i(t, t_0; \tau) \leq C_a \exp(-2\tau a g_i).$$

Note that ag_i equals the imaginary part of the integral of $g_i(z)$ from 0 to ia, so this result resembles the Landau formula.

The techniques we use are an extension of those introduced by Avron, Seiler, and Yaffe in [ASY], see also [KS]. The complex-analytic properties enter through the Cauchy integral formula, mainly in the guise of properties of analytic operator-valued functions in the Hardy class $\mathrm{H}^1(a)$.

We briefly mention some recent related work, with no pretense of completeness. K. Yajima has independently developed related ideas for two-level Hamiltonians [YAJ]. G. Hagedorn [HG2] has examined an exponential approach to the adiabatic limit for transitions between two eigenstates. Hagedorn techniques involve matching an adiabatic expansion near level crossing [HG1] to an adiabatic expansion away from level crossing. Several recent papers of Berry [BEX, BHI, BGE] address similar issues. Datta, Ghosh, and Engineer [DGE] have studied the time-dependent, two-level system.

We finally remark that application of the techniques developed in this part to the quantum Hall systems will be studied in [J].

Chapter 2: Prerequisites

2.1. Existence of Solutions, and Spectral Theorem

We briefly review the theory of existence of a solution to a time-dependent Schrödinger equation. If the Hamiltonian $H(t)$ is bounded, the existence and uniqueness of the solution is easily proved by differential equation techniques. We briefly outline some consequences of the work of Kato-Yosida [YOS], [RS2] for unbounded Hamiltonians. Our discussion follows [ASY], [KS], restricted to the C^∞ case. For a bounded open interval $I \subset \mathbf{R}$, consider a family of Hamiltonians $H(t)$, $t \in I$. We suppose that the following conditions are satisfied.

A1) $H(t)$ is self-adjoint, bounded from below, with a t-independent domain D, closed with respect to the graph norm of $H(0)$.

A2) The function $H(t)$, $t \in I$, mapping I to $\mathcal{L}(D, \mathcal{H})$, is C^∞.

Here $\mathcal{H}$ denotes the Hilbert space, and $\mathcal{L}(X, Y)$ is the normed space of linear maps from X to Y.

We then have ([ASY], Thm. 2.1.)

Proposition 2.1. The initial value problem

$$i\partial_t U(t,t_0)\phi = H(t)U(t_0,t_0)\phi, \qquad U(t_0,t_0)\phi = \phi \tag{2.1}$$

has a unique solution with the following properties: $U(t, t_0)$ is a unitary propagator, strongly continuous in t and t_0, and $U(t, t_0)\phi$ is continuously differentiable for all $\phi \in D$.

Recall that a *unitary propagator* is a two-parameter family of unitary operators $U(t, t_0)$, $(t, t_0) \in \mathbf{R} \times \mathbf{R}$, satisfying

$$U(t,t) = 1,$$
$$U(t,t_0) = U(t,t_1)U(t_1,t_0). \tag{2.2}$$

We now review the functional calculus of a self-adjoint operator. This is one formulation of the spectral theorem (see [RS1], Theorem VIII.5). Let H be a self-adjoint operator. Then to each bounded Borel function $f(\cdot)$ on $\mathbf{R}$ corresponds the operator

$$f(H) = \int_{-\infty}^{\infty} f(\lambda) dP_\lambda.$$

Furthermore, $f(H)$ is bounded, namely, $\|f(H)\| \leq \|f(\cdot)\|_{L^\infty(\mathbf{R})}$, and the assignment is an algebraic homomorphism, in the sense $(fg)(H) = f(H)g(H)$. Let $\beta \subset \mathbf{R}$ be a Borel set, and χ_β the characteristic function. $\chi_\beta(H)$ is then the spectral projection of H onto β. Denoting the spectrum of H by $\sigma(H)$, it is clear that $\chi_\beta(H) = \chi_{\beta\cap\sigma(H)}(H)$.

2.2. The Adiabatic Theorem, Spectral Bands and Spectral Gaps

We now turn to a discussion of the adiabatic theorem, following [ASY]. In the adiabatic limit, we consider Hamiltonians that vary slowly. We consider $H(t/\tau)$, as τ becomes large, and study the τ dependence of $U(t/\tau, t_0/\tau)$. Equivalently, a linear time rescaling gives

$$i\partial_s U_\tau(s,s_0) = \tau H(s) U_\tau(s,s_0), \qquad U_\tau(s_0,s_0) = 1. \tag{2.3}$$

We shall from now on work with the time-dependent Schrödinger equation of the form (2.3).

The adiabatic theorem basically states that if a time-dependent Hamiltonian has a spectral band that is separated for all s by gaps from the remainder of the spectrum, then as $\tau \to \infty$, $U_\tau(s,s_0)$ does not evolve states across the gaps. We make these concepts more precise.

Consider a single Hamiltonian H and a closed interval (not necessarily bounded)

$[a,b] \subset \mathbf{R}$. We shall frequently consider a collection $[a_i, b_i]$, where i belongs to some index set, and denote the corresponding spectral projections by $P_i = \chi_{[a_i,b_i]}(H)$. Denote by $H|_i$ the restriction of H to the range of P_i, and by $\sigma(H|_i)$ the spectrum of this restriction[1] .

We interchangeably call both P_i and $\sigma(H|_i) = [a_i, b_i] \cap \sigma(H)$ a *spectral band.*

The generalization to a time-dependent Hamiltonian $H(s)$ is immediate. Letting $a_i(s)$ and $b_i(s)$ be functions, the term *spectral band* refers to $[a_i(s), b_i(s)] \cap \sigma(H(s))$ and the corresponding spectral projection $P_i(s) = \chi_{[a_i(s),b_i(s)]}(H(s))$. By $H(s)|_i$ we denote the restriction of $H(s)$ to the range of $P_i(s)$. If $a_i(s)$ and $b_i(s)$ are locally bounded, we call the band *finite.*

There is nothing in the definition of a band implying that it is separated from the remainder of the spectrum. That information is described by the notion of spectral gap:

Definition 2.2. The *gap* $g_i(s)$ of a band $P_i(s)$ is the distance in $\mathbf{R}$ between $\sigma(H(s)|_i)$ and the complement of the spectrum, $\sigma(H(s)|_f)$, where $P_f(s) \equiv 1 - P_i(s)$;

$$g_i(s) \equiv \text{dist}[\sigma(H(s)|_i); \sigma(H(s)|_f)]. \tag{2.4}$$

We rephrase the gap condition for the adiabatic theorem of [ASY] with this terminology:

A3) The band $P_i(s)$ is finite, and there is an $\epsilon > 0$ such that $g_i(r) \geq \epsilon$ for all $r \in [s_0, s]$.

Associated with the band $P_i(s)$ is a unitary propagator $U_A(s, s_0; P_i)$, that is defined as the solution of a certain differential equation. It has the property that it intertwines $P_i(s)$; i.e.,

$$P_i(s) = U_A(s, s_0; P_i) P_i(s_0) U_A{}^{-1}(s, s_0; P_i).$$

[1] This is not in general the same as the spectrum of HP_i acting on $\mathcal{H}$, but does coincide on the complement of $\{0\}$.

The adiabatic theorem, in the version of [ASY], says that the adiabatic evolution $U_A(s, s_0; P_i)$ approximates the actual evolution $U_\tau(s, s_0)$ in the following sense[2].

Theorem 2.3. Supposing conditions A1), A2), and A3), and that the support of $P_i'(\cdot)$ is contained in the interior of the interval $[s_0, s]$; then

$$P_i(s) - U_\tau(s, s_0)P_i(s_0)U_\tau^{-1}(s, s_0) = O(1/\tau^\infty).$$

We shall require a more specific notion of spectral gap.

Definition 2.4. For a time-dependent Hamiltonian $H(s)$ with spectral bands $P_i(s)$ and $P_j(s)$, the *oriented gap* $g_{ki}(s)$ is defined by

$$g_{ki}(s) \equiv \inf \sigma(H(s)|_k) - \sup \sigma(H(s)|_i).$$

Remark 1: Definition 2.4 defines the oriented gap between two bands, whereas Definition 2.2 defines a related notion of gap between a single band and the remainder of the spectrum. While g_i is nonnegative, g_{ki} may be negative. Consider a band P_i with a nonzero gap g_i. Split the remaining spectrum $P_f = 1 - P_i = P_1 + P_2$, where P_1 is the spectrum strictly above P_i, and P_2 is the spectrum strictly below. Then

$$g_i = \min(g_{1i}, g_{i2}) > 0. \tag{2.5}$$

Remark 2: A band may consist of a single point of spectrum. Suppose that P_k and P_i are two such bands, with $\sigma(H|_k) = E_k \in \mathbf{R}$ and $\sigma(H|_i) = E_i \in \mathbf{R}$. Then

$$g_{ki} = -g_{ik} = E_k - E_i. \tag{2.6}$$

[2] The appendix of [KS] contains a revised proof of lemma 2.7 in [ASY].

Chapter 3: Intertwining

3.1. Transition Probabilities

We discuss transitions between bands. Let $P_i(s)$ and $P_j(s)$ be bands, with no gap assumptions at this point. Let $\phi \in \mathcal{H}$ be a normalized state in the range of $P_i(s_0)$, and ψ a normalized state in the range of $P_j(s)$. We consider a quantum mechanical system prepared in the state ϕ at scaled time s_0 (physical time τs_0). The time evolution of the state is prescribed by the Schrödinger equation, and a measurement is made at scaled time s (physical time τs). The probability that the system is measured to be in the state ψ is given by

$$p_{\psi,\phi}(s, s_0; \tau) \equiv |(\psi, U_\tau(s, s_0)\phi)|^2.$$

We define the *transition probability* $p_{k,i}(s, s_0; \tau)$ to be the supremum over all the normalized states in the respective subspaces of the probabilities,

$$\begin{aligned} p_{k,i}(s, s_0; \tau) &\equiv \sup_{\psi \in P_k(s)\mathcal{H}} \sup_{\phi \in P_i(s_0)\mathcal{H}} p_{\psi,\phi}(s, s_0; \tau) \\ &= \|P_k(s)U_\tau(s, s_0)P_i(s_0)\|^2. \end{aligned} \tag{3.1}$$

Let $P_f(s) = 1 - P_i(s)$ be the complementary band of P_i. Then $p_{f,i}(s, s_0)$ is the total transition probability for a state starting in the band P_i. We use the shorthand

$$p_i(s, s_0; \tau) \equiv p_{f,i}(s, s_0; \tau). \tag{3.2}$$

Remark: An immediate consequence of Theorem 2.3 is $p_i(s, s_0; \tau) = O(1/\tau^\infty)$.

3.2. Admissible Hamiltonians

We shall consider separately two types of time-dependent Hamiltonians. The first type is actually a special case of the second, but it provides a more transparent example of the techniques.

Suppose that for each $s \in \mathbf{R}$, $W(s)$ is a unitary operator and $W(0) = 1$. We further assume that the map $W : \mathbf{R} \to \mathcal{L}(\mathcal{H})$ is C^1; i.e., $W'(s)$ exists as a bounded operator, depending continously on s. We now define the less general case of our time-dependent Hamiltonians.

Definition 3.1. For $W(s)$ as above, we call the time-dependent Hamiltonian $H(s)$ *unitarily admissible* if it is of the form

$$H(s) = W(s)HW^{-1}(s) \tag{3.3}$$

for some self-adjoint operator H. If H is unbounded with domain D, we further assume that $W(s)D = D$ for all $s \in \mathbf{R}$, and that there exists a unique solution of the Schrödinger equation[3].

The admissible Hamiltonians exclude numerous interesting cases, so we generalize by letting pieces of the spectrum shift relative to each other. As before, take a self-adjoint operator H, with domain D. We now decompose H as a sum of operators acting on mutually orthogonal subspaces.

We consider a countable Borel partition of $\mathbf{R}$. Namely, let $\{\Omega_n\}, n \in J \subseteq \mathbf{Z}$ be disjont Borel sets with $\cup_n \Omega_n = \mathbf{R}$. Defining

$$Q_n = \chi_{\Omega_n}(H), \qquad n \in J, \tag{3.4}$$

the following properties are immediate from the functional calculus;

$$\sum_{n \in J} Q_n = 1; \qquad n \neq m \Rightarrow Q_n Q_m = 0;$$
$$Q_n H\phi = HQ_n\phi, \quad \phi \in D:$$

We call the $\{Q_n\}$ the *spectral partition* of H associated to $\{\Omega_n\}$.

[3] For example, it is sufficient that conditions A1) and A2) hold.

Definition 3.2. A time-dependent Hamiltonian $H(s)$ is *admissible* if it is of the form

$$H(s) = W(s)[H + \sum_{n \in J} \Delta_n(s) Q_n] W^{-1}(s), \tag{3.5}$$

where $\{Q_n\}$ is a spectral partition of H, and the functions $\Delta_n(s)$ are continuous, with $\sup_{n \in J} |\Delta_n(s)|$ locally bounded. If H is unbounded with domain D, we further assume that $W(s)D = D$, and that the Schrödinger equation has a unique solution.

We can assume $\Delta_n(0) = 0$ without loss of generality. We also note that if H is self-adjoint with domain D, then $H(s)$ is self-adjoint with the same domain. This follows from the fact that $\sum \Delta_n(s) Q_n$ is a bounded operator, and is from the Kato-Rellich theorem [RS2].

Taking $J = \{0\}$, the set with one element, and $Q_0 = 1$, one sees immediately that unitarily admissible, time-dependent Hamiltonians are admissible. This of course corresponds to the trivial partition $\Omega_0 = \mathbf{R}$.

3.3. INTERTWINING OF PROJECTIONS

Consider a unitarily admissible Hamiltonian $H(s)$. Consider the spectral band $P_i(s) = \chi_{[a_i, b_i]}(H(s))$, where a_i and b_i are constants that do not depend on s. We shall often use the shorthand $H = H(0)$, $P_i = P_i(0)$, etc. Then it is evident that

$$P_i(s) \equiv W(s) P_i W^{-1}(s). \tag{3.6}$$

This is the prototype of intertwining of spectral projections.

Let $P(s), s \in \mathbf{R}$, be a one-parameter family of self-adjoint projection operators.

Definition 3.3. A unitary propagator $U(s, s_0)$ is said to *intertwine* the time-dependent projection $P(s)$ if for all $s, s_0 \in \mathbf{R}$,

$$P(s) U(s, s_0) = U(s, s_0) P(s_0). \tag{3.7}$$

It is clear that

$$W_G(s, s_0) \equiv W(s)W^{-1}(s_0) \tag{3.8}$$

is a unitary propagator. Furthermore $W'_G(s, s_0)$ is a bounded operator, by the boundedness assumption on $W'(s)$. The following lemma is then immediate.

Lemma 3.4. Let $H(s)$ be a unitarily admissible Hamiltonian, and let $P_i(s) = \chi_{[a_i,b_i]}(H(s))$ be a spectral band with a_i and b_i constant. Then $W_G(s, s_0)$ intertwines $P_i(s)$.

Proof : Follows from the definitions and Equation (3.6). ∎

When generalizing to admissible Hamiltonians, one must keep in mind that the spectrum of $H(s)$ is no longer constant. Let $P_i = \chi_{[a_i,b_i]}(H)$ be a band of $H = H(0)$ such that for some $n \in J$, $P_iQ_n = P_i$. This condition is equivalent to $[a_i, b_i] \cap \sigma(H) \subset \Omega_n \cap \sigma(H)$.

Definition 3.5. A spectral band $P_i(s)$ of an admissible Hamiltonian $H(s)$ is called *compatible* if it is of the type

$$P_i(s) = \chi_{[a_i+\Delta_n(s), b_i+\Delta_n(s)]}(H(s)), \tag{3.9}$$

where a_i and b_i are the s-independent constants above.

Defining $Q_n(s) \equiv W(s)Q_nW^{-1}(s)$, the following lemma characterizes the (non-crossing) compatible spectral bands. We point out that the decomposition (3.5) of an admissible Hamiltonian is not unique.

Lemma 3.6.

a) Let $H(s)$ be unitarily admissible. A spectral band $P_i(s)$ is compatible if and only if it is of the form $P_i(s) = \chi_{[a_i,b_i]}(H(s))$ (as in Lemma 3.4).

b) Let $H(s)$ be admissible and $P_i(s)$ a compatible spectral band with nonzero gap, $g_i(s) > 0$. Then $H(s)$ can be decomposed in the form (3.5), in such a way that $P_i(s) = Q_{n_i}(s)$ for some $n_i \in J$.

Proof :

a) Taking $Q_0 = 1$, and $\Delta_0(s) = 0$, the result is immediate from Definition 3.9.

b) There exists by assumption an $n \in J$ such that $P_i(s)Q_n(s) = P_i(s)$. Split Q_n into two orthogonal projections, $Q_{n_1}(s) \equiv P_i(s)$ and $Q_{n_2}(s) \equiv (1 - P_i(s))Q_n(s)$. Taking $\Delta_{n_1}(s) = \Delta_{n_2}(s) = \Delta_n(s)$ and augmenting the index set accordingly gives the desired decomposition. ∎

We now consider the intertwining of compatible bands.

Lemma 3.7. Let $H(s)$ be an admissible Hamiltonian, and $P_i(s)$ a compatible spectral band. Then $W_G(s, s_0)$ intertwines $P_i(s)$.

Proof : The proof follows immediately from $P_i(s) = W(s)P_iW^{-1}(s)$. ∎

The following definition is motivated by the construction of [ASY].

Definition 3.8.

a) The self-adjoint operator $B(s)$ is given by

$$\begin{aligned} B(s) &\equiv iW'(s)W^{-1}(s) \\ &= iW_G'(s, s_0){W_G}^{-1}(s, s_0). \end{aligned} \tag{3.10}$$

b) The operator $V_\tau(s, s_0)$ is defined by the solution, if it exists, for a dense set of $\phi \in \mathcal{H}$, of the equation

$$i\frac{\partial V_\tau(s, s_0)\phi}{\partial s} = \tau[{W_G}^{-1}(s, s_0)H(s)W_G(s, s_0)]\ V_\tau(s, s_0)\phi; \qquad V_\tau(s_0, s_0) = 1. \tag{3.11}$$

c)

$$W_A(s, s_0) \equiv W_G(s, s_0)V_\tau(s, s_0). \tag{3.12}$$

It should come as no surprise that for admissible Hamiltonians, the solutions $V_\tau(s, s_0)$ of Equation (3.11) can be explicitly constructed.

Lemma 3.9.

a) For unitarily admissible Hamiltonians,

$$V_\tau(s,s_0) = W(s_0)[\exp(-i\tau(s-s_0)H)]W^{-1}(s_0). \tag{3.13}$$

b) For admissible Hamiltonians,

$$V_\tau(s,s_0) \equiv W(s_0)\exp(-i\tau[(s-s_0)H + \sum_{n\in J}\int_{s_0}^{s}\Delta_n(x)Q_n\,dx])W^{-1}(s_0).$$

Proof :

a) For unitarily admissible Hamiltonians,

$$\tau[W_G{}^{-1}(s,s_0)H(s)W_G(s,s_0)] = \tau H(s_0),$$

and the solution of Equation (3.11), with $\phi \in D$, is given by

$$V_\tau(s,s_0) = \exp(-i\tau(s-s_0)H(s_0)),$$

or equivalently by Equation (3.13).

b) The proof is analogous, using the additional fact that H commutes with all Q_n. ∎

From the explicit solutions, we have $V_\tau(s,s_0)D = D$.

Lemma 3.10. If $V_\tau(s,s_0)D = D$, then for $\phi \in D$,

$$i\frac{\partial W_A(s,s_0)\phi}{\partial s} = [\tau H(s) + B(s)]\; W_A(s,s_0)\phi; \qquad W_A(s,s_0) = 1.$$

Proof : Straightforward calculation. ∎

The following intertwining lemma is the analogue of Lemma 2.3 of [ASY]. Part a) actually follows from part b), but we prove a) separately to provide a simple example.

Lemma 3.11.

a) Let $H(s)$ be a unitarily admissible Hamiltonian, and $P_i(s)$ a compatible spectral band. Then $W_A(s, s_0)$ is a unitary propagator which intertwines $P_i(s)$.

b) Let $H(s)$ be an admissible Hamiltonian, and $P_i(s)$ a compatible spectral band. Then $W_A(s, s_0)$ is a unitary propagator that intertwines $P_i(s)$.

Proof :

a) Note that $P_i(s_0)$ commutes with $V_\tau(s, s_0)$, and use Lemma 3.4.

b) The proof is similar, using Lemma 3.7, and the fact that $P_i(s_0)$ commutes with $V_\tau(s, s_0)$ only if P_i commutes with all the Q_n. ∎

Remark: Both W_G and W_A mimic the physical time evolution U_τ in the adiabatic limit, in the sense that none of the evolutions allows the crossing of spectral gaps. One would expect W_A to be a better approximation than W_G, since it contains information of the dynamical phase V_τ. This is in fact the case, as is explained in [ASY] in a slightly different setting.

3.4. Discrete Spectrum

In this section, we analyze time-dependent Hamiltonians with discrete noncrossing spectrum, continuous in s. With mild regularity conditions, such Hamiltonians are automatically admissible. There is an explicit construction, that is due to Kato, of an intertwining operator (see [KAT1] and Chap. 2.4 of [KAT2]). This construction yields not only the admissibility, but also further regularity properties that shall be important for the discussion of the Landau-Zener formula.

The spectral representation of $H(s)$ is of the form

$$H(s) = \sum_{n \in J} E_n(s) P_n(s), \qquad n \in J \subseteq \mathbf{Z}. \tag{3.14}$$

For each s, the $P_n(s)$ form a complete orthonormal set of projections, and we assume that $P_n(s)$ depends continuously on s. We rewrite Equation (3.14) in a form more closely resembling Definition 3.2. Defining $\Delta_n(s) = E_n(s) - E_n(0)$,

$$H(s) = \sum_{n \in J} [E_n(0) + \Delta_n(s)] P_n(s). \tag{3.15}$$

By the spectral theorem, for each s, there exists a (nonunique) unitary $W(s)$ such that for all $n \in J$,

$$P_n(s) = W(s) P_n(0) W^{-1}(s).$$

Thus for each s, $H(s)$ can be written in the form (3.5), with $H = H(0)$ and $Q_n = P_n(0)$.

This does not suffice to show that $H(s)$ is admissible. $W(s)$ and $\Delta_n(s)$ have to satisfy further conditions. We assume that for all s, all $H(s)$ have a common domain D. Further, assume that all $P_n(s)$ are continuously differentiable, and the sum $\sum_n \|P_n'(s)\|$ converges in norm, uniformly on compact subsets of $\mathbf{R}$. With these assumptions,

$$L(s) \equiv \frac{i}{2} \sum_{n \in J} [P_n'(s), P_n(s)]$$

is a bounded self-adjoint operator, continuous in s.

Let $W(s)$ be the solution of the differential equation

$$iW'(s) = L(s)\, W(s), \qquad W(0) = 1. \tag{3.16}$$

Existence and uniqueness follow from standard techniques, discussed in the sequel. We now show that $W(s)$ intertwines all the levels.

Lemma 3.12. (Kato [KAT1])

a) For each $n \in J$,

$$[L(s), P_n(s)] = iP_n'(s). \tag{3.17}$$

b) For each $n \in J$,

$$P_n(s) = W(s) P_n(0) W^{-1}(s).$$

Proof :

a) We derive two simple identities. First, $0 = P[(P^2)' - P']P = PP'P$. Second, if

$n \neq k$, $0 = (P_n P_k)' = P_n' P_k + P_n P_k'$. Expanding the commutator and using these identities gives (3.17).

b) Applying $P_n(0)$ to the right-hand side of (3.16), obtain

$$i[W(s)P_n(0)]' = L(s)[W(s)P_n(0)], \qquad [W(0)P_n(0)] = P_n(0).$$

Compute the derivative,

$$\begin{aligned} i[P_n(s)W(s)]' &= iP_n'(s)W(s)P_n(s)W'(s) \\ &= (iP_n'(s) + P_n L(s))W(s) \\ &= L(s)[P_n(s)W(s)]. \end{aligned}$$

Here we first used (3.16) to obtain W', and then (3.17) to evaluate $iP_n' + P_n L$. $[P_n(s)W(s)]$ and $[W(s)P_n(0)]$ satisfy the same differential equation, with the same boundary condition at $s = 0$. They must then coincide by uniqueness of the solution. ∎

We now restrict ourselves to the finite-dimensional Hilbert space, which will appear naturally in the discussion of the Landau-Zener formula.

Proposition 3.13. Let $H(s)$ act on a finite-dimensional Hilbert space. Suppose $H(s)$ has a noncrossing spectrum continuous in s, and all $P_n(s)$ are continuously differentiable. Then $H(s)$ is admissible, with $W(s)$ given by Equation (3.16).

Proof : Follows from Definition 3.2 and Lemma 3.12. ∎

Remark: Suppose $H(s)$ acts on an infinite-dimensional Hilbert space, and has discrete noncrossing spectrum. In addition to the conditions of a), suppose that the sum $\sum_n P_n'(s)$ converges in norm, uniformly on compact sets. Further suppose that $\sup_n |E_n(s) - E_n(0)|$ is locally bounded. Then it follows that $H(s)$ meets all the conditions of admissibility, except possibly for the existence and uniqueness of the unitary propagator for the time-dependent Schrödinger equation. We outline the proof that $W(s)D = D$. By the assumption, all $H(s)$ have domain D. Since $\sup_n |\Delta_n(s)|$ is locally bounded, the operator $\sum_n \Delta_n(s)P_n(s)$ is bounded for any s. Using (3.15) and Kato-Rellich, we get that $\sum_n E_n(0)P_n(s)$ is self-adjoint with domain D. Now $\sum_n E_n(0)P_n(s)W(s) = W(s)H(0)$, so we see that $W(s)D = D$.

Certain of the operators associated to admissible Hamiltonians can be written more explicitly for Hamiltonians with discrete spectrum. Referring to Definition 3.8 a), we see that

$$B(s) = L(s) = \frac{i}{2}\sum_{n\in J}[P_n'(s), P_n(s)]. \tag{3.18}$$

We also have

$$V_\tau(s,s_0) = W(s_0)\exp(-i\tau\sum_{n\in J}\int_{s_0}^{s} E_n(s)ds\ P_n(0))W^{-1}(s_0).$$

Remark: We finish with a comparison of $W_A(s,s_0)$ with $U_A(s,s_0;P_n)$ of [ASY, KS]. For Hamiltonians with discrete spectrum,

$$W_A(s,s_0) = \sum_{n\in J} U_A(s,s_0;P_n)P_n(s_0).$$

While the $U_A(s,s_0;P_n)$ intertwine the single level $P_n(s)$, the $W_A(s,s_0)$ intertwine $P_k(s)$ for *all* $k \in J$ simultaneously.

3.5. Comparing Time Evolutions

We now introduce operators that will allow us to compare the physical time evolution $U_\tau(s,s_0)$ with the evolution $W_A(s,s_0)$. Following [ASY], we define the analog of the wave operator in scattering theory.

$$\begin{aligned}\Theta(s,s_0) &\equiv {W_A}^{-1}(s,s_0)U_\tau(s,s_0),\\ &= {V_\tau}^{-1}(s,s_0){W_G}^{-1}(s,s_0)U_\tau(s,s_0).\end{aligned} \tag{3.19}$$

Definition 3.14.

a)

$$K_G(s,s_0) \equiv {W_G}^{-1}(s,s_0)W_G'(s,s_0).$$

b)

$$K_\tau(s, s_0) \equiv V_\tau{}^{-1}(s, s_0) K_G(s, s_0) V_\tau(s, s_0).$$

`Remark 1:` Unlike $B(s)$ (Definition 3.8), $K_G(s, s_0)$ is *not* independent of s_0. In fact,

$$K_G(s, s_0) = W(s_0) W^{-1}(s) W'(s) W^{-1}(s_0).$$

Further, note that

$$K_\tau(s, s_0) = -i W_A{}^{-1}(s, s_0) B(s) W_A(s, s_0).$$

`Remark 2:` For discrete spectrum, our $K_\tau(s, s_0)$ is analogous to the $K_\tau(s, P)$ of [ASY]. The difference is that our $K_\tau(s, s_0)$ generates intertwining of all levels simultaneously.

Lemma 3.15.

$$\Theta'(s, s_0) = -K_\tau(s, s_0)\Theta(s, s_0), \qquad \Theta(s_0, s_0) = 1.$$

Proof : Since $B(s)$ is bounded, by the Kato-Rellich theorem [RS2], both $H(s)$ and $H(s) + B(s)/\tau$ are self-adjoint with the domain D. The rest is a direct computation, using part b) of Lemma 3.10. Since $U_\tau(s, s_0)$ preserves the domain D, we have

$$\begin{aligned} \frac{\partial[\Theta(x, s_0)\phi]}{\partial x}\Big|_s &= W_A{}^{-1} \frac{\partial[U_\tau(x, s_0)\phi]}{\partial x}\Big|_s + \frac{\partial[W_A{}^{-1}(x, s_0) U_\tau(s, s_0)\phi]}{\partial x}\Big|_s \\ &= -K_\tau(s, s_0)\Theta(s, s_0)\phi. \end{aligned}$$

Now $K_\tau(s, s_0)$ is bounded, and D is dense; the proof follows. ∎

We will be interested in the limit $s_0 \to -\infty$, $s \to \infty$. $\Theta(s, s_0)$ will not generally behave well in this limit. It is convenient to introduce a new wave unitary operator $\Omega(s, s_0)$ that behaves better in the limit.

Definition 3.16.

a)

$$\begin{aligned}\Omega(s,s_0) &\equiv W_A(0,s_0)\Theta(s,s_0){W_A}^{-1}(0,s_0) \\ &= W_A(0,s)U_\tau(s,s_0)W_A(s_0,0).\end{aligned} \tag{3.20}$$

b) If the following limit exists, define

$$\tilde{\Omega} \equiv \lim_{s\to\infty}\lim_{s_0\to-\infty}\Omega(s,s_0). \tag{3.21}$$

The following proposition will play a central role. We frequently use the shorthand of omitting a variable when it is set equal to 0, e.g., $K_\tau(s) \equiv K_\tau(s,0)$, $H \equiv H(0)$, and $P_i \equiv P_i(0)$.

Proposition 3.17.

$$\Omega'(s,s_0) = -K_\tau(s)\Omega(s,s_0), \qquad \Omega(s_0,s_0) = 1. \tag{3.22}$$

Proof : Use Lemma 3.15 and the unitary propagator composition property of W_A. ∎

We now discuss the computation of the transition probabilities for admissible Hamiltonians from the operators defined above. Recalling Equation (3.1), and assuming that the bands $P_i(s)$ and $P_k(s)$ are compatible with $H(s)$, we obtain

$$\begin{aligned}p_{k,i}(s,s_0;\tau) &= \|W_A(s,s_0)P_k(s_0){W_A}^{-1}(s,s_0)U_\tau(s,s_0)P_i(s_0)\|^2 \\ &= \|P_k(s_0)\Theta(s,s_0)P_i(s_0)\|^2 \\ &= \|P_k\Omega(s,s_0)P_i\|^2, \\ \tilde{p}_{k,i}(\tau) &\equiv \|P_k\tilde{\Omega}P_i\|^2 = \|P_i\tilde{\Omega}^\dagger P_k\tilde{\Omega}P_i\|, \\ \tilde{p}_i(\tau) &\equiv \|(1-P_i)\tilde{\Omega}P_i\|^2.\end{aligned} \tag{3.23}$$

We have used that $P_k(s) = W_A(s,s_0)P_k(s_0){W_A}^{-1}(s,s_0)$ by Lemma 3.11, and the unitarity of W_A.

In the sequel, we will consider data that is analytically extendible to regions of the complex plane. We retain the shorthand $K_G(z) = K_G(z, 0)$, etc.

Definition 3.18. Denote by $\mathcal{S}(b, a)$ the open strip in the complex plane

$$\mathcal{S}(b, a) \equiv \{z \in \mathbf{C} | b < \mathrm{Im}(z) < a\}. \tag{3.24}$$

We use the shorthand $\mathcal{S}(a)$ for the symmetric strip $\mathcal{S}(-a, a)$.

It is convenient to define Ω_c, an operator related to Ω, and the corresponding $K_{\tau c}$ analogous to K_τ.

Definition 3.19. Suppose $K_G(s)$ is analytically extendible (as an operator-valued function) to $\mathcal{S}(a)$. Then for $s, s_0 \in \mathbf{R}$, define $\Omega_c(s, s_0)$ as the solution of the following differential equation with the initial condition:

$$\Omega_c(s, s_0)' = -K_{\tau c}(s)\Omega_c(s, s_0); \qquad \Omega_c(s_0, s_0) = 1, \tag{3.25}$$

where

$$K_{\tau c}(s) \equiv V_\tau^{-1}(s) K_G(s + ic) V_\tau(s).$$

As before, if the following limit exists, define

$$\tilde{\Omega}_c \equiv \lim_{s \to \infty} \lim_{s_0 \to -\infty} \Omega_c(s, s_0). \tag{3.26}$$

Chapter 4: Technical Tools

4.1. Differential Equations on the Real Line

In this section, we collect some standard material about regularity of solutions of first-order linear differential equations. These are operator-valued, but this does not produce any complications. We will apply this to the differential equation for Ω, and will thus be dealing with bounded operators only, even though the time-dependent Hamiltonians may be unbounded. The basic method is the successive iteration of the corresponding Volterra integral equation.

We consider the operator-valued differential equation on $\mathbf{R}$,

$$\partial_s U(s, s_0) = -F(s)U(s, s_0); \qquad U(s_0, s_0) = 1, \tag{4.1}$$

Here $F(s)$ and $U(s, s_0)$ are operators on the Hilbert space $\mathcal{H}$, and $s, s_0 \in \mathbf{R}$.

Proposition 4.1. In the above equation, suppose $F : \mathbf{R} \to \mathcal{L}(\mathcal{H})$ is continuous. Then there exists a solution $U(s, s_0)$ with the following properties:

a)

$$U(s, s_0) = \sum_{j=0}^{\infty} U_j(s, s_0),$$

where

$$U_j(s, s_0) \equiv (-)^j \int_{s_0}^{s} dt_j \int_{s_0}^{t_j} dt_{j-1} \cdots \int_{s_0}^{t_2} dt_1 F(t_j)F(t_{j-1}) \dots F(t_1). \tag{4.2}$$

b)

$$\|U(s, s_0)\| \leq \exp\left(\int_{s_0}^{s} \|F(t)\| dt\right),$$

c) If furthermore $\|F(\cdot)\| \in L^1(\mathbf{R})$, then the following limits exist;

$$\tilde{U}_j \equiv \lim_{s\to\infty} \lim_{s_0\to-\infty} U_j(s,s_0),$$
$$\tilde{U} \equiv \lim_{s\to\infty} \lim_{s_0\to-\infty} U(s,s_0), \tag{4.3}$$

and $\tilde{U} = \sum_{j=0}^{\infty} \tilde{U}_j$.

d)

$$\|\tilde{U}\| \leq \exp\left(\|F(\cdot)\|_{L^1(\mathbf{R})}\right).$$

Proof : Integrating the differential equation (4.1),

$$U(s,s_0) = 1 - \int_{s_0}^{s} F(t)U(t,s_0)\, dt.$$

Part a) is the the formal iterative solution of this integral equation. To prove a) and b), we need to show convergence of the series. We have

$$\|U_j(s,s_0)\| \leq \int_{s_0}^{s} dt_j \int_{s_0}^{t_j} dt_{j-1} \cdots \int_{s_0}^{t_2} dt_1 G(t_j, t_{j-1}, \ldots, t_1), \tag{4.4}$$

with $G(t_j, t_{j-1}, \ldots, t_1) \equiv \|F(t_j)\|\ \|F(t_{j-1})\| \ \cdots \|F(t_1)\|$. Define $I = [s, s_0] \subset \mathbf{R}$. Then the region of integration in (4.4) is the quotient I^j/S_j, where S_j is the permutation group, acting by interchanging coordinates. Now G is S_j-invariant, so

$$\|U_j(s,s_0)\| \leq \frac{1}{j!}\left[\int_{s_0}^{s} dt\ \|F(t)\|\right]^j. \tag{4.5}$$

Summing the series, we get the bound b), and the convergence of a).

To prove c) and d), we use the same idea, and in addition show that the estimates are uniform in s and s_0. If $\|F(\cdot)\|_{L^1(\mathbf{R})} = f$, we see that the bound (4.5) gives

$$\|U_j(s,s_0)\| \leq \frac{1}{j!}[f]^j \tag{4.6}$$

for any s and s_0. ∎

The two-parameter family $U(s, s_0)$ of operators satisfies a composition law like Equation (2.2) for a unitary propagator, the difference, of course, being that if $F(s)$ is not anti-self-adjoint, then $U(s, s_0)$ is generally not unitary. We call a two-parameter family of invertible operators satisfying Equation (2.2) an *invertible propagator.* Decompose F into its self-adjoint and anti-self-adjoint parts, $F = F_+ + F_-$, with $F_+^\dagger = F_+$, and $F_-^\dagger = -F_-$.

Lemma 4.2. With the assumptions of Propostion (4.1),

a) $U(s, s_0)$ is an invertible propagator. Furthermore, if $F^\dagger(x) = -F(x)$ for all $x \in [s_0, s]$, then $U(s, s_0)$ is a unitary propagator.

b) $U(s, s_0)$ is the unique solution of Equation (4.1) .

Proof :

a) Repeating the arguments of Proposition (4.1) for the equation

$$L'(s, s_0) = L(s, s_0)F(s), \qquad L(s_0, s_0) = 1,$$

we find that $L(s, s_0)$ exists, and $L(s, s_0) = U(s_0, s)$. One checks from the series expansions that $L(s, s_0)U(s, s_0) = 1 = U(s, s_0)L(s, s_0)$, so $L(s, s_0) = U^{-1}(s, s_0)$. If $F = F_-$, one sees from the series that $U(s, s_0) = L^\dagger(s, s_0)$, so U is in fact unitary. The rest follows directly from the series expansion.

b) Suppose $B(s, s_0)$ is a solution of (4.1). Define $C(s, s_0) = U^{-1}(s, s_0)B(s, s_0)$. Then C satisfies the differential equation

$$C'(s, s_0) = 0, \qquad C(s_0, s_0) = 1,$$

which has the unique solution $C(s, s_0) = 1$, and $B(s, s_0) = U(s, s_0)$. ∎

Part b) of Lemma 4.2 suggests that we may be able to improve the bounds of parts b) and d) of Proposition 4.1. The self-adjoint part of $F(s)$ is responsible for the growth of $\|U(s, s_0)\|$, as we now make precise.

Corollary 4.3. With the assumptions of Proposition 4.1,

$$\|U(s,s_0)\| \leq \exp\left(\int_{s_0}^{s} \|F_+(t)\| dt\right),$$

$$\|\tilde{U}\| \leq \exp\left(\|F_+(\cdot)\|_{L^1(\mathbf{R})}\right).$$

Proof : Define $V(s,s_0)$ to be the solution of

$$V'(s,s_0) = -F_-(s)V(s,s_0), \qquad V(s_0,s_0) = 1.$$

$V(s,s_0)$ is unitary by part a) of Lemma 4.2.

Then defining $W(s,s_0) = V^{-1}(s,s_0)U(s,s_0)$, we find

$$W'(s,s_0) = -[V^{-1}(s,s_0)\ F_+(s)\ V(s,s_0)]W(s,s_0), \qquad W(s_0,s_0) = 1. \tag{4.7}$$

Applying part c) of Proposition 4.1 to Equation (4.7),

$$\|W(s,s_0)\| \leq \exp\left(\int_{s_0}^{s} \|F_+(t)\| dt\right),$$

$$\|\tilde{W}\| \leq \exp\left(\|F_+(\cdot)\|_{L^1(\mathbf{R})}\right),$$

where we have used the unitarity of V to obtain $\|V^{-1}F_+V\| = \|F_+\|$. Using once again the unitarity of V, $\|U\| = \|W\|$. ∎

4.2. Functions on the Complex Strip

In this section, we examine the solutions of first-order differential equations with coefficients that can be analytically extended from the real line to a strip in the complex plane. We will derive estimates on the analytic continuations of the solutions, using the series-expansion methods of the previous section. We will further define the Hardy class H^p of functions on the strip. We recall the notation $\mathcal{S}(b,a)$ of Definition 3.18.

We now consider Equation (4.1) with analytically extendible coefficients.

Lemma 4.4. Suppose $F(s)$ in Equation (4.1) is analytically extendible to $\mathcal{S}(b,a)$. Then:

a) The solution $U(s,s_0)$ is analytically extendible to $\mathcal{S}(b,a)$ in both variables.

b) For $z, z_0, w \in \mathcal{S}(b,a)$,

$$U(z,z_0) = U(z,w)U(w,z_0).$$

c) For $z, z_0 \in \mathcal{S}$,

$$\|U(z,z_0) - 1\| \leq \exp\left(\int_0^1 \|F(z_0 + t(z-z_0))\|\, dt\right) - 1.$$

Proof : We solve $\partial_z U(z,z_0) = -F(z)U(z,z_0)$ for $z, z_0 \in \mathcal{S}(b,a)$. The methods of Proposition 4.1 carry over, where we integrate over any continuous path joining z_0 and z. a) and b) follow trivially. To prove c), subtract 1 from both sides of the Volterra integral equation, and take norms. ∎

We now define a class of functions on $\mathcal{S}(b,a)$ for which the naive analogue of the Cauchy integral theorem holds on an infinite rectangle. The books [HOF], [KOOS] are general references on classical (complex-valued) Hardy classes, and [RSRV] covers some of the operator-valued theory.

Definition 4.5. Let $\mathrm{H}^p(b,a)$, $1 \leq p \leq \infty$, be the space of functions $T : \mathcal{S}(b,a) \to \mathcal{L}(\mathcal{H})$ that satisfy the conditions a) and b) below, and let $\mathrm{H}^p(a) \equiv \mathrm{H}^p(-a,a)$.

a) The $\mathrm{H}^p(b,a)$ norm of T is finite, where the norm is defined by

$$\|T\|_{\mathrm{H}^p(b,a)} \equiv \sup_{-a<c<a} \|T(\cdot + ic)\|_{L^p(\mathbf{R})}.$$

b) $T(z)$ is strongly analytic on $\mathcal{S}(b,a)$; i.e., for $h \in \mathbf{C}$, $\lim_{h\to 0}(T(z+h) - T(z))/h$ exists in the operator norm topology.

Remark 1: Since we are dealing with continuous functions,

$$\|T\|_{\mathrm{H}^\infty(b,a)} = \sup_{b<\mathrm{Im}(z)<a} \|T(z)\|,$$

and functions belonging to $\mathrm{H}^\infty(b,a)$ are uniformly bounded on the strip.

Lemma 4.6. If $T(\cdot) \in \mathrm{H}^p(b,a)$ and $R(\cdot) \in \mathrm{H}^\infty(b,a)$, then the pointwise product $T(\cdot)R(\cdot) \in \mathrm{H}^p(b,a)$.

Proof : Immediate. ∎

Remark 2: Condition b) of Definition 4.1 can be replaced by the apparently weaker condition b') below: (a)∧(b) is equivalent to (a)∧(b').

b') For any $\phi \in \mathcal{H}$, $T(z)\phi$ is analytic on $\mathcal{S}(b,a)$; i.e., for $h \in \mathbf{C}$, the limit $\lim_{h\to 0}(T(z+h)\phi - T(z)\phi)/h$ exists in the Hilbert space topology.

4.3. Properties of the Hardy Classes

This section describes results related to those of Paley and Wiener in their work on Fourier transforms of analytic functions [PLWI]. The first lemma is the Cauchy formula for an infinite rectangular contour.

Lemma 4.7. Let $T \in \mathrm{H}^1(b,a)$, and take real constants β and α such that $b < \beta < \alpha < a$. Then for $z \in \mathcal{S}(\beta,\alpha)$,

$$T(z) = \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{T(t+i\beta)}{t+i\beta-z}dt - \frac{1}{2\pi i}\int_{-\infty}^{\infty} \frac{T(t+i\alpha)}{t+i\alpha-z}dt.$$

Proof : Without loss of generality, take $z = i\gamma$, with $\beta < \gamma < \alpha$.

a) For $x > 0$, let Γ_x be the rectangular contour with vertices $(x, i\beta)$, $(x, i\alpha)$, $(-x, i\alpha)$, and $(-x, i\beta)$. By the ordinary Cauchy theorem, for any $x > 0$,

$$T(i\gamma) = \frac{1}{2\pi i}\oint_{\Gamma_x} \frac{T(w)}{w-i\gamma}dw. \tag{4.8}$$

We shall show that the contribution to the contour integral of the vertical segments vanishes as $x \to \pm\infty$. Define

$$G(x) = \int_{i\beta}^{i\alpha} \frac{T(x+iy)}{x+iy-i\gamma} dy.$$

By the Fubini theorem,

$$\begin{aligned} \int_{\pm 1}^{\pm\infty} dx \, \|G(x)\| &\le \int_{\pm 1}^{\pm\infty} dx \int_{\beta}^{\alpha} \|T(x+iy)\| \\ &\le (a-b)\|T\|_{\mathrm{H}^1(b,a)}. \end{aligned} \tag{4.9}$$

Taking the derivative,

$$\begin{aligned} \frac{dG(x)}{dx} &= \frac{T(x+i\alpha)}{x+i\alpha-i\gamma} - \frac{T(x+i\beta)}{x+i\beta-i\gamma} \\ \int_{\pm 1}^{\pm\infty} dx \, \left\| \frac{dG(x)}{dx} \right\| &\le 2\|T\|_{\mathrm{H}^1(a)}. \end{aligned} \tag{4.10}$$

Combining these bounds immediately implies

$$\lim_{x \to \pm\infty} G(x) = 0.$$

∎

Remark: This lemma is actually true for H^p, $1 \le p < \infty$. The proof is modified by using the Hölder inequality in (4.9) and (4.10).

Proposition 4.8. With the same assumptions as Lemma 4.7,

a)

$$\lim_{x \to \pm\infty} \int_{\beta}^{\alpha} \|T(x+ir)\| \, dr = 0.$$

b)

$$\int_{-\infty}^{\infty} T(t+i\beta) \, dt = \int_{-\infty}^{\infty} T(t+i\alpha) \, dt.$$

Proof :

a) Choose $\epsilon > 0$ such that $b < \beta - \epsilon$ and $\alpha + \epsilon < a$. By Lemma 4.7,

$$2\pi \|T(z)\| \leq \int_{-\infty}^{\infty} \frac{\|T(t + i(\beta - \epsilon))\|}{|t + i(\beta - \epsilon) - z|} dt + \int_{-\infty}^{\infty} \frac{\|T(t + i(\alpha + \epsilon))\|}{|t + i(\alpha + \epsilon) - z|} dt. \qquad (4.11)$$

Integrating, we find for $x \neq 0$,

$$\begin{aligned} 2\pi & \int_{\beta}^{\alpha} \|T(x + ir)\| dr \\ & \leq \int_{-\infty}^{\infty} dt \int_{\beta}^{\alpha} dr \left(\frac{\|T(t + i(\beta - \epsilon))\|}{|t - x + i(\beta - \epsilon - r)|} + \frac{\|T(t + i(\alpha + \epsilon))\|}{|t - x + i(\alpha + \epsilon - r)|} \right) \\ & \leq \int_{-\infty}^{\infty} dt \int_{\beta}^{\alpha} dr F_x(t, r), \end{aligned}$$

where we define

$$\begin{aligned} F_x(t, r) &\equiv \frac{\|T(t + i(\beta - \epsilon))\| + \|T(t + i(\alpha + \epsilon))\|}{|t - x + i\epsilon|}, \\ G(t, r) &\equiv \frac{\|T(t + i(\beta - \epsilon))\| + \|T(t + i(\alpha + \epsilon))\|}{\epsilon}. \end{aligned}$$

For any fixed $(t, r) \in \mathbf{R} \times [\beta, \alpha]$, one checks that $\lim_{x \to \pm\infty} F_z(t, r) = 0$. Furthermore, $G(t, r) \in L^1(\mathbf{R} \times [\beta, \alpha])$, and for each $x \in \mathbf{R}$, $F_x(t, r) \in L^1(\mathbf{R} \times [\beta, \alpha])$. Now the dominated convergence theorem ([RS1], thm. I.16), together with the bound $|F_x(t, r)| \leq G(t, r)$, yields the result.

b) For the rectangular contour Γ_x of Lemma 4.7,

$$\oint_{\Gamma_x} T(z)\, dz = 0.$$

Now the Cauchy theorem and part a) imply the statement. ∎

Corollary 4.9. $\mathrm{H}^1(-\infty, \infty) = \{0\}$.

Proof : Follows directly from Lemma 4.7, (or Equation (4.11)), by taking $\beta \to -\infty$ and $\alpha \to \infty$. ∎

The preceding results are essential for obtaining the exponential bounds for even the simplest case of bounded unitarily admissible Hamiltonians. The following result is used for more general Hamiltonians.

Lemma 4.10. Let $T \in \mathrm{H}^1(b,a)$, and $b < \gamma < \delta < a$. Then

a) $T(\cdot) \in \mathrm{H}^\infty(\gamma,\delta)$.

b) $T'(\cdot) \in \mathrm{H}^1(\gamma,\delta)$.

c) Let $\{c_n\}$, $\gamma < c_n < \delta$, be a sequence that

converges to c, $\gamma < c < \delta$. Then

$$\|T(\cdot + c_n) - T(\cdot + c)\|_{L^1(\mathbf{R})} \to 0.$$

Proof : Choose β such that $b < \beta < \gamma$, and α such that $\delta < \alpha < a$.

a) Use Lemma 4.7,

$$\|T(z)\| \le \frac{1}{2\pi}\frac{\|T(\cdot)\|_{\mathrm{H}^1(b,a)}}{|i\beta - \mathrm{Im}(z)|} + \frac{1}{2\pi}\frac{\|T(\cdot)\|_{\mathrm{H}^1(b,a)}}{|i\alpha - \mathrm{Im}(z)|}$$

$$\sup_{\gamma \le \mathrm{Im}(z) \le \delta} \|T(z)\| \le \frac{\|T(\cdot)\|_{\mathrm{H}^1(b,a)}}{2\pi}\left(\max(\frac{1}{\gamma-\beta},\frac{1}{\alpha-\gamma}) + \max(\frac{1}{\alpha-\delta},\frac{1}{\delta-\beta})\right).$$

b) Using Lemma 4.7 and the Lebesgue dominated convergence theorem, we get for $z \in S(\beta,\alpha)$

$$T'(z) = \frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{T(t+i\beta)}{(t+i\beta-z)^2}dt - \frac{1}{2\pi i}\int_{-\infty}^{\infty}\frac{T(t+i\alpha)}{(t+i\alpha-z)^2}dt.$$

Now for any c such that $\gamma < c < \delta$, we obtain the c-independent finite bound

$$\|T'(\cdot + ic)\|_{L^1(\mathbf{R})} \le \frac{1}{2\pi}\int dx \int dt \left[\frac{\|T(t+i\beta)\|}{(t-x)^2 + (\beta-\gamma)^2} + \frac{\|T(t+i\alpha)\|}{(t-x)^2 + (\alpha-\delta)^2}\right].$$

c) For $x \in \mathbf{R}$,

$$\|T(x+ic_n) - T(x+ic)\| \leq \left| \int_c^{c_n} \|T'(x+iy)\| dy \right| ,$$

$$\int_{-\infty}^{\infty} dx \|T(x+ic_n) - T(x+ic)\| \leq |c_n - c| \cdot \|T'(\cdot)\|_{H^1(\gamma,\delta)}.$$

The statement now follows from part b). ∎

If $\mathcal{S}(b,a)$ contains the real axis, and an element $T(\cdot) \in \mathrm{H}^1(b,a)$ is self-adjoint on the real axis, then by the Schwarz reflection principle, T is automatically an element of $\mathrm{H}^1(c)$, where the symmetric strip is defined by $c = \max(|b|, a)$.

4.4. Hardy Classes and Admissible Hamiltonians

In this section, we consider admissible Hamiltonians for which $W'(s)$ has an analytic extension that belongs to $\mathrm{H}^1(a)$. We show that this is equivalent to $K_G(\cdot) \in \mathrm{H}^1(a)$ and $B(\cdot) \in \mathrm{H}^1(a)$.

Proposition 4.11. Let $W(z)$ be an analytic operator-valued function on $\mathcal{S}(a)$ such that $W^\dagger(s) = W^{-1}(s)$ for all $s \in \mathbf{R}$. Then the following are equivalent:

a) $W'(z) \in \mathrm{H}^1(a)$.

b) $K_G(z) = W^{-1}(z)W'(z) \in \mathrm{H}^1(a)$.

c) $-iB(z) = W'(z)W^{-1}(z) \in \mathrm{H}^1(a)$.

Proof : On the real axis, $W^{-1}(z) = W^\dagger(z^*)$. Since $W^\dagger(z^*)$ is analytically extendible to $\mathcal{S}(a)$, $W^{-1}(z)$ is also analytically extendible, and the equality holds for all $z \in \mathcal{S}(a)$.

b) $\Leftarrow$ a) $\Rightarrow$ c): We start by proving that if $W' \in \mathrm{H}^1(a)$, then $W \in \mathrm{H}^\infty(a)$. For $x \in \mathbf{R}$, we denote by $C_x(z)$ the piecewise linear path from x to z that consists of the vertical line $[x, x+i\mathrm{Im}(z)]$ and the horizontal line $[x+i\mathrm{Im}(z), z]$. Take $W(0) = 1$;

then for $x > \max(0, \mathrm{Re}(z))$,

$$W(z) = W(x) + \int_{C_x(z)} W'(w)\, dw.$$

Taking the limit $x \to \infty$, the integral on the vertical line vanishes by part a) of Proposition 4.2, and the integral on the horizontal line is bounded since $W' \in \mathrm{H}^1(a)$. For any $z \in \mathcal{S}(a)$, we get by the triangle inequality the uniform bounds

$$\begin{aligned} \|W(z)\| &\le 2 + \|W'(\cdot)\|_{\mathrm{H}^1(a)} < \infty, \\ \|W^{-1}(z)\| &\le 2 + \|W'(\cdot)\|_{\mathrm{H}^1(a)} < \infty, \end{aligned} \tag{4.12}$$

where the bound on W^{-1} follows from $W^{-1}(z) = W^{\dagger}(z^*)$. The proof of *b)* $\Leftarrow$ *a)* $\Rightarrow$ *c)* follows from (4.12) and Lemma 4.6.

c) $\Rightarrow$ **a)**: We first prove that if *c)* holds, then $W \in \mathrm{H}^{\infty}(a)$. It is a tautology that $W(z) = W_G(z, 0)$, and that

$$W_G'(z, z_0) = -iB(z)W_G(z, z_0), \qquad W_G(z_0, z_0) = 1.$$

Take $x > \mathrm{Re}(z)$, and by Lemma 4.4 b),

$$W_G(z,0) = W_G(z, x + i\mathrm{Im}(z))\; W_G(x + i\mathrm{Im}(z), x)\; W_G(x, 0)$$

$$\lim_{x \to \infty} \|W_G(z,0)\| \le \|W_G(z, x + i\mathrm{Im}(z))\|.$$

Here we have used Lemma 4.4 c) to bound the second term by 1, and Corollary 4.3, along with the self-adjointness of $B(s)$ on the real axis, to bound the third term by 1. Using Proposition 4.1 d) on the remaining term, find

$$\|W(z)\| = \|W_G(z,0)\| \le \exp\left(\|B(\cdot)\|_{\mathrm{H}^1(a)}\right).$$

The result now follows from $W'(z) = -iB(z)W(z)$ and Lemma 4.6 .

b) $\Rightarrow$ a): Define $U_G(z, z_0)$ to be the solution of

$$U_G'(z, z_0) = -K_G(z)U_G(z, z_0), \qquad U_G(z_0, z_0) = 1.$$

As before, we find $U_G(\cdot, 0) \in \mathrm{H}^{\infty}(a)$. On the real axis, the solution is $U_G(s, 0) = W^{-1}(s)$. By analytic continuation, $U_G(z, 0) = W^{-1}(z) = W^{\dagger}(z^*)$, so $W(\cdot) \in$

$H^\infty(a)$. The result follows from $W' = WK_G$ and Lemma 4.6.

Chapter 5: Unitarily Related Hamiltonians

We now study transition probabilities for a unitarily admissible time-dependent Hamiltonian $H(s) = W(s)HW^{-1}(s)$. We consider the case where $W(s)$ is analytically extendible to the strip $\mathcal{S}(a)$. The main result is that if $W'(z)$ belongs to the Hardy class $\mathrm{H}^1(a)$, then the total transition probability from a compatible spectral band P_i, $\tilde{p}_i(\tau) = O(\exp(-2\tau a g_i))$, where g_i is the gap between the band P_i and the complementary spectral band $1 - P_i$. We recall that a compatible spectral band for a unitarily admissible Hamiltonian is specified by an interval $[a_i, b_i] \subset \mathbf{R}$, with $P_i(s) = \chi_{[a_i,b_i]}(H(s))$. We further recall that $\tilde{p}_i(\tau)$ is defined as the maximum probability that a state in the range of $P_i(s_0)$ evolves into a state in the range of $(1 - P_i(s))$, in the limit $s_0 \to -\infty$, $s \to \infty$. The assumptions we make will be sufficient for this limit to exist.

We first consider *bounded* unitarily admissible bounded Hamiltonians, and analytically continue the differential equation for Ω. This has the advantage of giving the exponential bound in a relatively transparent way. It has the disadvantage that the method does not generalize to unbounded Hamiltonians. In the second section, we generalize to unitarily admissible Hamiltonians that may be unbounded. The method is a term-by-term analysis of the series solution for the integral equation for Ω. We then apply these results to a simple class of Hamiltonians where the geometric context of the method, the appearance of Berry's phase in particular, is readily understood.

The following lemma is the key to the relative simplicity of the unitarily admissible Hamiltonians. Let $\mathbf{C}_\pm = \{z \in \mathbf{C} | 0 \leq \pm\mathrm{Im}(z)\}$.

Lemma 5.1. Consider a unitarily admissible Hamiltonian $H(s)$. Then

a) For $s, r \in \mathbf{R}$,

$$V_\tau(s + r) = V_\tau(s)V_\tau(r).$$

b) If H is bounded, then $V_\tau(s)$ is analytically extendible to the complex plane, and

$$V_\tau(w+z) = V_\tau(w)V_\tau(z), \qquad w,z \in \mathbf{C}.$$

c) Let P be a spectral projection of H. If PH is bounded below, then $PV^{-1}\tau(s)$ is analytically extendible to $\mathbf{C}_+$, and $V_\tau(s)P$ is extendible to $\mathbf{C}_-$. Furthermore,

$$PV_\tau{}^{-1}(w+z) = PV_\tau{}^{-1}(w)V_\tau{}^{-1}(z), \qquad w,z \in \mathbf{C}_+,$$
$$V_\tau(w+z)P = V_\tau(w)V_\tau(z)P, \qquad w,z \in \mathbf{C}_-.$$

Similarly, if PH is bounded below, then $PV_\tau{}^{-1}$ is extendible to $\mathbf{C}_-$, and $V_\tau P$ to $\mathbf{C}_+$.

Proof : The proofs follow from the functional calculus of the self-adjoint operators H and PH. ∎

5.1. Transition Probabilities in the Bounded Case

For bounded unitarily admissible Hamiltonians, the differential equation for Ω can be continued to the complex strip, giving exponential decay in a simple way.

Lemma 5.2. Let $H(s)$ be a bounded unitarily admissible Hamiltonian. Then for $s, s_0 \in \mathbf{R}$, and $-a < c < a$,

$$\Omega(s+ic, s_0+ic) = V_\tau{}^{-1}(ic)\Omega_c(s,s_0)V_\tau(ic), \qquad s,s_0 \in \mathbf{R}. \tag{5.1}$$

Proof : We prove that both sides are solutions of the same differential equation with the same initial conditions. By Proposition 3.17 and analytic extension, the left-hand side of Equation (5.1) satisfies

$$[\Omega(s+ic, s_0+ic)]' = -K_\tau(s+ic)[\Omega(s+ic,s_0+ic)], \qquad \Omega(s_0+ic,s_0+ic) = 1.$$

Taking the derivative of the right-hand side of (5.1),

$$\begin{aligned}[V_\tau^{-1}(ic)\Omega_c(s,s_0)V_\tau(ic)]' = \\ &- V_\tau^{-1}(s+ic)K_G(s+ic)V_\tau(s+ic)[V_\tau^{-1}(ic)\Omega_c(s,s_0)V_\tau(ic)], \\ &V_\tau^{-1}(ic)\Omega_c(s_0,s_0)V_\tau(ic) = 1.\end{aligned}$$

Here we have used the fact that Ω_c is the solution of the differential equation (3.25), and also the algebraic identity $V_\tau(s)V_\tau(ic) = V_\tau(s+ic)$ from Lemma 5.1 b). So both sides solve the same differential equation with the same boundary conditions, and are thus equal. ∎

The boundedness of H entered in the preceding lemma, as we needed to have $V_\tau(ic)$ bounded. The following proposition is the central identity from which the exponential bounds will easily follow.

Proposition 5.3. Let $H(s)$ be a bounded unitarily admissible Hamiltonian with $W'(\cdot) \in \mathrm{H}^1(a)$. Let P_i and P_k be spectral bands. Then for $-a < c < a$,

$$P_k\tilde{\Omega}P_i = P_k\exp(-\tau cHP_k)\tilde{\Omega}_c\exp(\tau cHP_i)P_i. \tag{5.2}$$

Proof : For $s, s_0 \in \mathbf{R}$, we have by Lemma 4.4 b),

$$\begin{aligned}\Omega(s,s_0) &= \Omega(s,s+ic)\Omega(s+ic,s_0+ic)\Omega(s_0+ic,s_0), \\ &= \Omega(s,s+ic)V_\tau^{-1}(ic)\Omega_c(s,s_0)V_\tau(ic)\Omega(s_0+ic,s_0).\end{aligned}$$

The second identity above follows from Lemma 5.2. We now show that in the limit,

$$\begin{aligned}\lim_{s_0\to-\infty}\Omega(s_0+ic,s_0) &= 1 \\ \lim_{s\to\infty}\Omega(s,s+ic) &= 1.\end{aligned} \tag{5.3}$$

Suppose $\|H\| = \gamma$. Then for $z \in \mathcal{S}(a)$,

$$\|V_\tau(z)\| \leq \exp(\tau a\gamma) \geq \|V_\tau^{-1}(z)\|.$$

Now by Proposition 4.11, $K_G(\cdot) \in \mathrm{H}^1(a)$, and

$$\begin{aligned} \|K_\tau(z)\| &= \|V_\tau^{-1}(z) K_G(z) V_\tau(z)\| \\ &\leq \exp(2\tau a\gamma)\|K_G(z)\| \\ \|K_\tau(\cdot)\|_{\mathrm{H}^1} &\leq \exp(2\tau a\gamma)\|K_G(\cdot)\|_{\mathrm{H}^1}, \end{aligned}$$

so $K_\tau \in \mathrm{H}^1(a)$. By Lemma 4.2 b)

$$\lim_{x\to\pm\infty} \int_0^c \|K_\tau(x+ir)\| dr = 0\,,$$

and (5.3) follows from Equation (3.22) by applying part c) of Lemma 4.4.

We now have

$$\tilde{\Omega} = V_\tau^{-1}(ic)\tilde{\Omega}_c V_\tau(ic),$$

and the proposition follows by sandwiching with projections, and expressing V_τ as an exponential using Lemma 3.13. ∎

Remark: When we generalize to unbounded and admissible Hamiltonians, the additional work will be obtaining the analogue of Proposition 5.3.

We recall the Definition 2.2 of the gap $g_i(s)$ between the compatible spectral band $P_i(s)$ and the complementary band $1 - P_i(s)$, and note that for unitarily admissible Hamiltonians, it is a constant g_i.

Theorem 5.4. Let $H(s)$ be a bounded unitarily admissible time-dependent Hamiltonian, and $P_i(s)$ the projection onto a compatible spectral band. If $W'(\cdot) \in \mathrm{H}^1(a)$, then there is a finite constant C_a such that the total transition probability

$$\tilde{p}_i(\tau) \leq C_a \exp(-2\tau a g_i).$$

Proof : If the gap g_i is not positive definite, the result follows trivially from unitarity of the time evolution, so assume $g_i > 0$. $P_f(s) = 1 - P_i(s)$ is the projection onto the complementary band. Split the projection $P_f = P_1 + P_2$, where P_1 projects onto the spectrum above P_i, and P_2 onto the spectrum below P_i. From Equation (2.5), $g_{1i} > 0$

and $g_{i2} > 0$.

By Proposition 4.11, $K_G(\cdot) \in \mathrm{H}^1(a)$. Take for F_a the finite constant

$$\begin{aligned} F_a &= \exp\left(\|K_{G+}(\cdot)\|_{\mathrm{H}^1(a)}\right) \\ &\le \exp\left(\|K_G(\cdot)\|_{\mathrm{H}^1(a)}\right), \end{aligned} \tag{5.4}$$

recalling that $K_{G+}(z)$ is the self-adjoint part of $K_G(z)$. Applying Corollary 4.3 to Equation (3.25), and using the unitarity of $V_\tau(s)$ for $s \in \mathbf{R}$,

$$\begin{aligned} \|\tilde{\Omega}_c\| &\le \exp\left(\|\{K_{\tau c}(\cdot)\}_+\|_{L^1(\mathbf{R})}\right) \\ &\le \exp\left(\|K_{G+}(\cdot + ic)\|_{L^1(\mathbf{R})}\right). \\ &\le \sup_{-a<c<a} \exp\left(\|K_{G+}(\cdot + ic)\|_{L^1(\mathbf{R})}\right). \\ &\le F_a. \end{aligned} \tag{5.5}$$

Now using Proposition 5.3, for $-a < c < a$,

$$\|P_k \tilde{\Omega} P_i\| \le F_a \; \|\exp(-\tau c H|_k)\| \; \|\exp(\tau c H|_i)\|. \tag{5.6}$$

Then for $P_k = P_1$, and $0 < c < a$,

$$\begin{aligned} \|P_1 \tilde{\Omega} P_i\| &\le F_a \exp(-\tau c \inf \sigma(H|_1)) \; \exp(\tau c \sup \sigma(H|_i)) \\ &\le F_a \exp(-\tau c g_{1i}), \end{aligned} \tag{5.7}$$

and taking a sequence $c_n < a$ that converges to a,

$$\|P_1 \tilde{\Omega} P_i\| \le F_a \exp(-\tau a g_{1i}). \tag{5.8}$$

Similarly, for $P_k = P_2$ and $-a < c < 0$,

$$\begin{aligned} \|P_2 \tilde{\Omega} P_i\| &\le F_a \exp(-\tau c \sup \sigma(H|_2)) \; \exp(\tau c \inf \sigma(H|_i)) \\ &\le F_a \exp(\tau c g_{i2}), \end{aligned} \tag{5.9}$$

and a sequence converging to $-a$ gives

$$\|P_2 \tilde{\Omega} P_i\| \le F_a \exp(-\tau a g_{i2}). \tag{5.10}$$

Recall that the transition probability is given by

$$
\begin{aligned}
\tilde{p}_i(\tau) &= \|(1-P_i)\tilde{\Omega}P_i\|^2 \\
&= \|P_i\tilde{\Omega}^\dagger(P_1+P_2)\tilde{\Omega}P_i\| \\
&\leq \|P_1\tilde{\Omega}P_i\|^2 + \|P_2\tilde{\Omega}P_i\|^2 \\
&\leq 2F_a^2\exp(-2\tau a g_i),
\end{aligned}
\tag{5.11}
$$

where we have first used (5.8) and (5.10), and then (2.5). ∎

Remark: We could have proved the theorem without decomposing K_G into K_{G+} and K_{G-}, but with a larger F_a. This can be done by using Proposition (4.1) d) instead of the refinement Corollary 4.3. The refinement is, however, particularly advantageous for small a, since $\|K_{G+}(\cdot + ic)\|_{L^1(\mathbf{R})}$ goes to 1 as $c \to 0$. Thus for small τ one might sometimes obtain a better bound by applying the theorem with some $a' < a$.

5.2. Transition Probabilities in the Unbounded Case

In this section, we generalize the proof of exponentially bounded transitions to unbounded unitarily admissible Hamiltonians. The technique is bounding the iterative solution of the differential equation for Ω termwise.

We assume as before that the analytic extension of $W'(\cdot) \in \mathrm{H}^1(a)$. That implies $K_G(\cdot) \in \mathrm{H}^1(a)$ by Proposition 4.11, and restricted to the real axis, $K_G(\cdot) \in L^1(\mathbf{R})$. By the unitarity of $V_\tau(\cdot)$ on the real axis, $K_\tau(\cdot) \in L^1(\mathbf{R})$. We can now apply Proposition 4.1 b), c) to the differential equation (3.22) that is solved by Ω, obtaining

$$
\begin{aligned}
\tilde{\Omega} &= \sum_{j=0}^{\infty} \tilde{\Omega}_j, \\
\tilde{\Omega}_j &= (-)^j \int_{-\infty}^{\infty} ds_j \int_{-\infty}^{s_j} ds_{j-1} \cdots \int_{-\infty}^{s_2} ds_1\; K_\tau(s_j)K_\tau(s_{j-1})\ldots K_\tau(s_1).
\end{aligned}
\tag{5.12}
$$

The integrand belongs to $L^1(\mathbf{R}^j)$, and changing coordinates is allowed by Fubini. With the coordinate transformation

$$\begin{aligned} x &= s_j, \quad w_k = s_k - s_{k+1}; \quad k = 1, \ldots, j-1, \\ s_j &= x, \quad s_k = x + \sum_{l=k}^{j-1} \omega_k; \quad k = 1, \ldots, j-1, \end{aligned} \tag{5.13}$$

and sandwiching with projections, Equation (5.12) gives

$$\begin{aligned} P_k \tilde{\Omega}_j P_i =& (-)^j \times P_k \Big[\int_{-\infty}^{0} dw_{j-1} \cdots \int_{-\infty}^{0} dw_1 \\ & \int_{-\infty}^{\infty} dx \; K_\tau(x) K_\tau(x + w_{j-1}) \ldots K_\tau(x + \textstyle\sum_{l=1}^{j-1} w_l) \Big] P_i. \end{aligned} \tag{5.14}$$

Recall the Definition 3.19 of $K_{\tau c}$.

Lemma 5.5. Let $H(s)$ be a unitarily admissible Hamiltonian with $W'(\cdot) \in \mathrm{H}^1(a)$. Let P_i and P_k be finite spectral bands; i.e., HP_i and HP_j are bounded operators. Fix any $(w_{j-1}, \ldots, w_1) \in \mathbf{R}^j$. Then for $-a < c < a$,

$$\begin{aligned} & P_k \Big[\int_{-\infty}^{\infty} dx \; K_\tau(x) K_\tau(x + w_{j-1}) \ldots K_\tau(x + \textstyle\sum_{l=1}^{j-1} w_l) \Big] P_i \\ & = P_k V_\tau^{-1}(ic) \Big[\int_{-\infty}^{\infty} dx \; K_{\tau c}(x) K_{\tau c}(x + w_{j-1}) \ldots K_{\tau c}(x + \textstyle\sum_{l=1}^{j-1} w_l) \Big] V_\tau(ic) P_i. \end{aligned}$$

Proof : Define the function

$$\begin{aligned} Z(\cdot) \equiv & P_k K_\tau(\cdot) K_\tau(\cdot + w_{j-1}) \ldots K_\tau(\cdot + \textstyle\sum_{l=1}^{j-1} w_l) P_i \\ = & P_k V_\tau^{-1}(\cdot) K_G(\cdot) V_\tau^{-1}(w_{j-1}) K_G(\cdot + w_{j-1}) \ldots \\ & K_G(\cdot + \textstyle\sum_{l=1}^{j-1} w_l) V_\tau(\textstyle\sum_{l=1}^{j-1} w_l) V_\tau(\cdot) P_i. \end{aligned} \tag{5.15}$$

Here we have used $K_\tau(s) = V_\tau^{-1}(s) K_G(s) V_\tau(s)$ and Lemma 5.1 a). By Proposition 4.11, $K_G(\cdot) \in \mathrm{H}^1(a)$. Since $Z(\cdot)$ is a product of functions that are analytically extendible to $\mathcal{S}(a)$, $Z(\cdot)$ is itself extendible. Now choose b such that $|c| < b < a$. Then by Lemma 4.10 a), $K_G(\cdot + w) \in \mathrm{H}^\infty(b)$ for any $w \in \mathbf{R}$. We conclude by Lemma 4.6 that

$Z(\cdot) \in \mathrm{H}^1(b)$. We can now apply Proposition 4.2 b) to $Z(\cdot)$,

$$\int_{-\infty}^{\infty} dx\ P_k K_\tau(x) K_\tau(x + w_{j-1}) \ldots K_\tau(x + \textstyle\sum_{l=1}^{j-1} w_l) P_i =$$

$$= \int_{-\infty}^{\infty} dx\ P_k V_\tau^{-1}(x+ic) K_G(x+ic) V_\tau^{-1}(w_{j-1}) K_G(x+ic+w_{j-1}) \ldots$$
$$V_\tau^{-1}(w_1) K_G(x+ic+\textstyle\sum_{l=1}^{j-1} w_l) V_\tau(\textstyle\sum_{l=1}^{j-1} w_l) V_\tau(x+ic) P_i,$$

and the result follows from the grouping of terms using Lemma 5.1. ∎

We now have the generalization of Proposition 5.3 to unbounded unitarily admissible Hamiltonians. The unbounded Hamiltonians cause slight complications.

Proposition 5.6. Let $H(s)$ be a unitarily admissible Hamiltonian with $W'(\cdot) \in \mathrm{H}^1(a)$. Let P_i and P_k be spectral bands.

a) If HP_i and HP_k are bounded, then

$$P_k \tilde{\Omega} P_i = P_k \exp(-\tau c H P_k) \tilde{\Omega}_c \exp(\tau c H P_i) P_i. \tag{5.16}$$

b) If HP_i is bounded above, HP_k is bounded below, and $0 < c < a$, then equation (5.16) holds.

c) If HP_i is bounded below, HP_k is bounded above, and $-a < c < 0$, then equation (5.16) holds.

Proof :

a) Use Lemma 5.5 in Equation (5.14), and then change coordinates back to the original set $(s_j, \ldots, s_1)$. Comparing the resulting expression with (5.12), immediately recognize

$$P_k \tilde{\Omega}_j P_i = P_k V_\tau^{-1}(ic) \tilde{\Omega}_{c,j} V_\tau(ic) P_i.$$

Now sum over j; the series converges by Proposition (4.1).

b),c): Decompose P_i and P_k as countable sums of orthogonal projections,

$$P_i = \sum_m P_{i,m}, \quad P_k = \sum_m P_{k,m},$$
$$P_{i,m}P_{i,m'} = \delta_{m,m'}P_{i,m}, \quad P_{k,m}P_{k,m'} = \delta_{m,m'}P_{k,m}.$$

Require further that $HP_{i,m}$ and $HP_{k,m}$ be bounded for all m. Then from part a),

$$P_{k,m}\tilde{\Omega}P_{i,m'} = P_{k,m}\exp(-\tau cHP_{k,m})\tilde{\Omega}_c\exp(\tau cHP_{i,m'})P_{i,m'}.$$

Summing over m and m' and using the functional calculus of H gives the result. ∎

The bound on the transition probabilities is the same as in Theorem 5.4:

Theorem 5.7. Let $H(s)$ be a unitarily admissible (possibly unbounded) time-dependent Hamiltonian, and $P_i(s)$ the projection onto a compatible spectral band (possibly not finite). If $W'(\cdot) \in \mathrm{H}^1(a)$, then there is a finite constant C_a such that the total transition probability

$$\tilde{p}_i(\tau) \leq C_a \exp(-2\tau a g_i).$$

Proof : Almost identical to the proof of Theorem 5.4, with Proposition 5.6 substituted for Proposition 5.3. We comment only on the parts that differ. As before, split $1 - P_i$ as $P_1 + P_2$. First note that either HP_1 is bounded below and HP_i is bounded above, or $P_1 = 0$. If the former holds, then by Proposition 5.6 b), the bound (5.7) is valid. If $P_1 = 0$, the bound (5.7) holds trivially. Similarly, either HP_2 is bounded above and HP_i is bounded below, or $P_2 = 0$. By proposition 5.6 c), the bound (5.9) is valid in the former case, and trivially valid in the latter. The remainder of the proof carries over without modification. ∎

5.3. Vector Operators and Berry's Phase

In this section, we consider a simple example of a unitarily admissible Hamiltonian.

The prototype for this type of Hamiltonian is $\mathbf{B}(s) \cdot J$, where $\mathbf{B}(s) \in \mathbf{R}^3$ is a time-dependent magnetic field, and J is the triplet of angular-momentum operators. This is perhaps the primary paradigm in the development of Berry's phase, and has been extensively analyzed in the adiabatic limit [B], [SIM1]. The geometric description of this system in the adiabatic limit is well known. We shall first obtain sufficient conditions for the applicability of Theorem 5.7 (or Theorem 5.4). We then give a geometric description of the operator $K_G(s)$, which turns out to be intimately related to Berry's phase. Recent work of Berry [BH], [BG] also addresses some related issues.

Choose a unitary representation of $SU(2)$ on the Hilbert space. The representation may be reducible. Let $\{J_1, J_2, J_3\}$ be the self-adjoint generators of the representation. We must assume that the J_i are bounded operators, which unfortunately excludes the interesting case of $\mathcal{H} = L^2(\mathbf{R}^3)$ with the natural action induced by the rotation group $SO(3)$. For $a \in \mathbf{R}^3$, use the notation $a \cdot J = a_1 J_1 + a_2 J_2 + a_3 J_3$. The commutation relations of the generators are, for $a, b \in \mathbf{R}^3$,

$$[a \cdot J, b \cdot J] = i(a \times b) \cdot J. \tag{5.17}$$

Definition 5.8. A triplet $V = \{V_1, V_2, V_3\}$ of self-adjoint operators is a *vector operator* if for $a, b \in \mathbf{R}^3$,

$$[a \cdot V, b \cdot J] = i(a \times b) \cdot V.$$

For example, the angular momentum operator J itself is a vector operator.

We now define our time-dependent Hamiltonians $H(s)$ [SEG]. Consider a smooth path $k(s)$ from $\mathbf{R}$ to the unit vectors in $\mathbf{R}^3$; i.e., $k(s) \cdot k(s) = 1$. The Hamiltonians we consider are of the form

$$H(s) = k(s) \cdot V + H_I, \tag{5.18}$$

with $[a \cdot J, H_I] = 0$, and V a vector operator. We will neglect domain questions in this section; the reader may alternately assume $H(s)$ is bounded. Let $W_R(s)$ be the solution of the equation

$$iW_R'(s) = [(k(s) \times k'(s)) \cdot J]\, W_R(s), \qquad W_R(0) = 1. \tag{5.19}$$

Lemma 5.9. For a time-dependent Hamiltonian of the form (5.18), W_R intertwines the Hamiltonian in the sense

$$H(s)W_R(s) = W_R(s)H(0). \tag{5.20}$$

Proof : Using $k' \cdot k = 0$, obtain

$$[(k \times k') \cdot J, k \cdot V] = ik' \cdot V \tag{5.21}$$

by applying (5.18). Now the right-hand side of Equation (5.20) satisfies

$$[W_R(s)H(0)]' = -i(k(s) \times k'(s) \cdot J)\ [W(s)H(0)].$$

Taking the derivative of the left-hand side of (5.20),

$$\begin{aligned}[H(s)W_R(s)]' &= (k' \cdot V)\ W_R - i(k \cdot V + H_I)(k \times k' \cdot J)W_R \\ &= -i(k \times k' \cdot J)(k \cdot V + H_I)W_R \\ &= -i(k(s) \times k'(s) \cdot J)\ [H(s)W_R(s)],\end{aligned}$$

where we have used (5.21), and the commutativity of H_I with J. Both sides of equation (5.20) thus satisfy the same differential equation, with the same boundary conditions, and the equality comes from the existence of a unique solution. ∎

Corollary 5.10. The time-dependent Hamiltonian (5.18) is unitarily admissible, with $W(s) = W_R(s)$. Furthermore, $B(s) = k(s) \times k'(s) \cdot J$.

Remark: The previous lemma resembles Lemma 3.12. In fact, when $H(s)$ of the form (5.18) has discrete spectrum of multiplicity one, $W_R(s)$ coincides with the intertwining operator of Lemma 3.12. Using

$$P_n'(s) = -i[k(s) \times k'(s) \cdot J, P_n(s)],$$

it follows that

$$\frac{i}{2}\sum_n [P_n'(s), P_n(s)] = (k(s) \times k'(s)) \cdot J.$$

Alternately, the equivalence of the intertwining operators follows from the uniqueness of $SU(2)$-invariant connections on line bundles over S^2. For $H(s)$ of the form (5.18), with discrete but not nondegenerate spectrum, the two intertwining operators are in general different. The actual evolution of the system in the adiabatic limit approximates the Kato form of the evolution. See [SEG] for details.

We say the vector-valued function $k'(s)$ belongs to $\mathrm{H}^p(a)$ if each component, with respect to a basis, has an analytic extension to $\mathcal{S}(a)$ that belongs to $\mathrm{H}^p(a)$.

Proposition 5.11. Let $H(s)$ be a Hamiltonian of the form (5.18). Let P_i be a spectral band with gap g_i. If $k'(\cdot) \in \mathrm{H}^1(a)$, then

$$\tilde{p}_i(\tau) = O(\exp(-2\tau a g_i)).$$

Proof : As in the proof of Proposition 4.11, one first checks that if $k' \in \mathrm{H}^1(a)$, then $k \in \mathrm{H}^\infty(a)$. By Lemma 4.6, $B(\cdot) = k' \times k \cdot J \in \mathrm{H}^1(a)$, and by Proposition 4.11, $W' \in \mathrm{H}^1(a)$. We can now apply Theorem 5.4 (or Theorem 5.7 if $H(s)$ is unbounded). ∎

By reparametrization of the time coordinate, we can consider a slight generalization. Letting $H_I = 0$, we have $H(s) = k(s) \cdot V$. Now let $r : \mathbf{R} \to \mathbf{R}$ be a C^1 diffeomorphism. By a simple application of the chain rule to the time-dependent Schrödinger equation, one checks that $U_\tau(s, s_0) = U_\tau^r(r^{-1}(s), r^{-1}(s_0))$, where U_τ^r is the solution of the Schrödinger equation for

$$H_r(s) \equiv \frac{H(r^{-1}(s))}{\partial_x r|_{x=r^{-1}(s)}} = \frac{1}{r'(r^{-1}(s))} k(r^{-1}(s)) \cdot V. \tag{5.22}$$

Thus a Hamiltonian of the form $H(s) = c(s)k(s) \cdot V$, with $c(s) \in \mathbf{R}_+$, is equivalent, by a reparametrization of the time coordinate, to a Hamiltonian of the form $k(s) \cdot V$, with $k(s) \in S^2 \subset \mathbf{R}^3$. The applicability of the time reparametrization is of course not limited to Hamiltonians of type (5.18).

We now turn to the geometric interpretation of $K_G(s)$. The geodesic curvature of the path $k(s)$ on the unit sphere S^2 is given by

$$\kappa_g(s) \equiv \frac{k''(s) \cdot (k'(s) \times k(s))}{|k'(s)|^3}.$$

Integrating the geodesic curvature with respect to the Riemannian length element $dl(s) = |k'(s)|ds$, define

$$\gamma(s) \equiv \int_0^s \kappa_g(x) dl(x) = \int_0^s C_g(x)\, dx,$$

where $C_g(s) \equiv |k'(s)|\kappa_g(s)$.

If we have a smooth, closed curve on S^2, i.e., for some s_c, $k(s_c) = k(0)$, and $k'(s_c) = k'(0)$, then the Gauss-Bonnet Theorem [SP], [KL] states that $\gamma(s_c)$ is equal to the spherical area of the region bounded by the curve. It is well known that the Berry's phase of a nondegenerate eigenstate around this path is proportional to the area [B], [SIM1], the constant of proportionality being the eigenvalue of $k \cdot J$. One may think of $C_g(s)$ as the local Berry's phase for this particular system.

The following proposition shows how these ideas enter into the expression for $K_G(s)$. Recall that $K_G(s)$ is the fundamental quantity for the computation of the transition probabilities, and it is only for $K_G(\cdot) \in \mathrm{H}^1(a)$ that Proposition 4.11 lets us phrase the results in terms of $W'(\cdot)$. We can without loss of generality take $k(0) \cdot J = J_3$, and $k'(0) \cdot J = |k'(0)| J_2$.

Proposition 5.12.

$$\begin{aligned} K_G(s, 0) &= i|k'(s)| \exp(-i\gamma(s)J_3)\ J_1\ \exp(i\gamma(s)J_3) \\ &= i|k'(s)|(\cos(\gamma(s))J_1 + \sin(\gamma(s))J_2) \end{aligned}$$

Proof : Define an orthonormal moving frame[4] of the curve $k(s) \subset \mathbf{R}^3$

$$e_1(s) = k(s), \qquad e_2(s) = \frac{k'(s)}{|k'(s)|}, \qquad e_3(s) = \frac{k(s) \times k'(s)}{|k'(s)|}.$$

[4] This particular frame is not a Frenet frame.

Since for any s this is an orthonormal basis, we have the obvious property that for any vector $a \in \mathbf{R}^3$, $a = (a \cdot e_1)\, e_1 + (a \cdot e_2)\, e_2 + (a \cdot e_3)\, e_3$. Define

$$L(s) = -iW^{-1}(s)(e_3(s) \cdot J)W(s).$$

From (5.19) it follows that $K_G(s,0) \equiv W^{-1}(s)W'(s) = |k'(s)|L(s)$.

Taking the derivative of $L(s)$, the term with W' cancels the term with $(W^{-1})'$, and we are left with

$$L'(s) = -iW^{-1}(s)(e_3'(s) \cdot J)W(s).$$

Now $e_3' \cdot e_3 = 0$ from the orthonormality, and

$$e_3'(s) \cdot e_1(s) = -e_3(s) \cdot e_1'(s) = -\frac{(k(s) \times k'(s)) \cdot k'(s)}{|k'(s)|} = 0,$$

and the orthonormal basis property yields

$$e_3'(s) = (e_3'(s) \cdot e_2(s))\; e_2(s) = -C_g(s)e_2(s).$$

Using this and $e_2 = -e_1 \times e_3$ and the commutation relations,

$$\begin{aligned} L'(s) &= -C_g(s)W^{-1}(s)[e_1(s) \cdot J, e_3(s) \cdot J]W(s) \\ &= [-iC_g(s)e_1(0) \cdot J, L(s)], \end{aligned}$$

where we have used the intertwining property. This differential equation for $L(s)$ can be integrated,

$$L(s) = \exp(-i\gamma(s)k(0) \cdot J)L(0)\exp(i\gamma(s)k(0) \cdot J). \qquad \blacksquare$$

Chapter 6: Admissible Hamiltonians

We first obtain a bound for the transition between two compatible bands of an admissible Hamiltonian. We then specialize to a finite-dimensional Hilbert space, where the connection with the Landau-Zener formula is most apparent. Finally, we discuss bounds on the total transition probability from a compatible band to the complement of the spectrum. Recall the abbreviated notation $H = H(0)$, $P_i = P_i(0)$, $g_{k,i} = g_{k,i}(0)$, etc.

6.1. Transitions Between Two Bands

In this section, we obtain an exponential bound on the transition probability $\tilde{p}_{k,i}(\tau)$ between two compatible spectral bands $P_i(s)$ and $P_k(s)$ of an admissible Hamiltonian

$$H(s) = W(s)[H + \sum_{n\in J} \Delta_n(s)Q_n]W^{-1}(s).$$

The exponential bound we obtain coincides in certain cases with the Landau expression, but is not in general identical. We will always assume, without loss of generality, that $\Delta_n(0) = 0$. Recall that by Lemma 3.6 b), we can without loss of generality assume that $P_i(s) = Q_{n_i}(s)$ for some $n_i \in J$. Since we are interested in transitions, we assume $P_k(s)P_i(s) = 0$, and thus we can take $P_k(s) = Q_{n_k}(s)$ for some $n_k \in J$. We abbreviate notation by using the same index; i.e., $P_i(s) = Q_i(s)$, $P_k(s) = Q_k(s)$, with i, k considered as elements of the index set J. Further assume $W'(\cdot) \in \mathrm{H}^1(a)$, as for unitarily admissible Hamiltonians, which implies $K_G(\cdot) \in \mathrm{H}^1(a)$. Finally, suppose all the functions $\Delta_n(s)$ are analytically extendible to $\mathcal{S}(a)$.

We now consider some gap properties of compatible spectral bands for admissible Hamiltonians. It is a consequence of the definitions of compatible bands that

$$g_{k,i}(z) = g_{k,i} + \Delta_k(z) - \Delta_i(z), \quad z \in \mathcal{S}(a), \tag{6.1}$$

where of course $g_{k,i} = g_{k,i}(0)$. We assume that $g_{k,i}(s) \neq 0$ for all $s \in \mathbf{R}$, making the choice of the origin $s = 0$ irrelevant.

Definition 6.1. For $k \in J$, define

$$\overline{g}_k(z) = i \sup_{n \in J} \operatorname{Im}(g_{n,k}(z)), \qquad z \in \mathcal{S}(a).$$

Then $\operatorname{Im}(\overline{g}_k(z)) \geq 0$, since $\operatorname{Im}(g_{k,k}(z)) = 0$.

Definition 6.2. Let $k, i \in J$. For $-a < c < a$, define

$$\underline{L}_{k,i}(c) \equiv \operatorname{Im}\left(\int_0^{ic} g_{k,i}(z)dz\right) - \int_{-\infty}^{0} \operatorname{Im}(\overline{g}_i(t+ic))dt - \int_0^{\infty} \operatorname{Im}(\overline{g}_k(t+ic))dt,$$

$$\overline{L}_{k,i}(c) \equiv \operatorname{Im}\left(\int_0^{ic} g_{k,i}(z)dz\right) + \int_{-\infty}^{0} \operatorname{Im}(\overline{g}_k(t+ic))dt + \int_0^{\infty} \operatorname{Im}(\overline{g}_i(t+ic))dt.$$

Remark: If the spectra of $H|_k$ and $H|_i$ are single points, then recalling (2.6), $g_{k,i} = -g_{i,k}$, and

$$\overline{L}_{i,k}(c) = -\underline{L}_{k,i}(c). \tag{6.2}$$

Defining

$$\overline{\Delta}(z) = i \sup_{n \in J} \operatorname{Im}(\Delta_n(z)), \quad z \in \mathcal{S}(a),$$

it is clear that

$$\operatorname{Im}(\overline{g}_k(z)) = \operatorname{Im}(\overline{\Delta}(z) - \Delta_k(z)). \tag{6.3}$$

Keeping in mind the Equation (2.6) for (6.2) levels, the following lemma indicates the connection with the Landau formula.

Lemma 6.3. For $r \in \mathbf{R}$,

a)

$$\operatorname{Im}\left(\int_0^{r+ic} g_{k,i}(z)dz\right) \geq \underline{L}_{k,i}(c).$$

b) The inequality of part a) is an equality if and only if for all $x \leq r$, $\overline{g}_i(x+ic) = 0$, and for all $x \geq r$, $\overline{g}_k(x+ic) = 0$.

c)

$$\operatorname{Im}\left(\int_0^{r+ic} g_{k,i}(z)dz\right) \leq \overline{L}_{k,i}(c).$$

d) The inequality of part c) is an equality if and only if for all $x \leq r$, $\overline{g}_k(x+ic) = 0$, and for all $x \geq r$, $\overline{g}_i(x+ic) = 0$.

Proof : First prove b) and d), using (6.3). Parts a) and c) then follow from the non-negativity of $\overline{g}_i$. ∎

For a fixed τ and $(w_{j-1}, \ldots, w_1) \in \mathbf{R}_-^j$, adopting the shorthand $w = \sum_{l=1}^{j-1} w_l$, define the function $Z_{k,i} : \mathcal{S}(a) \to \mathcal{L}(\mathcal{H})$ by

$$Z_{k,i}(q) \equiv Q_k K_\tau(q) K_\tau(q + w_{j-1}) \ldots K_\tau(q+w) Q_i. \tag{6.4}$$

Lemma 6.4. Let Q_i and Q_k be finite; i.e., HQ_i and HQ_k are bounded operators. Let $x \in \mathbf{R}$.

a) If $0 \leq c < a$, then assuming $\underline{L}_{k,i}(c)$ is finite,

$$\|Z_{k,i}(x+ic)\| \leq$$
$$\leq \exp(-\tau \underline{L}_{k,i}(c)) \|K_G(x+ic)\| \|K_G(x+ic+w_{j-1})\| \cdots \|K_G(x+ic+w)\|.$$

b) If $-a < c \leq 0$, then assuming $\overline{L}_{i,k}(c)$ is finite,

$$\|Z_{k,i}(x+ic)\| \leq$$
$$\leq \exp(\tau \overline{L}_{i,k}(c)) \|K_G(x+ic)\| \|K_G(x+ic+w_{j-1})\| \cdots \|K_G(x+ic+w)\|.$$

Proof : Using $K_\tau(s) = V_\tau^{-1}(s) K_G(s) V_\tau(s)$,

$$\begin{aligned} Z_{k,i}(q) = Q_k V_\tau^{-1}(q) K_G(q) V_\tau(q) V_\tau^{-1}(q+w_{j-1}) K_G(q+w_{j-1}) V_\tau(q+w_{j-1}) \\ V_\tau^{-1}(q+w_{j-1}+w_{j-2}) \ldots K_G(q+w) V_\tau(q+w) Q_i. \end{aligned} \tag{6.5}$$

Note however that Lemma 5.1 a) no longer holds. Consider the outer terms, and keep in mind that $w \leq 0$:

$$Q_k V_\tau^{-1}(x+ic) = Q_k \exp\left(i\tau(x+ic)HQ_k\right) \exp\left(i\tau \int_0^{x+ic} \Delta_k(z)dz\right),$$

$$V_\tau(x+ic+w)Q_i = \exp\left(-i\tau \int_0^{x+ic+w} \Delta_i(z)dz\right) \exp\left(-i\tau(x+ic+w)HQ_i\right) Q_i.$$

Now for any bounded operator $X \in \mathcal{L}(\mathcal{H})$ we obtain, by rearranging the scalar factors,

$$\begin{aligned} Q_k V_\tau^{-1}(x+ic)XV_\tau(x+ic+w)Q_i &= \exp\left(i\tau \int_0^{ic} (\Delta_k(z) - \Delta_i(z))dz\right) \times \\ \times \exp\left(i\tau\int_0^x \Delta_k(t+ic)dt\right) &\exp\left(i\tau\int_{x+w}^0 \Delta_i(t+ic)dt\right) Q_k \exp(i\tau(x+ic)HQ_k) \times \\ &\times X \exp(-i\tau(x+ic+w)HQ_i)Q_i, \end{aligned} \tag{6.6}$$

and taking the norm,

$$\begin{aligned} \|Q_k V_\tau^{-1}(x+ic)XV_\tau(x+ic+w)Q_i\| &\leq \exp\left(-\tau \mathrm{Im} \int_0^{ic} (\Delta_k(z) - \Delta_i(z))dz\right) \times \\ \times \exp\left(-\tau\int_{x+w}^0 \mathrm{Im}(\Delta_i(t+ic))dt\right) &\exp\left(-\tau\int_0^x \mathrm{Im}(\Delta_k(t+ic))dt\right) \times \\ \times \|Q_k \exp(-\tau c H Q_k)\| &\|X\| \|\exp(\tau c H Q_i))Q_i\|. \end{aligned}$$

We now consider the terms $V_\tau(x+ic)V_\tau^{-1}(x+ic+r)$, with $r \leq 0$.

$$V_\tau(x+ic)V_\tau^{-1}(x+ic+r) = \exp(i\tau r H) \exp\left(-i\tau \sum_{n\in J} Q_n \int_{x+r}^{x} \Delta_n(t+ic)dt\right)$$

$$\|V_\tau(x+ic)V_\tau{}^{-1}(x+ic+r)\| = \sup_{n\in J} \exp\left(\tau \int_{x+r}^{x} \mathrm{Im}(\Delta_n(t+ic))dt\right)$$
$$\leq \exp\left(\tau \int_{x+r}^{x} \mathrm{Im}(\overline{\Delta}(t+ic))dt\right). \tag{6.7}$$

Using the composition property of the exponential,

$$\|V_\tau(x+ic)V_\tau{}^{-1}(x+ic+w_{j-1})\| \cdots \|V_\tau(x+ic+\textstyle\sum_{l=2}^{j-1} w_l)V_\tau{}^{-1}(x+ic+w)\|$$
$$\leq \exp\left(\tau \int_{x+w}^{x} \mathrm{Im}(\overline{\Delta}(t+ic))dt\right).$$

Combining these estimates, and using the fact that $\mathrm{Im}(\overline{\Delta} - \Delta_n) \geq 0$,

$$\|Z_{k,i}(x+ic)\| \leq \exp\left(-\tau \mathrm{Im}\int_0^{ic}(\Delta_k(z) - \Delta_i(z))dz\right)\exp\left(\tau \int_{-\infty}^{0}\mathrm{Im}(\overline{\Delta}(t+ic) - \Delta_i(t+ic))dt\right)$$

$$\times \exp\left(\tau \int_0^{\infty} \mathrm{Im}(\overline{\Delta}(t+ic) - \Delta_k(t+ic))dt\right) \|\exp(-\tau c H|_k)\| \|\exp(\tau c H|_i))\| \times$$

$$\times \|K_G(x+ic)\| \|K_G(x+ic+w_{j-1})\| \cdots \|K_G(x+ic+w)\|,$$

the result follows by using bounds of the form (5.6) through (5.9), and rearranging terms using (6.1) and (6.3). ∎

We now obtain a generalization of Lemma 5.5.

Lemma 6.5. Let $H(s)$ be an admissible Hamiltonian with $W'(\cdot) \in \mathrm{H}^1(a)$. Let Q_i and Q_k be finite spectral bands. Fix $(w_{j-1}, \ldots w_1) \in \mathbf{R}_-^j$.

a) If

$$\inf_{0<b<a} \underline{L}_{k,i}(b) > -\infty,$$

then for any c, $0 \le c < a$,

$$\|Q_k\Big[\int_{-\infty}^{\infty} dx\ K_\tau(x)K_\tau(x+w_{j-1})\dots K_\tau(x+w)\Big]Q_i\|$$

$$\le \exp(-\tau \underline{L}_{k,i}(c)) \int_{-\infty}^{\infty} dx \|K_G(x+ic)\| \cdots \|K_G(x+ic+w)\|.$$

b) If

$$\sup_{-a<b<0} \overline{L}_{i,k}(b) < \infty,$$

then for any c, $-a < c \le 0$,

$$\|Q_k\Big[\int_{-\infty}^{\infty} dx\ K_\tau(x)K_\tau(x+w_{j-1})\dots K_\tau(x+w)\Big]Q_i\|$$

$$\le \exp(\tau \overline{L}_{i,k}(c)) \int_{-\infty}^{\infty} dx \|K_G(x+ic)\| \cdots \|K_G(x+ic+w)\|.$$

Proof : The proof mirrors the proof of Lemma 5.5, with some complications. As before, $K_G(\cdot) \in \mathrm{H}^1(a)$. It is clear that $Z_{k,i}(q)$ is analytic on $\mathcal{S}(a)$.

a) Fix b such that $c < b < a$. Then $K_G(\cdot + w_i) \in \mathrm{H}^\infty(0,b)$ by Lemma 4.10 a). By assumption, the $\mathrm{H}^\infty(0,b)$ norm of the (nonanalytic) bounding function of Lemma 6.4,

$$h(x+ic) \equiv \exp(-\tau \underline{L}_{k,i}(c)),$$

is finite. Then by Lemma 4.6, $Z_{k,i}(\cdot) \in \mathrm{H}^1(0,b)$. For $0 < \epsilon < b$, use Proposition 4.2 b) to obtain

$$\int_{-\infty}^{\infty} Z_{k,i}(t+ic)dt = \int_{-\infty}^{\infty} Z_{k,i}(t+i\epsilon)dt. \tag{6.8}$$

Consider the limit $\epsilon \to 0$. By Lemma 4.10 c), $K_G(\cdot + i\epsilon)$ converges in $L^1(\mathbf{R})$ to $K_G(\cdot)$. The restriction of $Z_{k,i}(\cdot)$ to $\mathcal{S}(0,c)$ is a product of $K_G(\cdot)$ and terms that belong to $\mathrm{H}^\infty(0,c)$. Thus $Z_{k,i}(\cdot + i\epsilon)$ converges in $L^1(\mathbf{R})$ to $Z_{k,i}(\cdot)$, and Equation (6.8) holds for $\epsilon = 0$.

The result now follows from Lemma 6.4 a).

b) The proof of part b) is completely analogous. ∎

The next result is our version of the Landau formula.

Theorem 6.6. Let $H(s)$ be an admissible Hamiltonian, $P_i(s)$ and $P_k(s)$ compatible spectral bands (not necessarily finite) which we take to be of the form $Q_i(s)$ and $Q_k(s)$ with $i, k \in J$. Assume $W'(\cdot) \in \mathrm{H}^1(a)$.

a) If $g_{k,i} > -\infty$ (equivalently $g_{k,i}(s) > -\infty$ for all $s \in \mathbf{R}$), and

$$\inf_{0<b<a} \underline{L}_{k,i}(b) > -\infty, \tag{6.9}$$

then for any c, $0 < c < a$,

$$\tilde{p}_{k,i}(\tau) \leq C_a \exp(-2\tau \underline{L}_{k,i}(c)), \tag{6.10}$$

where C_a is a finite constant independent of c.

b) If $g_{i,k} > -\infty$ (equivalently $g_{i,k}(s) > -\infty$ for all $s \in \mathbf{R}$), and

$$\sup_{-a<b<0} \overline{L}_{i,k}(b) < \infty, \tag{6.11}$$

then for any c, $-a < c < 0$,

$$\tilde{p}_{k,i}(\tau) \leq C_a \exp(\tau \overline{L}_{i,k}(c)), \tag{6.12}$$

where C_a is a finite constant independent of c.

Proof :

a) We first obtain a bound on $\|Q_k \tilde{\Omega} Q_i\|$ assuming that HQ_i and HQ_k are bounded. This follows the proof of Proposition 5.6. Define the finite constants[5] $G_a \equiv \exp(\|K_G(\cdot)\|_{H^1(a)})$, and $C_a \equiv G_a^2$. Use (5.14) and Lemma 6.5 to bound $\|Q_k \tilde{\Omega}_j Q_i\|$. Then change coordinates back to the $(s_j, \ldots, s_1)$ of (5.13). We then obtain the

[5] $G_a \geq F_a$, with F_a defined in (5.4), as we are bypassing the analogue of Proposition 5.6.

bound

$$\|Q_k\tilde{\Omega}_j Q_i\| \leq \exp(-\tau \underline{L}_{k,i}(c)) \frac{(\|K_G(\cdot)\|_{H^1(a)})^j}{j!}.$$

The factor $1/j!$ comes from the fact that the region of integration is a simplex in $\mathbf{R}^j$ (as in Equation (5.12)). Then summing over j and squaring to obtain a bound on the transition probability via (3.23) completes the proof of part a) for the special case that HQ_i and HQ_k are bounded.

To extend the proof to the more general situation $g_{k,i} > -\infty$, we use a technique similar to that in the proof of Proposition 5.6 b) and c). Decompose Q_i and Q_k as sums of orthogonal projections,

$$Q_i = \sum_{m=0}^{\infty} Q_{i,m}, \qquad Q_k = \sum_{m=0}^{\infty} Q_{k,m},$$
$$Q_{i,m}Q_{i,m'} = \delta_{m,m'}Q_{i,m}, \qquad Q_{k,m}Q_{k,m'} = \delta_{m,m'}Q_{k,m}.$$

Require as before that $HQ_{i,m}$ and $HQ_{k,m}$ are bounded for all m. We can always perform this decomposition such that for any $y > 0$,

$$g_{k,m;i,m'} \equiv \inf \sigma(H|_{k,m}) - \sup \sigma(H|_{i,m'}) = g_{k,i} + y(m + m').$$

Then we have

$$\sum_{m,m'} \|Q_{k,m}\tilde{\Omega}Q_{i,m'}\| \leq G_a \exp(-\tau \underline{L}_{k,i}(c)) \sum_m \exp(-\tau c y m) \sum_{m'} \exp(-\tau c y m')$$
$$\leq \frac{G_a \exp(-\tau \underline{L}_{k,i}(c))}{(1 - \exp(-\tau c y))^2},$$

where we have summed the product of the two geometric series. Since y can be taken arbitrarily large, the proof of part a) in the general case follows.

b) Part b) is proved the same way. ∎

In certain special cases, this result is equivalent to the Landau formula. In general, we see from Lemma 6.3 that the exponential approach is slower than that given by the naive Landau formula, possibly even an *increasing* exponential which does not give a useful bound.

6.2. Finite Dimension and Landau-Zener Formula

We now return to admissible Hamiltonians on a finite-dimensional Hilbert space. First recall Proposition 3.13, which states that a finite-dimensional Hamiltonian $H(s)$, with noncrossing spectrum and certain mild regularity conditions, is admissible. Furthermore, there are explicit prescriptions for the intertwining operators. We shall now suppose that the Hamiltonian $H(s)$ is analytically extendible as an operator-valued function to a strip $\mathcal{S}(b)$ in the complex plane. We refer to [DY2], [DVPE], [HWPE] for a previous discussion of analyticity and the Landau-Zener formula for finite-dimensional Hilbert space.

We briefly review some general results concerning such matrix-valued analytic functions, following Kato (Chap. 2.1 in [KAT2]). Let N be the dimension of the Hilbert space. In any compact subset of $\mathcal{S}(b)$, there are a finite number of *exceptional points*, where eigenvalues cross. At all other points, the number of distinct eigenvalues is constant, which is of course bounded by N. If the number of distinct eigenvalues is less than N, then some eigenvalues are permanently degenerate. We can write the admissible Hamiltonian in such a way that the number of distinct eigenvalues away from an exceptional point is equal to $|J|$, the cardinality of the index set. On a simply connected region that does not contain any exceptional points, the eigenvalues $E_n(z)$ and spectral projections $P_n(z)$ are analytic functions.

At an exceptional point, there are two possibilities. The first possibility is that all the eigenfunctions are analytic. In this case, the projections may either be analytic or have poles of integer order. A special case is an exceptional point that occurs on the real axis, since all the $H(s)$ are self-adjoint on the real axis. At an exceptional point on the real axis, the projections are analytic (Thm. 1.10, Chap. 2.1 [KAT2]). We can use this fact to relax the restriction on noncrossing eigenvalues in Proposition 3.13.

The second possibility is that some of the eigenvalues are sheets of an analytic function that has a branch point at the exceptional point. The eigenvalues are still continuous at such a branch point, but clearly are not analytic. Using a theorem of

Butler ([BUTL], Thm. 1.9, Chap. 2.1 [KAT2]), one can show that unless all of the eigenvalues are single-valued analytic functions at the exceptional point, not all the spectral projections can be analytic at the exceptional point. However, even if all the eigenvalues are single-valued, spectral projections can still have poles.

At an exceptional point, we then generally expect $B(s)$ as given by Equation (3.18) to be nonanalytic. Let $a < b$ be the distance from the real axis to the nearest such exceptional point. Then for all n, $P_n(s)$ and $P_n'(s)$ are extendible to analytic functions on the strip $\mathcal{S}(a)$. We suppose further that $P_n'(\cdot) \in \mathrm{H}^1(a-\epsilon)$, for some small positive ϵ. Duplicating the argument in the proof of Lemma 4.10, we conclude that $P_n(\cdot) \in \mathrm{H}^\infty(a-\epsilon)$. Now by Lemma 4.6, it easily follows that $B(s) = L(s) \in \mathrm{H}^1(a-\epsilon)$. By Lemma 4.10, both $W'(\cdot) \in \mathrm{H}^1(a-\epsilon)$, and we can apply Theorem (6.6).

We first adapt some of the notation to this simple case. Defining

$$\overline{E}(z) \equiv i \sup_{n \in J} \mathrm{Im}(E_n(z)),$$

Definition 6.2 becomes

$$\begin{aligned}\underline{L}_{k,i}(c) \equiv \mathrm{Im}\left(\int_0^{ic} (E_k(z) - E_i(z))dz\right) &- \int_{-\infty}^{0} \mathrm{Im}(\overline{E}(t+ic) - E_i(t+ic))dt \\ &- \int_0^{\infty} \mathrm{Im}(\overline{E}(t+ic) - E_k(t+ic))dt, \\ \overline{L}_{i,k}(c) = -\underline{L}_{k,i}(c).\end{aligned}$$

Let the exceptional point be at $r + ia$, $r \in \mathbf{R}$. Now recall Lemma 6.3. If for all $x \le r$, $\mathrm{Im}(\overline{E}(x+ic)) = \mathrm{Im}(E_i(x+ic))$, and for all $x \ge r$, $\mathrm{Im}(\overline{E}(x+ic)) = E_k(x+ic)$, we obtain

$$\underline{L}_{k,i}(c) = \mathrm{Im}\left(\int_0^{r+ic} (E_k(z) - E_i(z))dz\right).$$

An analogous result holds for $\overline{L}_{i,k}(c)$. Now for $c = a - \epsilon$, assuming the conditions of Theorem 6.6 are satisfied, we obtain an expression similar to that of Landau. The exponential rate can be made arbitrarily close to the Landau rate, but the multiplicative constant need not be uniform in ϵ.

We summarize the above discussion, assuming for concreteness that $E_k(0) > E_i(0)$.

Theorem 6.7. Let $H(s)$ be a finite-dimensional Hamiltonian that is analytically extendible to $\mathcal{S}(b)$. Let $r + ia$ be the point of eigenvalue crossing that is closest to the real axis. Assume that all $P_n'(\cdot) \in \mathrm{H}^1(a - \epsilon)$, and

$$\inf_{0<b<a-\epsilon} \underline{L}_{k,i}(b) > -\infty.$$

If there is a sequence $r_n + ic_n$ in $\mathcal{S}(a)$ converging to $r + i(a-\epsilon)$ such that for all $x \leq r_n$, $\mathrm{Im}(\overline{E}(x + ic_n)) = \mathrm{Im}(E_i(x + ic_n))$, and for all $x \geq r_n$, $\mathrm{Im}(\overline{E}(x + ic_n)) = E_k(x + ic_n)$, then the transition probability is bounded by

$$\tilde{p}_{k,i}(\tau) \leq C_{a-\epsilon} \exp\left(-2\tau \mathrm{Im}\left[\int_0^{r+i(a-\epsilon)} (E_k(z) - E_i(z))dz\right]\right).$$

Proof : Evident from the above discussion.

Remark 1: Note that *any* eigenvalue crossing can ruin the analyticity of $W'(z)$; it does not have to be crossing of E_i with E_k.

Remark 2: The conditions in the theorem single out two unique levels i and k for which the Landau formula holds (within ϵ). For other levels, one can obtain a weaker exponential bound using $\underline{L}_{n,m}$, which is generally not equal to the Landau expression; recall Lemma 6.3.

6.3. TOTAL TRANSITION PROBABILITY

We now consider transitions from a compatible band P_i to the remainder of the spectrum, instead of transitions to a given compatible band P_k as above. We again assume that $P_i(s) = Q_i(s)$. We can use Theorem 6.6 to bound $\tilde{p}_{k,i}(\tau)$ for all $k \neq i$ in J, and sum to obtain a bound on $\tilde{p}_i(\tau)$. If the index set J is finite, and $\tilde{p}_{k,i}(\tau)$ is exponentially for each $k \neq i$, then the total transition probability is exponentially bounded. If the index set is infinite, even if each $\tilde{p}_{k,i}(\tau)$ is exponentially bounded, the total transition probability may not be exponentially bounded, because the sum over $k \neq i$ may diverge, or the rate of exponential approach may not be bounded away from zero. We now formalize these rather simple notions.

If the gap $g_i > 0$, then we can without loss of generality write $H(s)$ as an admissible Hamiltonian in such a way that $g_{k,i} > 0$ for all $k > i$, and $g_{i,k} > 0$ for all $k < i$.

Definition 6.8.

a) If $i < k$, define

$$L_{k,i} = \sup_{0<c<a} \underline{L}_{k,i}(c);$$

if $k < i$, define

$$L_{k,i} = \sup_{-a<c<0} (-\overline{L}_{i,k}(c)).$$

b) The *Landau constant* L_i is defined by

$$L_i = \inf_{k \neq i} L_{k,i}.$$

c) We say the levels are *nonaccumulating* with respect to Q_i if

$$\sum_{k \neq i} \exp(-L_{k,i}) < \infty.$$

Remark 1: If J is finite, and $L_i > -\infty$, then the levels are clearly nonaccumulating. If J is infinite, and for all but a finite number of k, $L_{k,i} \geq \lambda|k - i| + \alpha$ for some real constants α and $\lambda > 0$, then the levels are nonaccumulating with respect to Q_i. This is the motivation for the terminology.

Remark 2: Note from part a) that if the transitions increase energy, we go to the upper half plane, and if they decrease energy, we go to the lower half plane, in accord with the arguments of Landau and Lifshitz [LNLF].

Theorem 6.9. Suppose that $g_i(s) > 0$ for all $s \in \mathbf{R}$, and the Q_n are indexed as above.

Suppose that for all $k > i$,

$$\inf_{0<b<a} \underline{L}_{k,i}(b) > -\infty,$$

and for all $k < i$,

$$\sup_{-a<b<0} \overline{L}_{i,k}(b) < \infty.$$

If the levels are nonaccumulating with respect to Q_i then there is a finite constant D_a such that for $\tau \geq 1$,

$$\tilde{p}_i(\tau) \leq D_a \exp(-\tau L_i).$$

Proof : From Theorem 6.6 , we have

$$\tilde{p}_{k,i}(\tau) \leq C_a \exp(-2\tau L_{k,i}).$$

Summing over $k \neq i$ gives, as in (5.11), for $\tau \geq 1$,

$$\begin{aligned}\tilde{p}_i(\tau) &\leq C_a \sum_{k\neq i} \exp(-2\tau L_{k,i}) \\ &\leq C_a \exp(-2\tau L_i) \sum_{k\neq i} \exp(-2\tau(L_{k,i} - L_i)) \\ &\leq C_a \exp(-2\tau L_i) \sum_{k\neq i} \exp(-2(L_{k,i} - L_i)),\end{aligned}$$

which is finite. ∎

Part II

Eigenvalue Asymptotics of the Neumann Laplacian of Regions and Manifolds with Cusps

Chapter 7: Introduction

Let Ω be a region in $\mathbf{R}^d$. We recall that the Neumann Laplacian $H_N = -\Delta_N^\Omega$ is the unique self-adjoint operator whose quadratic form is

$$g(f,f) = \int_\Omega |\nabla f|^2\,dx \tag{7.1}$$

on the domain $H^1(\Omega) = \{f \in L^2(\Omega) \mid \nabla f \in L^2(\Omega)\}$, where the gradient is taken in the distributional sense. One similarly defines the Dirichlet Laplacian $H_D = -\Delta_D^\Omega$ as the unique self-adjoint operator whose quadratic form is given by the closure of (7.1) on the domain $C_0^\infty(\Omega)$. If Ω is a bounded region with a smooth boundary it is well known that both H_N and H_D have compact resolvent and that their eigenvalue distributions are given by Weyl's law

$$N_E(H_N) \sim N_E(H_D) \sim \frac{\tau_d}{(2\pi)^d}\mathrm{Vol}(\Omega)E^{d/2}, \tag{7.2}$$

where by $f(E) \sim g(E)$ we mean $\lim_{E\to\infty} f(E)/g(E) = 1$. We denote by τ_d the volume of a unit ball in $\mathbf{R}^d$, by $\mathrm{Vol}(\Omega)$ the Lebesgue measure of Ω and by $N_E(A)$ the number of eigenvalues of the operator A which are less than E. If one drops the condition that Ω has a smooth boundary, nothing dramatic happens with the Dirichlet Laplacian H_D. As long as $\mathrm{Vol}(\Omega) < \infty$, H_D will have a compact resolvent and (7.2) remains true [ROS1]. On the other hand, the spectrum of H_N can undergo rather spectacular changes. The following theorem was proved in [HSS]:

Theorem. Let S be a closed subset of the positive real axis. Then there exists a bounded domain Ω for which

$$\sigma_{\mathrm{ess}}(H_N) = S.$$

In the previous Theorem, Ω can be chosen in such a way that its boundary has a singularity at exactly one point. We will be interested in the other extreme, namely when the domain Ω retains a nice boundary, but is unbounded, and in particular is of the form

$$\Omega = \{ (x,y) \in \mathbf{R}^2 \,:\, x > 1, |y| < f(x) \} . \tag{7.3}$$

In the sequel we will suppose that f is $C^\infty[1,\infty)$, strictly positive, and that its first three derivatives are bounded (although less regularity could be required). If $f(x) \to 0$, the Dirichlet Laplacian still has a compact resolvent [MOLA], but if $f(x) = x^{-1}$, or even if $f(x) = \exp(-x)$ (so $\mathrm{Vol}(\Omega) < \infty$), Davies and Simon [DVSM] showed that $\sigma_{\mathrm{ac}}(H_N)$ is nonempty. The difference in the spectral behavior is again striking, and one feels that a rather rapid decay of f should be required to ensure compactness of the resolvent of H_N. The following beautiful theorem was proven in [EVHR].

Theorem. If Ω is given by (7.3), H_N has a compact resolvent if and only if

$$\lim_{x\to\infty} \left(\int_1^x \frac{1}{f(t)}\, dt \right) \left(\int_x^\infty f(t)\, dt \right) = 0. \tag{7.4}$$

In this part we will study the large E asymptotic of the eigenvalue distribution of H_N in the regions (7.3). As in [DVSM], the main role is played by the one-dimensional Schrödinger operator

$$H_V = -\frac{d^2}{dx^2} + V(x), \qquad V(x) = \frac{1}{4}\left(\frac{f'}{f}\right)^2 + \frac{1}{2}\left(\frac{f'}{f}\right)', \tag{7.5}$$

acting on $L^2[1,\infty)$, and with Dirichlet boundary condition at 1. We make the following two hypotheses:

$$V(x) \to \infty, \qquad f''(x) \to 0 \;\text{ as } x \to \infty\,; \tag{H1}$$

$$\text{if } 0 < \epsilon < 1,\;\; N_E((1\pm\epsilon)H_V) = N_E(H_V)(1+O(\epsilon)). \tag{H2}$$

Our main result is

Theorem 7.1. If (H1) and (H2) are satisfied, we have

$$N_E(H_N) \sim N_E(H_V) + \frac{E}{2}\mathrm{Vol}(\Omega). \tag{7.6}$$

Remark 1: (H1) implies that

$$f(x) + f'(x)^2/f(x) \to 0 \qquad \text{as } x \to \infty \tag{7.7}$$

(see Section 8.1). In turn, Davies and Simon [DVSM] showed that if (7.7) is satisfied, H_N will have compact resolvent if and only if H_V does. Consequently, both sides in (7.6) are finite, and in particular (H1) implies that $\mathrm{Vol}(\Omega) < \infty$. (H2) prevents $N_E(H_V)$ from growing too rapidly (e.q. exponentially), which is needed to make our perturbation argument work. For example, it is satisfied if V is convex functions [TTCH] or if $V(x) \sim x^\alpha (\ln x)^\beta, \alpha > 0$. On the other hand, if $V(x) \sim \ln x$ (e.g. $f(x) = \exp(-x \ln x)$), it is not, and our argument does not apply.

`Remark 2:` The fact that Ω is symmetric is irrelevant. If $\Omega = \{(x, y) : x > 1, -f_1(x) < y < f_2(x)\}$, (7.6) remains valid providing that $f_1'' \to 0$, $f_2'' \to 0$, and that H_V, defined with $f = (f_1 + f_2)/2$, satisfies (H1), (H2). Also, if (H1) is replaced by a more involved hypothesis, the result extends (as usual [ROS1], [DVSM]) to the case when $\mathbf{R}^2$ is replaced by $\mathbf{R}^{d+1}$, $(x_1, x_\perp) \in \mathbf{R}^{d+1}$, $x_\perp \in \mathbf{R}^d$, $\Omega = \{x \mid x_\perp / f(x_1) \in G, 1 \leq x_1 \leq \infty\}$, where G is a bounded connected set. The asymptotic is given by (8.6) (replacing M with Ω).

`Example 1:` Let $f(x) = \exp(-x^\alpha)$. H_N has a compact resolvent if and only if $\alpha > 1$. One calculates

$$V(x) = \frac{\alpha^2}{4} x^{2(\alpha-1)} - \frac{\alpha(\alpha-1)}{2} x^{\alpha-2}.$$

The semiclassical formula [TTCH] yields

$$N_E(H_V) \sim \frac{1}{4(\alpha-1)\sqrt{\pi}} \left(\frac{\alpha}{2}\right)^{1/(1-\alpha)} \frac{\Gamma(1/(2(\alpha-1)))}{\Gamma(3/2 + 1/(2(\alpha-1)))} E^{1/2+1/(2(\alpha-1))}, \tag{7.8}$$

and thus both (H1) and (H2) are satisfied. (7.6) and (7.8) imply that the asymptotics of $N_E(H_N)$ satisfies Weyl's law if $\alpha > 2$, and is given by (7.8) if $1 < \alpha < 2$. If $\alpha = 2$ we have $N_E(H_N) \sim E/2\,(\mathrm{Vol}(\Omega) + 1/2)$. The leading order is the same as in Weyl's law but the constant is larger. We observe a phase transition in the eigenvalue asymptotics for the value $\alpha_c = 2$. In [DVSM] it was shown that for $\alpha = 1$, $\sigma_{\mathrm{ac}}(H_N) = [1/4, \infty)$, and for $0 < \alpha < 1$, $\sigma_{\mathrm{ac}}(H_N) = [0, \infty)$. In both cases $\sigma_{\mathrm{sing}}(H_N) = \emptyset$, and $\sigma_{\mathrm{pp}}(H_N)$ consists of a discrete set $0 = \lambda_1 < \lambda_2 \leq \ldots \leq \lambda_n \to \infty$ of embedded eigenvalues of finite multiplicity. (See the Appendix.)

Example 2: Let $f(x) = \exp(-x^2 g(x))$, $g(x) = 1 + \cos^2(\sqrt{\ln(1+x)})$. We have $V(x) \sim x^2 g(x)^2$ and the semiclassical formula yields

$$N_E(H_V) \sim \frac{E}{4g(E)}.$$

(H1), (H2) are satisfied, and we observe that $N_E(H_N)/E$ stays bounded above and below, but $\lim_{E\to\infty} N_E(H_N)/E$ does not exist.

The simplest way to understand the result of Theorem 7.1 is to consider a subspace P of $L^2(\Omega)$ consisting of functions u, which depend on the x variable only. On $C_0^2(\overline{\Omega}) \cap P$ the form (7.1) acts as

$$\int_1^\infty \left| \frac{d}{dx} u(x) \right|^2 2f(x)dx,$$

and viewed as a form on $L^2([1,\infty), 2f(x)dx)$ yields an operator that is (up to a minor change of boundary condition at $x = 1$) unitarily equivalent to H_V. It is now immediate that $N_E(-\Delta_N^\Omega) \succeq N_E(H_V)$ ($f(E) \succeq g(E)$ means that $\liminf_{E\to\infty} f(E)/g(E) \geq 1$), but in an equally simple way we can say even more. Denote $\Omega_L = \{(x,y) : 1 < x < L, |y| < f(x)\}$ and put an additional Dirichlet boundary condition along the line $x = L$. Dirichlet-Neumann bracketing yields

$$N_E(-\Delta_N^\Omega) \succeq N_E(H_V) + \frac{E}{2}\mathrm{Vol}(\Omega_L).$$

Letting $L \to \infty$, we obtain the one-sided inequality in (7.6), which is obviously true under the sole condition that f is a $C^2[1,\infty)$ function. It is the other, nontrivial direction of (7.6) which forces us to place conditions on f and V, and which could be proven using techniques developed in [SIM3], [DVSM] . The main technical point in such an approach is to obtain control of H_N on the subspace orthogonal to P. Here we will adopt a different strategy which, we believe, sheds some new light on the problem. Let $M = (-1,1) \times (1,\infty)$ be a strip with the metric

$$ds_M^2 = dx^2 + f(x)^2 dy^2, \tag{7.9}$$

and denote by H_N the Laplace-Beltrami operator on M with the Neumann boundary condition. Separating the variables we obtain that H_N is unitarily equivalent to the operator $\bigoplus_{n\geq 0} H_n$ acting on $\bigoplus_{n\geq 0} L^2([1,\infty), dx)$, where

$$H_n = H_V + \left(\frac{n\pi}{2f(x)}\right)^2$$

with the boundary condition $\psi'(1) = (f'(1)/2f(1))\psi(1)$. The main technical ingredient in this approach is to show that $N_E(\bigoplus_{n\geq 1} H_n)$ satisfies Weyl's law. Then the analog of Theorem 7.1 for H_N is immediate. After a suitable coordinate change, the region Ω is transformed into the strip M, with a metric that is (under the conditions of the Theorem 7.1) asymptotically of the form (7.9). At this point, a relatively easy perturbation argument will yield (7.6).

Finally, we remark that the above approach appears useful in studying eigenvalue asymptotics of a Dirichlet Laplacian in a region Ω given by (7.3), with $f(x) \to 0$ and $\mathrm{Vol}(\Omega) = \infty$. While we can recover most of the known results on the asymptotics of $N_E(H_D)$ in such regions (but not all, e.g., we cannot treat the case $f(x) = (\ln(1+x))^{-1}$, see [ROS1], [BER]), here we restrict ourselves to giving a new proof of the well-known

Theorem 7.2.(Rosenblum-Simon) Let $\Omega = \{(x,y) : |x|^\alpha |y| \leq 1\}$. Then

$$N_E(H_D) \sim \frac{1}{\sqrt{\pi}}\left(\frac{2}{\pi}\right)^{1/\alpha}\zeta(1/\alpha)\frac{\Gamma(1+1/2\alpha)}{\Gamma(3/2+1/2\alpha)}E^{1/2+1/2\alpha}, \text{ if } 0 < \alpha < 1,$$

$$N_E(H_D) \sim \frac{1}{\pi}E\ln E, \qquad \text{if } \alpha = 1,$$

where ζ is the standard zeta function. The case $\alpha > 1$ follows by symmetry.

Chapter 8: Neumann Laplacians on Manifolds and Regions with Cusps

We begin by studying the eigenvalue distribution of a Laplace-Beltrami operator on a Riemannian manifold of the form $M = N \times [1, \infty)$, with a metric ds_M^2, $\text{Vol}(M) < \infty$. Here, N is a compact, oriented Riemannian manifold (with or without boundary), $\dim(N) = d$, with a metric ds_N^2, and a volume element dm_N. We remark that the boundary of M does not have to be C^∞, but it is certainly piecewise C^∞, and therefore causes no problem in the discussion below (see, e.g., [CH]). In Sections 8.1 and 8.2 we treat the case when the metric on M has a warped product form. Perturbations are studied in Section 8.3. Finally, in Section 8.4, we derive Theorem 7.1 as an easy consequence of the results obtained for manifolds.

8.1. Preliminaries

We suppose that the metric on M is given by

$$ds_M^2 = dx^2 + f(x)^2 ds_N^2, \tag{8.1}$$

where f is a positive $C^\infty[1, \infty)$ function, and that

$$\text{Vol}(M) = \text{Vol}(N) \int_1^\infty f(x)^d dx < \infty. \tag{8.2}$$

If $d = 1$, (8.2) is a consequence of (H1). H_N, the Laplace-Beltrami operator on M with Neumann boundary conditions, acts on a Hilbert space $L^2(M, dm_M)$ and is the unique self-adjoint operator whose quadratic form is given by the closure of

$$q(\phi, \phi) = \int_M |\nabla \phi|^2 dm_M \tag{8.3}$$

on $C_0^2(\overline{M})$. In (8.3), $dm_M = f^d dm_N dx$ and ∇ is the gradient on M. Of equal importance for us is the Laplace-Beltrami operator $H_{N,D}$ on M with the Dirichlet boundary condition along $\{1\} \times N$, and the Neumann one on the rest of the boundary. It is defined as a closure of the form (8.7) on the subspace of $C_0^2(\overline{M})$ consisting of functions that vanish along $\{1\} \times N$. The analog of (7.5) is the one-dimensional Schrödinger operator of the form

$$H_V = -\frac{d^2}{dx^2} + V(x), \quad V(x) = \frac{d^2}{4}\left(\frac{f'}{f}\right)^2 + \frac{d}{2}\left(\frac{f'}{f}\right)', \tag{8.4}$$

with the Dirichlet boundary condition at 1. Denote by

$$C_d = \left((4\pi)^{(d+1)/2}\Gamma((d+3)/2)\right)^{-1}. \tag{8.5}$$

The following lemma, which we prove in Section 8.2, is the main technical ingredient in our approach.

Lemma 8.1. Suppose that $V(x) \to \infty$, $f(x)^2V(x) \to 0$ as $x \to \infty$. Then

$$N_E(H_N) \sim N_E(H_{N,D}) \sim N_E(H_V) + E^{(d+1)/2}C_d\mathrm{Vol}(M). \qquad (8.6).$$

In the sequel we collect, for reader's convenience, a few simple results that will be needed later. Let

$$D_N = \{\phi : \phi \in C_0^2(\overline{M}), \nu\phi = 0\},$$

where ν is the outward unit normal vector field on ∂M. H_N acts on D_N as

$$H_N(\phi) = -\frac{1}{f(x)^d}\frac{\partial}{\partial x}f(x)^d\frac{\partial}{\partial x}\phi + \frac{1}{f(x)^2}H_N^N(\phi),$$

where H_N^N is a Laplace-Beltrami operator of N. H_N^N has a compact resolvent [CH]; its spectrum consists of discrete eigenvalues $0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \ldots \leq \lambda_n \to \infty$, and we denote by ϕ_n^N the corresponding eigenfunctions. Introducing

$$L_n^2(M) = \{g : g(x,t) = \psi(x)\phi_n^N(t), \int_1^\infty |\psi(x)|^2 f(x)^d dx < \infty\},$$

we obtain the decomposition

$$L^2(M) = \bigoplus_{n\geq 0} L_n^2(M) = \bigoplus_{n\geq 0} L_n^2([1,\infty), f(x)^d dx).$$

The operator H_N splits accordingly

$$H_N = \bigoplus_{n\geq 0} H_{N,n},$$

where $H_{N,n}$ acts on $L_n^2([1,\infty), f(x)^d dx)$ as

$$H_{N,n} = -\frac{1}{f(x)^d}\frac{\partial}{\partial x} f(x)^d \frac{\partial}{\partial x} + \frac{\lambda_n}{f^2(x)}.$$

Under the unitary map

$$U : L^2([1,\infty), dx) \to L_n^2([1,\infty), f(x)^d dx), \quad U(\phi) = f^{-d/2}\phi$$

$H_{N,n}$ transforms as

$$H_n = U^{-1} H_{N,n} U = -\frac{d^2}{dx^2} + V(x) + \frac{\lambda_n}{f^2(x)}, \tag{8.7}$$

and (if V is bounded below) is essentially self-adjoint on

$$D_V = \{\psi : \psi \in C_0^2[1,\infty),\ \psi'(1) = d/2(f'(1)/f(1))\psi(1)\}. \tag{8.8}$$

H_N is unitarily equivalent to the operator $\bigoplus_{n\geq 0} H_n$ acting on $\bigoplus_{n\geq 0} L^2([1,\infty), dx)$. Similarly, $H_{N,D}$ is unitarily equivalent to $\bigoplus_{n\geq 0} H_n^D$, where H_n^D is the operator (8.7) with the Dirichlet boundary condition at 1. The spectral analysis of H_N and $H_{N,D}$ reduces to the spectral analysis of the one-dimensional Schrödinger operators H_n, H_n^D. We will need

Lemma 8.2. If $V(x) \to \infty$ as $x \to \infty$, we have

$$N_E(H_n^D) \leq N_E(H_n) \leq 1 + N_E(H_n^D) \tag{8.9}$$

for all $n \geq 0$.

Proof : We just sketch the well-known argument. $C_0^\infty[1,\infty)$ is a form core for H_n^D, and thus $N_E(H_n^D) \le N_E(H_n)$ follows from the min-max principle [RS4]. Let

$$D = \{\psi : \psi \in C_0^2[1,\infty),\ \psi(1) = 0\}.$$

If L stands for an arbitrary vector subspace of $L^2[1,\infty)$, the min-max principle yields

$$N_E(H_n) = \sup_{\substack{L\subset D_V \\ (H_n\psi,\psi)<E \\ \psi\in L, \|\psi\|=1}} \dim L, \qquad N_E(H_n^D) = \sup_{\substack{L\subset D \\ (H_n^D\psi,\psi)<E \\ \psi\in L, \|\psi\|=1}} \dim L.$$

Fix $L \subset D_V$ and let $L_0 = \{\psi \in L : \psi(1) = 0\}$. Observing that $\dim L/L_0 \le 1$ we derive (8.9). ∎

We finish with the following

Lemma 8.3. If $d = 1$ and (H1) is satisfied, we have

$$f(x) + |f'(x)| + f'(x)^2/f(x) + f(x)V(x) \to 0 \text{ as } x \to \infty. \tag{8.10}$$

Furthermore, for large x, f is convex and strictly decreasing.

Proof : The result follows from

$$f''(x) = 2f(x)V(x) + \frac{f'(x)^2}{2f(x)}.$$

∎

8.2. Proof of Lemma 8.1

Denote $A_N = \bigoplus_{n\ge1} H_n$, $A_D = \bigoplus_{n\ge1} H_n^D$. (8.6) will follow if we prove that

$$\lim_{E\to\infty} \frac{N_E(A_N)}{E^{(d+1)/2}} = \lim_{E\to\infty} \frac{N_E(A_D)}{E^{(d+1)/2}} = C_d \mathrm{Vol}(M). \tag{8.11}$$

Let

$$m = \max_{x>1} f(x)^2, \qquad M = \max_{x>1} |V(x)f(x)^2|.$$

We have that $N_E(H_n^D) = 0$ if $\lambda_n > mE + M$, and thus

$$\begin{aligned} N_E(A_D) \leq N_E(A) &\leq N_E(A_D) + \#\{\lambda_n \, : \, \lambda_n \leq mE + M\} \\ &= N_E(A_D) + O(E^{d/2}), \end{aligned}$$

since Weyl's law applies for H_N^N. Consequently, it suffices to prove (8.11) for A_D. By the Karamata-Tauberian Theorem [SIM1], (8.11) will follow if we prove

$$\lim_{t \to 0} t^{(d+1)/2} \operatorname{Tr}(\exp(-tA_D)) = (4\pi)^{-(d+1)/2} \operatorname{Vol}(M). \tag{8.12}$$

First, note that

$$\lim_{t \to 0} t^{d/2} \sum_{k \geq 1} \exp(-t\lambda_k) = (4\pi)^{-d/2} \operatorname{Vol}(N) \tag{8.13}$$

[CH], and in addition

$$t^{d/2} \sum_{k \geq 1} \exp(-t\lambda_k) < L \tag{8.14}$$

for a uniform constant L and for all $t > 0$. The Golden-Thompson inequality [SIM1] yields

$$\operatorname{Tr}(\exp(-tH_k^D)) \leq \frac{1}{2\sqrt{\pi t}} \int_1^\infty \exp(-t \cdot (V(x) + \lambda_k / f(x)^2)) dx.$$

Fix $\varepsilon > 0$, $\lambda_1 > \varepsilon > 0$, and let $R > 0$ be big enough so that $|f^2(x)V(x)| < \varepsilon$ if $x > R$. Let $c = \inf_{x \in [1,R]} V(x)$. We have

$$\operatorname{Tr}(\exp(-tH_k^D)) \leq \frac{e^{-ct}}{2\sqrt{\pi t}} \int_1^\infty \exp\left(-t \cdot (\lambda_k - \varepsilon) / f(x)^2\right) \, dx$$

$$\begin{aligned} t^{(d+1)/2} \operatorname{Tr}(\exp(-tA_D)) &= \sum_{k \geq 1} t^{(d+1)/2} \operatorname{Tr}(\exp(-tH_k)) \\ &\leq \frac{e^{-ct}}{2\sqrt{\pi}} \int_1^\infty f(x)^d \cdot \sum_k \left(t/f(x)^2\right)^{d/2} \exp\left(-t(\lambda_k - \varepsilon)/f(x)^2\right) \, dx. \end{aligned}$$

Using (8.14) and the Lebesgue dominated convergence theorem, we obtain

$$\limsup_{t \to 0} t^{(d+1)/2} \operatorname{Tr}(\exp(-tA_D)) \leq \frac{\operatorname{Vol}(N)}{(4\pi)^{(d+1)/2}} \int_1^\infty f(x)^d dx.$$

It remains to show

$$\liminf_{t\to 0} t^{(d+1)/2}\operatorname{Tr}(\exp(-tA_D)) \geq (4\pi)^{-(d+1)/2}\mathrm{Vol}(M). \tag{8.15}$$

Let $R > 1$ be a positive number; make a partition of $[1, R)$ into k intervals I_m of equal size. Denote by H_D^m the Dirichlet Laplacian on I_m, and let

$$d_m = \sup_{x\in I_m} f(x)^{-2}, \qquad c = \sup_{x\in[1,R]} |V(x)|.$$

Dirichlet-Neumann bracketing yields

$$\operatorname{Tr}(\exp(-tH_n)) \geq \sum_{m=1}^{k} \exp(-t(c + \lambda_n d_m))\operatorname{Tr}(\exp(-tH_D^m)).$$

Obviously, $\operatorname{Tr}(\exp(-tH_D^m)) = \operatorname{Tr}(\exp(-tH_D^1))$ for all m, and

$$\lim_{t\to 0} t^{1/2}\operatorname{Tr}\exp(-tH_D^1) = \frac{1}{2\sqrt{\pi}}\frac{R}{k}.$$

We have

$$\begin{aligned}\liminf_{t\to 0} t^{(d+1)/2}\sum_{n>0}\operatorname{Tr}(\exp(-tH_n)) &\geq \frac{1}{2\sqrt{\pi}}\sum_{m=1}^{k}\frac{R}{k}d_m^{-d/2}\liminf_{t\to 0}(td_m)^{d/2}\sum_{n>0}\exp(-td_m\lambda_n)\\ &= \mathrm{Vol}(N)(4\pi)^{-(d+1)/2}\sum_{m=1}^{k}\frac{R}{k}d_m^{-d/2}.\end{aligned}$$

Using that f is continuous and passing to the limit $k\to\infty$ we have

$$\liminf_{t\to 0} t^{(d+1)/2}\operatorname{Tr}(\exp(-tA_D)) \geq (4\pi)^{-(d+1)/2}\,\mathrm{Vol}(N)\int_1^R f(x)^d dx.$$

Letting $R\to\infty$ we obtain (8.15) and (8.12).

8.3. Metric Perturbations

In this section we suppose that a metric on M is given by

$$ds_M^2 = \alpha(t,x)^2 dx^2 + \beta(t,x)^2 ds_N^2, \tag{8.16}$$

where α, β are two positive, C^∞ functions on M. We also suppose that

$$\mathrm{Vol}(M) = \int_M \alpha \cdot \beta^d dm_N dx < \infty.$$

After a suitable coordinate change, the region Ω, given by (8.3) (if (H1) is satisfied), transforms into $(-1,1) \times (1,\infty)$ with a metric of the form (8.16). That is the reason why we choose to discuss (8.16), even if a much larger class of perturbations can be treated along the same lines (see [FRHS], [PR1] for related discussions). H_N, $H_{N,D}$ are defined, as in the previous section, via the closure of the quadratic form (8.3) (with $dm_M = \alpha \cdot \beta^d dm_N dx$) on the appropriate subspace. If there exists a function f, satisfying the condition of Lemma 8.1, such that $\alpha \to 1$, $\beta \to f$ as $x \to \infty$, one expects that $N_E(H_N)$ should not be too far from $N_E(\widehat{H}_N)$, where $\widehat{H}_N$ is the Laplace-Beltrami operator on M for the metric

$$d\widehat{s}_M^2 = dx^2 + f(x)^2 ds_N^2. \tag{8.17}$$

It is indeed the case. Denote $M_L = N \times [L, \infty)$,

$$\|g\|_L = \sup_{(t,x) \in M_L} |g(t,x)|,$$

and let

$$\nu(L) = \|\alpha - 1\|_L + \|f/\beta - 1\|_L + \||\widehat{\nabla}\alpha|\|_L + \||\widehat{\nabla}(f/\beta)|\|_L, \tag{8.18}$$

where $\widehat{\nabla}$ is the gradient on M with the metric (8.17). For H_V given by (8.4), we have

Lemma 8.4. Suppose that $\nu(L) \to 0$ as $L \to \infty$, that f and V satisfy the conditions of Lemma 8.1, and that $N_E(H_V)$ satisfies (H2). Then

$$N_E(H_N) \sim N_E(H_{N,D}) \sim N_E(H_V) + E^{(d+1)/2} C_d \mathrm{Vol}(M).$$

We remark that while $\mathrm{Vol}(M)$ is calculated in the metric (8.16), the operator H_V arises from the metric (8.17).

Proof : We will consider only H_N. A virtually identical argument applies for $H_{N,D}$. For $L > 1$, denote by $H_{L,D}^-$, $H_{L,D}^+$ the Laplace-Beltrami operators acting on $N \times [1, L]$,

M_L, with the metric (8.16) and the Dirichlet boundary condition along $N \times \{L\}$, on the rest of boundary we take the Neumann one. Denote by $\widehat{H}^+_{L,D}$ the Laplace-Beltrami operator on M_L with the metric (8.17) and with same boundary condition as $H^+_{L,D}$. Let

$$U : L^2(M_L, \alpha\beta^d dm_N dx) \to L^2(M_L, f^d dm_N dx)$$

be a unitary mapping defined as

$$U(\phi) = (\alpha \cdot (\beta/f)^d)^{1/2}\phi = (1/g) \cdot \phi.$$

The operator $H^+_{L,D}$ is then unitarily equivalent to the operator acting on $L^2(M, f^d dm_N dx)$, which we again denote by $H^+_{L,D}$ and whose quadratic form is given by the closure of

$$\int_{M_L} |\nabla(g\phi)|^2 \alpha\beta^d dm_N dx \tag{8.19}$$

on the subspace

$$C^2_{0,L}(\overline{M}_L) = \{\phi \, : \, \phi \in C^2_0(\overline{M}_L), \, \phi(t, L) = 0\}.$$

Vector fields $\nabla\phi$, $\widehat{\nabla}\phi$ are given as

$$\nabla\phi = \frac{1}{\alpha^2}\frac{\partial\phi}{\partial x}\frac{\partial}{\partial x} + \frac{1}{\beta^2}\nabla_N\phi,$$
$$\widehat{\nabla}\phi = \frac{\partial\phi}{\partial x}\frac{\partial}{\partial x} + \frac{1}{f^2}\nabla_N\phi,$$

where ∇_N is the gradient on N. If $\phi \in C^2_{0,L}(\overline{M}_L)$ and has norm 1 as an element of $L^2(M_L, f^d dm_N dx)$, we estimate

$$\left|((H^+_{L,D} - \widehat{H}^+_{L,D})\phi, \phi)\right| \leq \int_{M_L} \left||\nabla(g\phi)|^2 \alpha\beta^d - |\widehat{\nabla}\phi|^2 f^d\right| dm_N dx$$
$$\leq \int_{M_L} A(L)|\widehat{\nabla}(g\phi)|^2 + \left||\widehat{\nabla}(g\phi)|^2 - |\widehat{\nabla}\phi|^2\right| f^d dm_N dx,$$

where

$$A(L) = \|1/g\|^2_L \left(\|(1/\alpha)^2 - 1\|_L + \|(f/\beta)^2 - 1\|_L\right) + \|(1/g)^2 - 1\|_L.$$

Furthermore, we have

$$|\widehat{\nabla}(g\phi)|^2 \leq |\widehat{\nabla}\phi|^2 \cdot (\|g\|_L^2 + \|g\|_L \cdot \||\widehat{\nabla}g|\|_L) + \\ + |\phi|^2 \cdot (\||\widehat{\nabla}g|\|_L^2 + \|g\|_L \cdot \||\widehat{\nabla}g|\|_L),$$

$$\left||\widehat{\nabla}(g\cdot\phi)|^2 - |\widehat{\nabla}\phi|^2\right| \leq |\widehat{\nabla}\phi|^2 \cdot (\|g^2 - 1\|_L + \|g\|_L \cdot \||\widehat{\nabla}g|\|_L) + \\ + |\phi|^2 \cdot (\||\widehat{\nabla}g|\|_L^2 + \|g\|_L \cdot \||\widehat{\nabla}g|\|_L).$$

Because $\nu(L) \to 0$, all the constants in the above estimates are $O(\nu(L))$, and we conclude that

$$\left|((H_{L,D}^+ - \widehat{H}_{L,D}^+)\phi, \phi)\right| \leq D\nu(L)\left((\widehat{H}_{L,D}^+\phi, \phi) + 1\right), \tag{8.20}$$

for an L-independent constant D. In the sequel we take L large enough so that $D\nu(L) < 1$, and then absorb D into $\nu(L)$. (8.20), min-max principle, and Lemma 8.1 yield (recall that $f(E) \succeq g(E)$ means $\liminf_{E\to\infty} f(E)/g(E) \geq 1$)

$$N_E(H_{L,D}^+) \succeq N_{E-\nu(L)}((1+\nu(L))\widehat{H}_{L,D}^+) \sim N_E((1+\nu(L))\widehat{H}_{L,D}^+). \tag{8.21}$$

If $H_{V,L}$ is the operator (8.6) acting on $L^2([L,\infty), dx)$, we observe that the asymptotic of $N_E(H_{V,L})$ does not depend on the boundary condition at L, nor on L itself. Consequently, in the sequel we will deal only with H_V. Denote

$$C_1(L) = \liminf_{E\to\infty} \frac{N_E((1-\nu(L))H_V)}{N_E(H_V)}, \qquad C_2(L) = \limsup_{E\to\infty} \frac{N_E((1+\nu(L))H_V)}{N_E(H_V)}.$$

(H2) implies

$$\lim_{L\to\infty} C_1(L) = 1, \qquad \lim_{L\to\infty} C_2(L) = 1. \tag{8.22}$$

(8.21), (8.22) were the two essential ingredients of the argument. Denote by $\mathrm{Vol}(\widehat{M}_L)$ the volume of M_L in the metric (8.16). We have

$$\begin{aligned} N_E(H_N) &\succeq N_E(H_{L,D}^-) + N_E(H_{L,D}^+) \\ &\succeq E^{(d+1)/2} C_d \mathrm{Vol}(N \times [1,L]) + N_E((1+\nu(L))\widehat{H}_{L,D}^+) \\ &\succeq I(L)\left(E^{(d+1)/2} C_d(\mathrm{Vol}(N \times [1,L)) + \mathrm{Vol}(\widehat{M}_L)) + N_E(H_V)\right), \end{aligned} \tag{8.23}$$

where

$$I(L) = \min\left\{(1+\nu(L))^{-((1+d)/2}, C_2(L)\right\}.$$

(8.23) follows from Dirichlet-Neumann bracketing, Lemma 8.1 and the fact that the eigenvalue distribution of a Laplace-Beltrami operator on a compact manifold with a piecewise smooth boundary and mixed boundary conditions satisfies Weyl's law [CH]. Replacing the boundary condition along $N \times \{L\}$ with the Neumann b. c., we get the operators $H_{L,N}^-$ and $H_{L,N}^+$, and a completely analogous argument gives

$$
\begin{aligned}
N_E(H_N) &\preceq N_E(H_{L,N}^-) + N_E(H_{L,N}^+) \\
&\preceq S(L)\left(E^{(d+1)/2}C_d(\mathrm{Vol}(N \times [1, L)) + \mathrm{Vol}(\widehat{M}_L)) + N_E(H_V)\right),
\end{aligned}
\tag{8.24}
$$

where

$$S(L) = \max\left\{(1 - \nu(L))^{-(1+d)/2}, C_1(L)\right\}.$$

As $L \to \infty$, $I(L) \to 1$, $S(L) \to 1$, $\mathrm{Vol}(\widehat{M}_L) \to 0$, $\mathrm{Vol}(N \times [1, L)) \to \mathrm{Vol}(M)$, and the lemma follows from (8.23), (8.24). ∎

It is now obvious why our argument fails in the case when $N_E(H_V)$ grows exponentially fast ($C_1(L) = C_2(L) = \infty$). It is natural to conjecture that in such cases $N_E(H_N) \sim N_E(H_V)$, but it is unlikely that the above argument can be modifed to prove it.

8.4. Proof of Theorem 7.1

One consequence of hypothesis (H1) (see Lemma 8.3) is that f is a strictly decreasing function for large x. The familiar Dirichlet-Neumann bracketing argument, which will be repeated in detail once again below, implies that without loss of generality we can assume $f'(x) < 0$ for $x > 1$. We construct a change of variable as follows: Let

$$\varepsilon(x, y) = \frac{y}{f(x)}, \qquad -1 \leq \varepsilon \leq 1.$$

ε is the first integral of the equation

$$\frac{dy}{dx} = y \cdot \frac{f'}{f}.$$

The equation for the orthogonal lines is given by

$$y \cdot \frac{dy}{dx} = -\frac{f}{f'},$$

whose first integral is

$$\frac{y^2}{2} + \int_1^x \frac{f(t)}{f'(t)} dt = c.$$

Any C^1 function of this first integral is an orthogonal coordinate to ε. Let

$$F(x) = \int_1^x \frac{f(t)}{f'(t)} dt;$$

note that F is a decreasing function ($f' < 0$) and denote $a = \lim_{x\to\infty} F(x)$. The inverse function F^{-1} is well defined on $(a, 0]$, and for R large enough we have

$$\frac{y^2}{2} + F(x) \in (a, 0], \qquad x > R, \quad (x, y) \in \Omega.$$

Let

$$\eta(x, y) = F^{-1}\left(y^2/2 + F(x)\right), \, (x, y) \in \Omega, \, x > R.$$

It is easy to check that (ε, η) is one-one, and that Jacobian $D(\varepsilon, \eta)/D(x, y) \sim 1/f(x) \neq 0$ for x large. Denoting (for $c > R$)

$$\Omega_1 = \{(x, y) : (x, y) \in \Omega, \, \eta(x, y) > c\}, \tag{8.25}$$

we conclude that for a large c, (ε, η) is a C^∞-bijection between Ω_1 and half-strip $M = (-1, 1) \times (c, \infty)$ with a C^∞-inverse. The eigenvalue asymptotics of a Laplacian on a bounded region with piecewise C^∞ boundary and with mixed boundary conditions satisfies Weyl's law. Consequently, putting an additional Dirichlet or Neumann b. c. along $\eta(x, y) = c$, we observe that it is enough to prove the statement for H_N, $H_{N,D}$, the Laplacians on Ω_1 with respectively Neumann or Dirichlet b. c. along $\eta(x, y) = c$, and the Neumann b. c. on the rest of the boundary. The above change of variables transforms H_N, $H_{N,D}$ into Laplace-Beltrami operators on M, with the metric $ds_M^2 = dx(\varepsilon, \eta)^2 + dy(\varepsilon, \eta)^2$, the Neumann or Dirichlet b. c. along $[-1, 1] \times \{c\}$, and the

Neumann b. c. along $\{\pm 1\} \times [c, \infty)$. An easy calculation shows

$$dx^2 + dy^2 = \left(1 + y^2\left(\frac{f'(x)}{f(x)}\right)^2\right)^{-1}\left(d\varepsilon^2 f^2(x) + d\eta^2\left(\frac{f'(x)}{f(x)}\right)^2\left(\frac{f(\eta)}{f'(\eta)}\right)^2\right). \qquad (8.26)$$

In the notation of Section 8.3

$$\alpha(\varepsilon,\eta) = \left(\frac{f'(x)}{f(x)}\right)\left(\frac{f(\eta)}{f'(\eta)}\right)\cdot\left(1 + y^2\left(\frac{f'(x)}{f(x)}\right)^2\right)^{-1/2}$$

$$\beta(\varepsilon,\eta) = f(x)\cdot\left(1 + y^2\left(\frac{f'(x)}{f(x)}\right)^2\right)^{-1/2},$$

and it is a straightforward (but rather long) exercise in differentiation to show that

$$\begin{aligned} |\alpha(\varepsilon,\eta) - 1| = O(F(\eta)), \qquad & |f(\eta)/\beta(\varepsilon,\eta) - 1| = O(F(\eta)), \\ |\widehat{\nabla}\alpha(\varepsilon,\eta)| \le \left|\frac{1}{f(\eta)}\frac{\partial\alpha(\varepsilon,\eta)}{\partial\varepsilon}\right| + & \left|\frac{\partial\alpha(\varepsilon,\eta)}{\partial\eta}\right| = O(F(\eta)), \\ |\widehat{\nabla}(f(\eta)/\beta(\varepsilon,\eta))| \le \left|\frac{1}{f(\eta)}\frac{\partial(f/\beta)}{\partial\varepsilon}\right| + & \left|\frac{\partial(f/\beta)}{\partial\eta}\right| = O(F(\eta)), \end{aligned} \qquad (8.27)$$

where

$$F(\eta) = |f(\eta)| + |f'(\eta)| + |f''(\eta)| + |f'(\eta)^2/f(\eta)|.$$

In obtaining (8.27) we have used the fact that the third derivative of f is bounded (recall 7.3). Lemma 8.3 implies that $F(\eta) \to 0$ as $\eta \to \infty$. Theorem 7.1 is now an immediate consequence of Lemmas 8.3, 8.4.

Chapter 9: Dirichlet Laplacians on Regions with Cusps

9.1. Some Generalities

There have been quite a few results [ROS1], [TAM], [SIM3], [BER] on the asymptotics of the eigenvalue distribution of H_D in regions Ω given by (7.3) when $f(x) \to 0$ and $\mathrm{Vol}(\Omega) = \infty$. Here we give a new treatment which, besides being elementary, seems to cover most of the interesting examples. We refer to the papers of Rosenblum [ROS1] and Davies [DV2] for a detailed discussion of the spectral properties of H_D in limit-cylindrical domains.

We suppose that f is convex and that

$$f(x) + f''(x) + f'(x)^2/f(x) \to 0 \text{ as } x \to \infty. \tag{9.1}$$

If $\mathrm{Vol}(\Omega) = \infty$, $\lim_{E\to\infty} N_E(H_D)/E = 0$, and we restrict ourselves to studying the operators H_D, $H_{D,N}$ on Ω_1 given by (8.25), with respectively Dirichlet or Neumann boundary condition on $\eta(x,y) = c$. Performing the same change of variable as in the previous section, we obtain the Laplace-Beltrami operators on $M = (-1,1) \times (c,\infty)$ with the metric (7.9) and with the Dirichlet boundary conditions on $\{\pm 1\} \times [c,\infty)$ and the Dirichlet or Neumann b. c. on $[-1,1] \times \{c\}$. Let us first analyze $H_{D,N}$. If $\widehat{H}_{D,N}$ is the Laplace-Beltrami operator on M with metric (8.26) and with the same boundary condition as $H_{D,N}$, we obtain, as in Sections 8.3, 8.4, that for any $\epsilon > 0$ we can find c big enough so that

$$N_E((1-\epsilon)\widehat{H}_{N,D}) \succeq N_E(H_{N,D}) \succeq N_E((1+\epsilon)\widehat{H}_{N,D}). \tag{9.2}$$

Separating the variables, we obtain that $\widehat{H}_{D,N}$ is unitarily equivalent to $\bigoplus_{n\geq 1} H_n$, given by (8.7), acting on $\bigoplus_{n\geq 1}^{\infty} L^2[c,\infty)$, and with the boundary conditions (8.8) at $x = c$. (9.1) implies that $V(x)f(x)^2 \to 0$, and (eventually increasing ϵ in (9.2)) we can restrict ourselves to studying

$$A = \bigoplus_{n\geq 1} -\frac{d^2}{dx^2} + \left(\frac{n\pi}{2f(x)}\right)^2 . \tag{9.3}$$

Starting with H_D on Ω_1, we end up with operator (9.3) with Dirichlet boundary condition at c, which we denote by A_D. (9.2) implies that $\lim_{E\to\infty} N_E(A)/E = \infty$, and, as in Section 8.2, we observe that the asymptotic of $N_E(A)$ does not depend on the boundary condition at c, nor on c itself. Consequently, we can restrict ourselves to studying A_D with $c = 1$. The strategy is now clear: If we show that

$$\lim_{\epsilon\to 0}\lim_{E\to\infty} \frac{N_E((1\pm\epsilon)A_D)}{N_E(A_D)} = 1, \tag{9.4}$$

we have $N_E(H_D) \sim N_E(A_D)$, and the asymptotics of the original problem follows.

To demonstrate the effectiveness of the above strategy, we prove Theorem 7.2.

9.2. Proof of Theorem 7.2

We can obviously restrict ourselves to studying only the horn $\Omega_1 = \{x : x > 1, |y| < x^{-\alpha}\}$, and multiplying the result by 2 if $0 < \alpha < 1$, or with 4 if $\alpha = 1$. (9.1) is trivial. The operators A_D become

$$\bigoplus_{n\geq 1} -\frac{d^2}{dx^2} + \left(\frac{n\pi}{2}\right)^2 x^{2\alpha}$$

acting on $L^2[1,\infty)$. Suppose that we prove

$$\lim_{t\to 0} t^{1/2+1/2\alpha}\mathrm{Tr}(\exp(-tA_D)) = \frac{1}{2\sqrt{\pi}}\left(\frac{2}{\pi}\right)^{1/\alpha}\zeta\left(\frac{1}{\alpha}\right)\Gamma\left(\frac{1}{2\alpha}+1\right), \text{ if } 0<\alpha<1 \tag{9.5}$$

and

$$\lim_{t\to 0} t(\ln t^{-1})^{-1}\mathrm{Tr}(\exp(-tA_D)) = \frac{1}{4\pi}, \qquad \text{if } \alpha = 1. \tag{9.6}$$

Then, by the Karamata-Tauberian Theorem ([SIM1], [SIM3]),

$$N_E(A_D) \sim \frac{1}{2\sqrt{\pi}}\left(\frac{2}{\pi}\right)^{1/\alpha}\zeta(1/\alpha)\frac{\Gamma(1/(2\alpha)+1)}{\Gamma(3/2+1/(2\alpha))}E^{1/2+1/(2\alpha)}, \text{ if } 0<\alpha<1,$$

$$N_E(A_D) \sim \frac{1}{4\pi}E\ln E \qquad \text{if } \alpha = 1,$$

(9.4) is immediate and the theorem follows. It remains to prove (9.5), (9.6). It should not come as a surprise that the argument closely follows the one of Section 8.2.

Case $0 < \alpha < 1$: The Gordon-Thompson inequality yields

$$\begin{aligned} t^{1/2+1/2\alpha}\mathrm{Tr}(\exp(-tA_D)) &\leq t^{1/2+1/2\alpha}\sum_{n>0}\frac{1}{2\sqrt{\pi t}}\int_1^\infty \exp(-t(n\pi/2)^2x^{2\alpha})dx \\ &\leq \frac{1}{2\sqrt{\pi}}\left(\frac{2}{\pi}\right)^{1/\alpha}\zeta\left(\frac{1}{\alpha}\right)\int_0^\infty \exp(-x^{2\alpha})dx \\ &\leq \frac{1}{2\sqrt{\pi}}\left(\frac{2}{\pi}\right)^{1/\alpha}\zeta\left(\frac{1}{\alpha}\right)\Gamma\left(\frac{1}{2\alpha}+1\right), \end{aligned}$$

and it is immediate that

$$\limsup_{t\to 0} t^{1/2+1/2\alpha}\mathrm{Tr}(\exp(-tA_D)) \leq \frac{2}{\sqrt{\pi}}\left(\frac{2}{\pi}\right)^{1/\alpha}\zeta\left(\frac{1}{\alpha}\right)\Gamma\left(\frac{1}{2\alpha}+1\right).$$

It remains to prove

$$\liminf_{t\to 0} t^{1/2+1/2\alpha}\mathrm{Tr}(\exp(-tA_D)) \geq \frac{2}{\sqrt{\pi}}\left(\frac{2}{\pi}\right)^{1/\alpha}\zeta\left(\frac{1}{\alpha}\right)\Gamma\left(\frac{1}{2\alpha}+1\right). \qquad (9.7)$$

Make a partition of $[1,\infty)$ into intervals I_k of equal size $1/m$. Denote by H_k^D the Dirichlet Laplacian on I_k, and by

$$d_k = \sup_{x\in I_k} x^{2\alpha}, \qquad Q_m(t) = mt^{1/2}\mathrm{Tr}(\exp(-tH_k^D)),$$

$$V_m(x) = \sum_{k>0} d_k\cdot\chi_k(x), \qquad (9.8)$$

where χ_k is the characteristic function of the interval I_k. Putting additional

Dirichlet boundary conditions at the end points of intervals I_k, we get

$$t^{1/2+1/2\alpha}\mathrm{Tr}(\exp(-tA_D)) \geq t^{1/2+1/2\alpha}\sum_{k>0}\mathrm{Tr}(\exp(-tH_k^D))\sum_{n>0}\exp(-t(n\pi/2)^2 d_k)$$
$$\geq Q_m(t)t^{1/2\alpha}\sum_{n>0}\int_1^\infty \exp(-t(n\pi/2)^2 V_m(x))dx$$
$$= Q_m(t)\left(\frac{2}{\pi}\right)^{1/\alpha}\sum_{n>0}\left(\frac{1}{n}\right)^{1/\alpha}\int_{t^{1/2\alpha}(n\pi/2)^{1/\alpha}}^\infty \exp(-V_m(x))dx$$
$$\geq Q_m(t)\left(\frac{2}{\pi}\right)^{1/\alpha}\sum_1^N\left(\frac{1}{n}\right)^{1/\alpha}\int_{t^{1/2\alpha}(N\pi/2)^{1/\alpha}}^\infty \exp(-V_m(x))dx.$$

Using that

$$\lim_{t\to 0} Q_m(t) = \frac{1}{2\sqrt{\pi}},$$

we get

$$\liminf_{t\to 0} t^{1/2+1/2\alpha}\mathrm{Tr}(\exp(-tA_D)) \geq \frac{2}{\sqrt{\pi}}\left(\frac{2}{\pi}\right)^{1/\alpha}\sum_1^N\left(\frac{1}{n}\right)^{1/\alpha}\int_0^\infty \exp(-V_m(x))dx.$$

Letting $N\to\infty$ and $m\to\infty$, we obtain (9.7) and (9.5).

Case $\alpha = 1$: As before

$$\begin{aligned}\mathrm{Tr}(\exp(-tA_D)) &\leq \frac{1}{2\sqrt{\pi t}}\sum_{n>0}\int_1^\infty \exp(-t(n\pi/2)^2x^2)dx \\ &= \frac{1}{t\pi\sqrt{\pi}}\sum_{n>0}\frac{1}{n}\int_{\sqrt{t}n\pi/2}^\infty \exp(-x^2)dx.\end{aligned} \tag{9.9}$$

Split the positive integers into two sets, $I_1 = \{n : n\sqrt{t} \leq 2/\pi\}$ and $I_2 = \{n : n\sqrt{t} \geq 2/\pi\}$. We have

$$\begin{aligned}\sum_{n\in I_2}\frac{1}{n}\int_{\sqrt{t}n\pi/2}^\infty \exp(-x^2)dx &\leq \frac{\pi\sqrt{t}}{2}\sum_{n\in I_2}\exp(-\sqrt{t}n\pi/2) \\ &= O(1) \text{ as } t\to 0,\end{aligned} \tag{9.10}$$

$$\sum_{n\in I_1}\frac{1}{\pi\sqrt{\pi}}\int_{\sqrt{t}n\pi/2}^{\infty}\exp(-x^2)dx \le \frac{1}{2\pi}\sum_{n\in I_1}\frac{1}{n} \sim \frac{1}{4\pi}\ln t^{-1} \text{ as } t\to 0. \tag{9.11}$$

In (9.11) we used that $1+1/2+\ldots+1/n-\ln n\to\gamma$, as $n\to\infty$, where γ is the Euler constant. From (9.9), (9.10), (9.11) we get that

$$\limsup_{t\to 0} t(\ln t^{-1})^{-1}\mathrm{Tr}(\exp(-tA_D)) \le \frac{1}{4\pi}.$$

To prove that

$$\liminf_{t\to 0} t(\ln t^{-1})^{-1}\mathrm{Tr}(\exp(-tA_D)) \ge \frac{1}{4\pi}, \tag{9.12}$$

we proceed as follows. Let $I=\{n : n\sqrt{t}<2\epsilon/\pi\}$, and with notation (9.8) we have

$$\begin{aligned} t(\ln t^{-1})^{-1}\mathrm{Tr}(\exp(-tA_D)) &\ge Q_m(t)t^{1/2}(\ln t^{-1})^{-1}\sum_{n>0}\int_1^\infty \exp(-t(n\pi/2)^2V_m(x))dx \\ &= Q_m(t)\frac{2}{\pi}\sum_{n>0}\frac{1}{n}(\ln t^{-1})^{-1}\int_{\sqrt{t}n\pi/2}^{\infty}\exp(-V_m(x))dx \\ &\ge Q_m(t)\frac{2}{\pi}(\ln t^{-1})^{-1}\sum_{n\in I}\frac{1}{n}\int_\epsilon^\infty \exp(-V_m(x))dx. \end{aligned}$$

As $t\to 0$,

$$Q_m(t)\to\frac{1}{2\sqrt{\pi}}, \qquad (\ln t^{-1})^{-1}\sum_{n\in I}\frac{1}{n}\to\frac{1}{2},$$

and consequently,

$$\liminf_{t\to 0} t(\ln t^{-1})^{-1}\mathrm{Tr}(\exp(-tA_D)) \ge \frac{1}{2\pi\sqrt{\pi}}\int_\epsilon^\infty \exp(-V_m(x))dx.$$

Letting $\epsilon\to 0$ and $m\to\infty$, we obtain (9.12) and (9.6).

Appendix

If Ω is given by (7.3) and V by (7.5), let us make the following two hypotheses: For some $\epsilon > 0$,

$$|f'(x)| + f'(x)^2/f(x) = O(x^{-1-\epsilon})\,; \tag{HA1}$$

$$|V(x)| = O(x^{-1-\epsilon}). \tag{HA2}$$

Recently, Davies and Simon [DVSM] proved the following

Theorem A.1. If (HA1) and (HA2) are satisfied, we have

a) $\sigma_{\text{ac}}(H_N) = [0, \infty)$ of uniform multiplicity.

b) $\sigma_{\text{sing}}(H_N) = \emptyset$.

c) The pure point spectrum consists of a discrete set of eigenvalues, λ_n, each of finite multiplicity with $\lambda_n \to \infty$.

For example, (HA1) and (HA2) are satisfied if $f(x) = x^{-\beta}, \beta > 0$, or if $f(x) = \exp(-x^\alpha)$ for $0 < \alpha < 1/2$. On the other hand, if $1/2 \le \alpha \le 1$, (HA1) remains valid, but (HA2) does not; namely, V is not a short-range potential any more. (We remark that the case $\alpha = 1$ is somewhat special, because then $V = 1/4$; the argument of [DVSM] shows that Theorem A.1 remains valid with the stipulation that $\sigma_{\text{ac}}(H_N) = [1/4, \infty)$.) Anyhow, for $1/2 \le \alpha < 1$, V is certainly a long-range potential ([HOR4], [PR2]), and authors of [DVSM] conjectured "that it is likely that one can modify ...[their]... argument" to prove the analog of Theorem A.1. While it is certainly the case that Theorem A.1 remains valid if (HA2) is replaced with the sole condition that V is a long-range potential, the technicalities of the long-range scattering theory (whose role is to become clear soon) tend to obscure the simplicity and beauty of the argument in [DVSM]. There is, however, an important special case (which covers the above examples) which is easily technically tractable.

In the sequel, H_0 stands for the one-dimensional free Laplacian. Let $u(\theta) : L^2(\mathbf{R}) \to$

$L^2(\mathbf{R})$ be a unitary mapping defined as

$$u(\theta)\phi(x) = \exp(\theta/2)\phi(\exp(\theta)x).$$

A potential $\widehat{V}$, defined on the whole real line, is dilation-analytic ([PR2], [RS4]), if $\widehat{V}$ is H_0-compact and the operator-valued function

$$C(\theta) = u(\theta)\widehat{V}u(\theta)^{-1}(H_0+1)^{-1}$$

extends to an analytic operator-valued function on the strip $\mathcal{S}(a) = \{z : -a < \mathrm{Im}(z) < a\}$ for some $a > 0$.

We make the the following hypothesis on V, given by (7.5):

$$\begin{aligned} &V \text{ is a } C^\infty[1,\infty) \text{ function and all derivatives of } V \text{ are bounded;} \\ &|V'(x)| = O(x^{-1-\epsilon}). \end{aligned} \tag{HA3}$$

Define

$$\widehat{V}(x) = V(|x|+1), \qquad x \in \mathbf{R}.$$

Theorem A.2. If (HA1) and (HA3) are satisfied, and $\widehat{V}$ is a dilation-analytic potential, all three conclusions of Theorem A.1 remain valid.

Remark 1: The requirement that V be C^∞ with bounded derivatives is somewhat artificial, and can definitely be dropped by slightly extending the argument below (see Remark 3). Nevertheless, the assumption of dilation analyticity of $\widehat{V}$ is essential, and our proof does not extend to a larger class of potentials.

Example : If $f(x) = \exp(-x^\alpha)$ for $0 < \alpha < 1$,

$$\widehat{V}(x) = \frac{\alpha^2}{2}(|x|+1)^{2(\alpha-1)} - \frac{\alpha(\alpha-1)}{2}(|x|+1)^{\alpha-2},$$

and one easily checks that the conditions of Theorem A.2 are satisfied. The theorem also covers the case $f(x) = x^{-\beta}$, $\beta > 0$.

We will prove Theorem A.2 below, using ideas of Davies and Simon. Nevertheless, assuming additionally that f is a convex function for large x, Theorems A.1 and A.2 can both be proved using ideas developed in Chapter 2 (and indirectly ones from [DVSM], see also [FRHS]). Such an approach clarifies where the above result comes from, and we just sketch the main steps. Let us start again with the half-strip $M = (-1,1) \times (1,\infty)$ with the metric

$$ds_M^2 = dx^2 + f(x)^2 dx^2, \qquad (A.1)$$

and let $\widehat{H}_N$ be the Laplace-Beltrami operator on M with the Neumann boundary condition. Separating the variables, we obtain that $\widehat{H}_N$ is unitarily equivalent to $\bigoplus_{n\geq 0} H_n$, where H_n is given by (9.7). If V is bounded and $f(x) \to 0$, $\bigoplus_{n\geq 1} H_n$ will have a discrete spectrum and any nontrivial spectral behavior can come only from H_V. For V short- or long-range, all three conclusions of Theorem A.1 are valid. If Ω is given by (7.3), performing the same change of variable as in Section 8.4, we obtain the Laplace-Beltrami operator on M with a distorted metric (8.26), which is asymptotically of the form (A.1). Perturbations can be controlled as in Sections 8.3 and 8.4, and assuming (HA1), it is easy to show that the two Laplace-Beltrami operators, arising from the metrics (A.1), (8.26), are the short-range Enss-pair (see [PR2]), regardless of V being a short- or long-range potential. Now, $\widehat{H}_N$, the operator in the metric (A1), plays the role which is usually played by the free Laplacian. It causes no problems when potential V is short-range, because then H_V and H_0 are again the short-range Enss pair, and Theorem A.1 follows by a straightforward application of the short-range Enss theory [DVSM], [PR2]. In the long-range case the above strategy obviously does not apply. Neverthless, the uniform propagation estimates, which are valid for H_0 and which are the essential ingredient of the Enss theory, are now valid for H_V, *providing* V is dilation-analytic [PR2]. Then, a long-range modification of the Enss theory argument follows basically line by line the simple short-range case, and Theorem A.2 follows.

Instead of making the above argument rigorous, we will give a modification of the original Davies and Simon argument (in fact, since we are relying so heavily on the Enss theory, the discussion above can also be considered as a modification of their argument). The two approaches seem to be complementary and each of them reveals a part of the picture. The reader, already familiar with the change of variable trick, should see the other part of the story, namely, the direct spectral analysis approach of [DVSM].

Proof of Theorem A.2

Needless to say, our argument follows the one in [DVSM] almost line by line. Let H_V be the operator (8.5) with the Neumann boundary condition at 1, and denote by

$$D = \{\psi : \psi \in C^2[1,\infty), \psi'(1) = 0\}$$

its domain of essential self-adjointness. Let $J : L^2(R) \to L^2(\Omega)$ be the embedding

$$J\phi(x) = \phi(x)/\sqrt{2f(x)},$$

and denote $Q = 1 - JJ^*$. The following theorem is the backbone of Davies and Simon's, and hence our, argument.

Theorem A.3. [DVSM] If (HA1) is satisfied, we have:

a) If $\phi \in D$,

$$\|(H_N+1)^{-1/2}(H_N J - JH_V)\phi\| \leq 2 \cdot \|f'\phi\|_2 + \|(f')^2)/f)\phi\|_2 + C|\phi(1)|,$$

where C is a uniform constant.

b) $Q(H_N+1)^{-1/2}$ is a compact operator.

c) If g is a continuous function on $R \cup \{\infty\}$, $g(H_N)J - Jg(H_V)$ is a compact operator.

Remark 2: The part a) is independent of (HA1), and for parts b) and c) it suffices to assume that $f + (f')^2/f \to 0$. As we already remarked in the Introduction, the form of H_N, restricted to the subspace consisting of functions which depend on x-variable only, naturally yields the operator H_V. The control of perturbations, viewing H_N as a perturbation of H_V, is given by the above theorem. Having complete knowledge of the spectral properties of H_V, and with Theorem A.2 at hand, it is fairly obvious how to use the scattering theory to deduce spectral information about H_N. While we are going to use the time-dependent approach of Enss, as was done in [DVSM], one can equivalently use the stationary scattering theory, as in [PR1], [HOR], and presumably a modification of the Mourre theory, as in [FRHS]. While the above two approaches are somewhat more lengthy (and less elegant), they yield more information: One can construct a generalized eigenfunction expansion (see [PR2], [HOR]), and tackle the issue of the structure of the embedded eigenvalues. We are not going to discuss those methods here.

We now collect some standard results from the Enss theory. Extend V as an even function around the point $x = 1$. If $\widehat{H}_V$ is the operator (8.5) on the whole real line, its restriction to the subspace consisting of functions that are even around the point $x = 1$ coincides with H_V. Translating by 1, we observe that $\widehat{H}_V$ is unitarily equivalent to $H_0 + \widehat{V}$, which we also denote by $\widehat{H}_V$. Let A be a scale transformation around $x = 1$ (see [CFKS], [PR2]),

$$A = \frac{1}{2}((x-1)\cdot p + p\cdot(x-1)),$$

where $p = -iD = -i\partial/\partial x$ in an x-space representation. A is essentally self-adjoint on $C_0^\infty(R)$, its spectrum is purely absolutely continuous on $(-\infty, \infty)$, and A leaves invariant the subspace of functions that are even around 1. By $P_\pm$ we denote the spectral projections of A on $\pm(0,\infty)$, and by $P_\pm^a$ the spectral projections on $\pm(\pm a, \infty)$. Obviously, $P_+ + P_- = 1$. It is a standard result that (under conditions (HA1) and (HA3)) the operator H_V has no (strictly) positive eigenvalues, and that $\sigma_{\text{ac}}(H_V) = [0,\infty)$, $\sigma_{\text{sing}}(H_V) = \emptyset$. In the sequel we will use Enss' notation where $F(M)$ stands for the characteristic function of the set M, and P_{ac} will denote the spectral projection on the absolutely continuous subspace of H_V. Because of the view of H_V as a restriction of $\widehat{H}_V$ (keeping the above translation in mind), we have

Lemma A.4.

a) Let g be a C^∞ function with support in $[\alpha, \beta]$, $\alpha > 0$. Then for any $\delta > 0$, $N > 0$, and a,

$$\|F(1 \le x < |t|^{1-\delta}) \exp(-itH_V) g(H_V) P_\pm^a\| = O(|t|^{-N}) \qquad (A.2))$$

as $t \to \pm\infty$.

b) $\text{s} - \lim_{t\to\pm\infty} P^a_\pm \exp(-itH_V) = 0.$

Remark 3: For a proof we refer to [PR2], Theorem 12.4. The fact that $\widehat{V}$ is infinitely differentiable (and that its derivatives are bounded) is used in the proof. Strictly speaking, $\widehat{V}$ does not have to be differentiable at the point $x = 0$. Nevertheless, it is C^∞ away from 0, with derivatives that remain bounded on the whole real line, so a glance at the proof in [PR2] shows that it causes no difficulties. Another way of resolving the issue is to decompose $\widehat{V}$, using the Weierstrass transformation [PR2], into a smooth, long-range, dilation-analytic part and a short-range part. The short-range part will contribute to the estimate a) of Theorem A.3, while (A.2) certainly holds for the long-range part, and the argument below carries over without changes. Using the Weierstrass transform trick, one can also drop the assumption that V is C^∞.

The final preparative Lemma is the following

Lemma A.5. Let

$$S(R) = \|(H_N+1)^{-1/2}(HJ - JH_V)(H_V+1)^{-1}F(x > R)\|.$$

Then, if (HA1) is satisfied, $\int_0^\infty S(R)dR < \infty$.

Proof : The proof is standard, and follows line by line the argument of Lemma 5.4 in [CFKS]. Let j be a C^∞ function with $0 \le j(x) \le 1$ and $j(x) = 1$ for $x < 1/2$, $j(x) = 1$ for $x \ge 1$. Denote $j_R(x) = j(x/R)$. We have $j_R F(x \ge R) = F(x \ge R)$, and

$$[(H_V+1)^{-1}, j_R] = (H_V+1)^{-1}(D^2 j_R + Dj_R \cdot D)(H_V+1)^{-1}.$$

It is trivial to estimate $|D^2 j_R|, |Dj_R| \le (C/R)\cdot j_{R/2}$, and thus

$$\begin{aligned}
S(R) &\le \|(H_N+1)^{-1/2}(H_N J - JH_V)(H_V+1)^{-1}j_R\| \\
&\le \|(H_N+1)^{-1/2}(H_N J - JH_V)j_R(H_V+1)^{-1}\| + \\
&\qquad + \|(H_N+1)^{-1/2}(H_N J - JH_V)(H_V+1)^{-1}(D^2 j_R + Dj_R\cdot D)(H_V+1)^{-1}\| \\
&\le O(R^{-1-\epsilon}) + C'S(R/2)/R.
\end{aligned}$$

We used Theorem A.3 and (HA1) in the above estimates. Iterating the last inequality and using that $S(R)$ is bounded, we derive

$$S(R) \leq O(R^{-1-\epsilon}) + C''/R^2,$$

and the lemma follows. ∎

We now follow step by step the argument of [DVSM].

Step 1: $\mathrm{s} - \lim_{t\to\pm\infty} (H_N+1)^{-1/2} \exp(itH_N) J \exp(-itH_V) P_{\mathrm{ac}}$ exists.

Let us consider only the limit $t \to \infty$; a similar consideration applies to the other one. By Cook's criterion, it suffices to show that

$$\int_0^\infty \|(H_N+1)^{-1/2}(HJ - JH_V)\exp(-itH_V) g(H_V) P_+^a\| dt \leq \infty,$$

where g is as in Lemma A.4, since $\cup_{a,g} \mathrm{Ran} g(H_V) P_+^a$ is dense in $\mathcal{H}_{\mathrm{ac}}(H_V)$. Denote

$$A(t) = \|(H_N+1)^{-1/2}(HJ - JH_V)\exp(-itH_V) g(H_V) P_+^a\|.$$

Choosing $\delta < \epsilon$ in (A.2), we estimate, using Lemmas A.3 and A.4,

$$\begin{aligned} A(t) \leq & \|(H_N+1)^{-1/2}(HJ - JH_V)(H_V+1)^{-1} F(x \geq t^{-1-\delta})\| + \\ & + \|F(1 \leq x < t^{-1-\delta}) \exp(-itH_V)(H_V+1) g(H_V) P_+^a\| \\ \leq & \, O(t^{-1-\epsilon+\delta}) + O(t^{-2}). \end{aligned}$$

Step 2: The wave operators $\Omega^\pm = \mathrm{s} - \lim_{t\to\mp\infty} \exp(itH_N) J \exp(-itH_V) P_{\mathrm{ac}}$ exist.

$(H_N+1)^{-1/2} J - J(H_V+1)^{-1/2}$ is compact by Theorem A.3, and thus

$$\mathrm{s} - \lim_{t\to\mp\infty} \exp(-itH_N)((H_N+1)^{-1/2} J - J(H_V+1)^{-1/2}) \exp(-itH_V) P_{\mathrm{ac}} = 0.$$

By Step 1, $\Omega^\pm \phi$ exist if $\phi \in \mathrm{Ran}(H_V+1)^{-1/2} P_{\mathrm{ac}}$, and the last set coincides with $\mathcal{H}_{ac}(H_V)$.

Step 3: $(H_N+1)^{-1/2}(\Omega^\pm - J) g(H_V) P_\pm$ is a compact operator.

First, $(H_N+1)^{-1/2}(\exp(itH_N)J\exp(-itH_V)-J)g(H_V)P_\pm$ converges in the operator norm, and thus it suffices to show that each of these operators is compact. Such operators are finite integrals of the operators of the form

$$(H_N+1)^{-1/2}(HJ-JH_V)\exp(-itH_V)g(H_V)P_\pm, \tag{A.3}$$

and thus it suffices to show that operators (A.3) are compact. But it is a consequence of the part c) of Theorem A.3.

`Step 4:` If $\phi_n \in \mathcal{H}_{\mathrm{ac}}(H_N)^\perp$, with $\|(H_N+1)\phi_n\|$ bounded and $(H_N+1)^{1/2}\phi_n \to 0$ weakly, then $\|\phi_n\| \to 0$ as $n \to \infty$.

First, $(\Omega^\pm)^*\phi_n = 0$ for all n, and thus for any $C_0^\infty((0,\infty))$ function g, step 3 yields

$$P_\pm g(H_V)J^*\phi_n \to 0.$$

Since $P_+ + P_- = 1$ and $g(H_V)J^* - J^*g(H_N)$ is a compact operator, we obtain that $J^*g(H_V)\phi_n \to 0$. Since $\|(H_N+1)\phi_n\|$ is bounded, we estimate

$$\|g(H_N)\phi_n - \phi_n\| \leq C\|g(H_N)-1\|. \tag{A.4}$$

Since g is arbitrary, the left-hand side of (A.4) can be made arbitrarily small, and thus $J^*\phi_n \to 0$, and so $JJ^*\phi_n \to 0$. By Theorem A.3, $Q\phi_n = (1-JJ^*)\phi_n \to 0$, and we conclude that $\phi_n \to 0$.

`Step 5:` $\sigma_{\mathrm{sing}}(H_N) = \emptyset$ and in any finite interval H_N has only finitely many eigenvalues.

If any of the statements is not valid, we can construct an orthonormal sequence ϕ_n so that $\phi_n \in \mathcal{H}_{\mathrm{ac}}(H_N)^\perp$, $\|(H_N+1)\phi_n\|$ is bounded, and $(H_N+1)^{1/2}\phi_n \to 0$ weakly. Step 4 implies then that $\phi_n \to 0$, which contradicts the fact that the sequence ϕ_n is orthonormal.

`Step 6:` $\sigma_{\mathrm{ac}}(H_N)$ has multiplicity one.

It suffices to show that $\mathrm{Ran}\,\Omega^+ = \mathcal{H}_{\mathrm{ac}}(H_N)$. Suppose that it is not, namely that we can find a non-zero vector $\phi \in \mathcal{H}_{\mathrm{ac}}(H_N) \cap (\mathrm{Ran}\,\Omega^+)^\perp \cap D(H_N)$. Define $\phi_n = \exp(-inH_N)\phi$.

The part b) of Lemma A.4 yields

$$P_{\pm}(\Omega^{-})^{*}\phi_{n} = P_{\pm}\exp(-inH_{V})P_{\mathrm{ac}}(\Omega^{-1})^{*}\phi \to 0, \qquad \text{as } n \to \infty.$$

Thus, as in the step 4, $\|\phi_n\| \to 0$, and we derive that $\phi = 0$, a contradiction.

`Step 7:` There exists a discrete set of embedded eigenvalues.

This is a consequence of symmetry of Ω with respect to the axes $x = 0$. Let E be the subspace of $L^2(\Omega)$ consisting of those functions that are even under reflection $(x, y) \to (x, -y)$. That subspace is invariant under Q and H_N and thus H_N restricted to it has a compact resolvent, by Theorem A.3.

Part III

Spectral Properties of Random Schrödinger Operators with Unbounded Potentials

Chapter 10: Introduction

It is already a part of folklore that multiplicative perturbations of the Anderson model show rather "unusual" spectral behavior. The basic paradigm is the discrete Schrödinger operator on $l^2(\mathbf{Z}^1)$

$$H_\omega = H_0 + V_\omega(n), \qquad V_\omega(n) = \lambda \xi_n(\omega)|n|^\alpha,$$

$$H_0 u(n) = 2u(n) - u(n+1) - u(n-1),$$

where $\xi_n(\omega)$ are independent random variables with bounded, compactly supported density $r(x)$, and λ is a parameter. For $\alpha < 0$, the above model has been extensively studied in [SIM7], [DSS1], [DSS2], [DEY], and their main results can be summarized as follows (note that for $\alpha < 0$, $V_\omega(n) \to 0$ as $|n| \to \infty$ and thus $\sigma_{\text{ess}}(H_\omega) = [0,4]$).

Theorem With probability 1 :

(a) For $-1/2 < \alpha < 0$, spectrum in $[0,4]$ is pure point with eigenfunctions decaying as $\exp(-C|n|^{1+2\alpha})$.

(b) For $\alpha < -1/2$, spectrum in $[0,4]$ is purely absolutely continuous.

(c) For $\alpha = -1/2$ and λ large, spectrum in $[0,4]$ is pure point with polynomially decaying eigenfunctions, while for λ small H_ω will have some singular continuous spectrum.

For $\alpha > 0$, $|n|^\alpha \to \infty$, but this does not imply that spectrum is necessarily discrete: If $r(x)$ does not vanish in some neighborhood of 0, ξ_n can get arbitrarily small with positive probability and thus eventually compensate for growth of $|n|^\alpha$ within infinitely many sites. That in turn can lead to a nontrivial spectral behavior. Let us consider the simplest case when ξ_n are independent random variables uniformly distributed on $[0,1]$: It was shown in [GMO] that for a. e. ω, H_ω will have a discrete spectrum if and only if $\alpha > 1$. Furthermore, if $d/k \geq \alpha > d/(k+1)$, $\sigma_{\text{ess}}(H_\omega) = [a_k, \infty)$, where a_k is a strictly decreasing sequence of positive numbers, $\sigma(H_\omega) = \sigma_{\rm pp}(H_\omega)$, and the eigenfunctions decay superexponentially. Thus, while for $\alpha < 0$ the essential spectrum is always $[0,4]$ with a phase transition in its nature at $\alpha_c = -1/2$, for $\alpha > 0$, the essential spectrum is always pure point but its endpoints are piecewise constant functions of the parameter α(!). In this part we are interested in obtaining the multidimensional analog of the above results when $\alpha > 0$; namely, we will study the operator

$$H_\omega = H_0 + \xi_n(\omega)(1 + |n|^\alpha), \qquad \alpha > 0, \tag{10.1}$$

acting on $l^2(\mathbf{Z}^d)$. In (10.1), $|n| = (\sum n_i^2)^{1/2}$, $\xi_n(\omega)$ are independent, random variables uniformly distributed on $[0,1]$, and

$$H_0\phi(n) = \sum_{|n-m|_+=1} \phi(n) - \phi(m), \qquad \|H_0\| = 4d, \tag{10.2}$$

where $|n|_+ = \sum |n_i|$. We view $\xi_n(\omega)$ as a random field on $\bigotimes_{n\in\mathbf{Z}^d}[0,1] = \Omega$, and denote by P the corresponding probability measure, and by $\mathbf{E}$ the mathematical expectation on Ω. Before stating our main results, we introduce some notation. For $X \subset \mathbf{Z}^d$ denote by $\mathrm{C_{fin}}(X)$ the set of all $\phi \in l^2(\mathbf{Z}^d)$ with support in X. Let $\mathcal{D}$ be the form associated to H_0,

$$\mathcal{D}(\phi) = \sum_{\substack{\langle n,m\rangle \\ |n-m|_+=1}} |\phi(m) - \phi(n)|^2, \tag{10.3}$$

where $\langle n, m\rangle$ reminds that each pair appears only once in the summation. Denote

$$\Lambda(X) = \inf_{\substack{\|\phi\|=1 \\ \phi\in \mathrm{C_{fin}}(X)}} \mathcal{D}(\phi).$$

If $\#X < \infty$, $\Lambda(X)$ is the smallest eigenvalue of the spectral problem

$$H_0\phi = \lambda\phi, \qquad \phi(n) = 0 \text{ if } n \in \mathbf{Z}^d \setminus X.$$

Following [GR], we say that a set $A_k \subset \mathbf{Z}^d$ is a k-animal (or just animal) if A_k is connected and $\#A_k = k$. Modulo translation, there are only finitely many animals of the size k. Let

$$a_k = \inf_{A_k} \Lambda(A_k). \tag{10.4}$$

Obviously, a_k is a strictly decreasing sequence of positive numbers. Those animals for which the infimum in (10.4) is attained we will denote by $A_{T,k}$ and call them tamed animals. As we will see later, taming the animals (namely, obtaining control over a_k, $A_{T,k}$) is not an easy task at all.

In the sequel, $f(x) \sim g(x)$ stands for $\lim_{x\to\infty} f(x)/g(x) = 1$. With the above notation, our main results are stated as follows.

Theorem 10.1. H_ω has a discrete spectrum $P-$a.s. if and only if $\alpha > d$. Furthermore, if $N_\omega(E)$ denotes the number of eigenvalues of H_ω that are less then E, we have that for $\alpha > d$ and for a. e. ω

$$N_\omega(E) \sim \frac{\tau_d}{\alpha - d} \cdot E^{d/\alpha}, \tag{10.5}$$

where τ_d denotes the volume of a unit ball in $\mathbf{R}^d$.

Theorem 10.2. If $d/k \geq \alpha > d/(k+1)$ for positive integer k, we have for a. e. ω

a) $\sigma_{\text{ess}}(H_\omega) = [a_k, \infty)$

b) $\sigma_{\text{ac}}(H_\omega) = \emptyset$.

Theorem 10.3.(A. Gordon) Let λ_D be the lowest eigenvalue of a Dirichlet Laplacian of a unit ball in $\mathbf{R}^d$. Then

$$a_k \sim k^{-d/2} \cdot \lambda_D.$$

Remark 1: Only affecting the values of constants, we can suppose random variables ξ_n have common nonnegative absolutely continuous density which is of the form x^β on $[0, \delta)$ for some $\beta, \delta > 0$. On the other hand if ξ_n are uniformly distributed on $[-1, 1]$, Theorem 10.1 remains valid (with appropriate reformulation of (10.5)), while part a) of Theorem 10.2 has to be replaced with $\sigma(H_\omega) = (-\infty, \infty)$ (part b) also remains valid).

Remark 2: The constant λ_D, introduced in Theorem 10.3, coincides with the smallest zero of the Bessel function $J_{d/2-1}$. So, if $d = 2$, $\lambda_D = 2.4048...$, if $d = 3$, $\lambda_D = \pi$ and $\lambda_D \sim d/2$ for d large.

The above results are the first part of a program of investigation of random

Schrödinger operators with nonstationary potentials. Already for the model (10.1) we have right now much more detailed spectral information. In [GJMS] we will show that $\sigma(H_\omega) = \sigma_{\text{pp}}(H_\omega)$ with superexponentially decaying eigenfunctions and that $\#\sigma_{\text{disc}}(H_\omega) < \infty$ for typical ω. In [GJMS] we also study the integrated density of states of H_ω. These results are somewhat technically involved and we will not discuss them here (partly because some details still have to be worked out).

The continuous analog of the above theorems exists and will be discussed in Chapter 13.

We finally remark that Theorem 10.3 is entirely a contribution of A. Gordon. Although the author has previously proven the continuous analog of it, Theorem 13.3, he even had a wrong conjecture for the discrete case! For the sake of completeness, Gordon's beautiful result is included here.

Chapter 11: On the Discrete and Essential Spectrum

This chapter is devoted to proofs of Theorems 10.1 and 10.2.

11.1. On the Essential Spectrum

In this section we prove that for a. e. ω, H_ω has discrete spectrum iff $\alpha > d$ and that for $d/k \geq \alpha > d/(k+1)$, $\sigma_{\text{ess}}(H_\omega) = [a_k, \infty)$.

A sufficient and necessary condition for $H_0 + V_\omega(n)$ to have discrete spectrum is that

$$|V_\omega(n)| \to \infty \text{ as } |n| \to \infty. \tag{11.1}$$

Let $c > 0$ be fixed and denote

$$A_n^c = \{\omega : \xi_n(\omega) \cdot (1 + |n|^\alpha) < c\}.$$

$P(A_n^c) = c/(1+|n|^\alpha)$ and $\sum_n P(A_n^c)$ converges if and only if $\alpha > d$. Borel-Cantelli lemma implies that (11.1) holds iff $\alpha > d$, and thus the first part of Theorem 10.1 follows.

Let us suppose that $d/k \geq \alpha > d/(k+1)$. Denote $I = 2k \cdot \mathbf{Z}^d$, and decompose $\mathbf{Z}^d = \cup_{n \in I} \mathcal{J}_n$, where $\mathcal{J}_n$ is the cube of volume $(2k)^d$ centered at n. Let A_T be an arbitrary tamed k-animal that contains 0, and denote by A_T^n its translation by the vector $n \in I$. To show that

$$\sigma_{\text{ess}}(H_\omega) \supset [a_k, \infty) \qquad P\text{-a.s.} \tag{11.2}$$

it suffices (using Weyl's criterion and the fact that the essential spectrum is a closed set) to construct for every rational $\lambda > 0$ and for a. e. ω a sequence φ_i, satisfying

$$\lim_{i \to \infty} \|(H_\omega - \lambda - a_k)\varphi_i\| = 0. \tag{11.3}$$

Fix a sequence $b_i \to 0$, and denote for $n \in I$

$$A_n^{b_i} = \{\omega : \lambda - b_i < V_\omega(x) < \lambda + b_i \text{ for } x \in A_T^n\}.$$

$P(A_n^{b_i}) \geq b_i C/(1 + |n|^\alpha)^k$ for a suitable uniform constant C, and thus $\sum_{n\in I} P(A_n^{b_i})$ diverges. The Borel-Cantelli lemma and diagonal argument implies that there exists with probability 1 a strictly increasing (ω-dependent) sequence n_i such that

$$|V_\omega(n) - \lambda| < b_i \qquad \text{for } n \in A_T^{n_i}.$$

If φ_0 is an eigenfunction corresponding to a_k, set φ_0 to be zero outside A_T and denote $\varphi_i(n) = \varphi_0(n - n_i)$. It is trivial to check that (11.3) is satisfied and (11.2) follows.

It remains to show that

$$\inf \sigma_{\text{ess}}(H_\omega) \geq a_k \qquad P\text{-a.s.} \tag{11.4}$$

The following simple lemma is the backbone of our argument.

Lemma 11.1. For $\gamma > 0$ let

$$B_n = \{\omega : \text{in the ball } B(n, |n|^\gamma) \text{ there exist } k+1 \text{ points } n_i \text{ such that } V_\omega(n_i) \leq |n_i|^\gamma\}. \tag{11.5}$$

Then, for γ small enough, with probability 1, only finitely many events B_n take place.

Proof : It is easy to show that for γ small enough

$$P(B_n) \leq C \cdot |n|^{(k+1)(d\gamma+\gamma-\alpha)} \leq C|n|^{-d-\epsilon},$$

where C is a uniform constant. Thus, for such γ, $\sum_n P(B_n) < \infty$, and the Borel-Cantelli lemma implies the statement. ∎

The discrete version of Persson theorem ([CFKS], Theorem 3.12) states

$$\inf \sigma_{\text{ess}}(H_\omega) = \sup_{\substack{K\subset \mathbf{Z}^d \\ \#K<\infty}} \inf_{\substack{\phi\in C_{\text{fin}}(\mathbf{Z}^d\setminus K) \\ \|\phi\|=1}} (\phi, H_\omega\phi).$$

Let K be a ball, centered at 0, of large enough radius so that outside K no event B_n takes place for a. e. ω. Let

$$R = \inf_{n \notin K} |n|^\gamma,$$

and let

$$A_\omega = \{n \in \mathbf{Z}^d \setminus K \,:\, V_\omega(n) < 1\}.$$

For a. e. ω, A_ω is a disjoint union of animals of size $\# \leq k$. Let $B = \mathbf{Z}^d \setminus (K \cup A_\omega)$, and for $\phi \in C_{\text{fin}}(\mathbf{Z}^d \setminus K)$, $\|\phi\| = 1$ denote

$$\phi_1 = \begin{cases} \phi(n), & \text{if } n \in A_\omega; \\ 0, & \text{otherwise;} \end{cases} \qquad \phi_2 = \begin{cases} \phi(n), & \text{if } n \in B_\omega; \\ 0, & \text{otherwise.} \end{cases}$$

Obviously,

$$(\phi_1, \phi_2) = 0, \qquad \|\phi_1\|^2 + \|\phi_2\|^2 = 1.$$

For $R > a_k$, we have

$$\begin{aligned}
(H_\omega\phi, \phi) &= (H_\omega\phi_1, \phi_1) + (H_\omega\phi_2, \phi_2) + 2\text{Re}(H_\omega\phi_1, \phi_2) \\
&\geq a_k\|\phi_1\|^2 + R\|\phi_2\|^2 + 2\text{Re}(H_\omega\phi_1, \phi_2) \\
&\geq a_k + (R - a_k)\|\phi_2\|^2 - 2\|H_0\| \cdot \|\phi_1\| \cdot \|\phi_2\| \\
&\geq a_k - \frac{16d^2}{R - a_k}.
\end{aligned}$$

Consequently,

$$\inf \sigma_{\text{ess}}(H_\omega) \geq a_k - \frac{16d^2}{R - a_k} \qquad P-\text{a.s.}$$

By taking K big enough, R can be made arbitrarily large and (11.4) follows.

11.2. Absence of Absolutely Continuous Spectrum

The following simple consequences of Lemma 11.1 will be of use below (and are of essential importance in [GJMS], where we prove localization). Let $d/k \geq \alpha > d/(k+1)$, and for a suitable γ let

$$A_\omega = \{\, n \,:\, V_\omega(n) \leq |n|^\gamma\}.$$

According to Lemma 11.1, for a. e. ω we have a decomposition

$$A_\omega = \bigcup_{n\geq 0} A(n,\omega), \qquad A(n,\omega)\cap A(m,\omega) = \emptyset.$$

(In the sequel we drop the ω-dependence, which is clear within the context.) $A(0)$ is a finite region chosen in such a way that for $n \notin A(0)$, no events B_n take place (see (11.5)), and $A(n)$ are animals of size $\leq k$. For $X, Y \subset \mathbf{Z}^d$, we define

$$d(X,Y) = \min\{\,|s-s'|\,:\, s\in X,\, s'\in Y\},$$

and let $\sim$ be a relation of equivalence on $\{A(n)\,:\, n>0\}$ defined as

$$A(n)\sim A(m) \Leftrightarrow (\exists\, n_1 = n, n_2, \ldots, n_l \text{ such that}$$
$$d(A(n_i), A(n_{i+1})) \leq C\max\{\,|s|^\gamma,\, |s'|^\gamma \,:\, s\in A(n_i),\, s'\in A(n_{i+1})\},$$

for a suitable constant C. Let $G^{(i)}$ be the union of the elements of the i-th class of equivalence. By taking C small enough, it is trivial to show that $\#G^{(i)} \leq k$ (otherwise some event B_n happens for $n\notin A(0)$) and that for $i\neq k$

$$d(G^{(i)}, G^{(k)}) > C\max\{\,|s|^\gamma,\, |s'|^\gamma \,:\, s\in G^{(i)},\, s'\in G^{(k)}\}.$$

The point of the above is the following. Think about $G^{(i)}$ as potential wells. Then, for typical ω and outside a finite (ω-dependent) set, wells have no more then k points and are separated by high and long potential barriers. These barriers make tunneling difficult, and one should expect that (at least) there is no a. c. spectrum. That intuition is very close to the one in [SIMSP], where among others the following (deterministic) theorem was proven.

Theorem 11.2. Let $\{C_n\}_{n=1}^\infty$ be a sequence of disjoint cubes in $\mathbf{Z}^d$ of side l_n and let $d_n = d(C_n, C_m)$. Suppose that potential V satisfies

$$V(k)\geq 0 \text{ for } \qquad k\notin \bigcup_{n\geq 1} C_n,$$

and that, for any $\epsilon > 0$,

$$\sum_n l_n^{d-1}\exp(-\epsilon d_n) < \infty.$$

Then

$$\sigma_{\rm ac}(H_0+V)\cap(-\infty,0)=\emptyset.$$

The above theorem is quite general. For example, its immediate consequence is that if in addition we have

$$\lim_{\substack{|m|\to\infty\\ m\notin\cup C_n}} V(m)=\infty, \tag{11.6}$$

then

$$\sigma_{\rm ac}(H_0+V)=\emptyset. \tag{11.7}$$

Thus, that in our model we have

$$\sigma_{\rm ac}(H_\omega)=\emptyset \qquad P\text{-a.s.} \tag{11.8}$$

can be shown as follows. To every $G^{(i)}$ we associated the point $n_i\in G^{(i)}$ in such a way that $G^{(i)}$ is contained in cube C_i, centered at n_i and of side $C|n_i|^\gamma$, and moreover

$$d(C_i,C_j)\geq D\max\{|n_i|^\gamma,|n_j|^\gamma\}. \tag{11.9}$$

Since for every p and any $\epsilon>0$,

$$\sum_{n\in\mathbf{Z}^d}|n|^p\exp(-\epsilon|n|^\gamma)<\infty,$$

the result follows.

11.3. Proof of Theorem 10.1

To calculate the eigenvalue asymptotics, first note that monotonicity of $N_\omega(E)$ implies that it is enough to consider the case when $E\to\infty$ is an integer. We proceed as follows. Denote by

$$\chi_E^{\pm}(n,\omega)=\begin{cases}1, & \text{if } \xi_n(\omega)\cdot(1+|n|^\alpha)\leq E\pm 4d;\\ 0, & \text{otherwise.}\end{cases}$$

and set $S_E^{\pm}(\omega)=\sum_{n\in\mathbf{Z}^d}\chi_E^{\pm}(n,\omega)$. Because $\|H_0\|=4d$, we have

$$S_E^-(\omega)\leq N_\omega(E)\leq S_E^+(\omega).$$

Since

$$E(S_E^{\pm}) = \#\{n : (1+|n|^\alpha) \le E \pm 4d\} + \sum_{n:1+|n|^\alpha > E\pm 4d} \frac{E \pm 4d}{1+|n|^\alpha},$$

one easily obtains

$$\begin{aligned}\lim_{E\to\infty} E^{-d/\alpha}\mathbf{E}(S_E^{\pm}) &= \tau_d + \int_{|x|>1} \frac{1}{|x|^\alpha}\,dx \\ &= \frac{\tau_d}{\alpha - d}.\end{aligned} \tag{11.10}$$

It remains to show that

$$E^{-d/\alpha}(S_E^{\pm} - \mathbf{E}(S_E^{\pm})) \to 0 \text{ as } E \to \infty \ P\text{-a.s.} \tag{11.11}$$

First note that

$$\mathbf{E}((S_E^{\pm})^k) \le 2^{k-1} \cdot \left((\#\{n : (1+|n|^\alpha) < E \pm 4d\})^k + \sum_{\substack{(n_1,\dots,n_k)\\ n_i > E\pm 4d}} \frac{E \pm 4d}{\prod_{i=1}^k (1+|n_i|^\alpha)} \right)$$

and thus (as in (11.11)) $\limsup_{E\to\infty} E^{-dk/\alpha}\mathbf{E}((S_E^{\pm})^k) \le C$, where C is a uniform constant. Let $\eta_E^{\pm}(n,\omega) = \chi_E^{\pm}(n,\omega) - \mathbf{E}(\chi_E^{\pm}(n,\omega))$. $\eta_E^{\pm}(n)$ is a sequence of independent (but not identically distributed) random variables satsfying $|\eta_E^{\pm}(n)| \le 2$, $\mathbf{E}(\eta_E^{\pm}(n)) = 0$. We have

$$\begin{aligned}\mathbf{E}((S_E^{\pm} - E(S_E^{\pm}))^{2k}) &= \mathbf{E}((\sum_{n\in\mathbf{Z}^d} \eta_E^{\pm}(n))^{2k}) \\ &\le C \cdot \mathbf{E}((S_E^{\pm})^k) \\ &\le C \cdot E^{dk/\alpha}\end{aligned} \tag{11.12}$$

for a uniform constant C. The first inequality in (11.13) follows from simple combinatorics and the observations that

$$\#\{\, n\ : \eta_E^{\pm}(n,\omega) \ne 0\} \le S_E^{\pm} \qquad \mathbf{E}(\sum_{n\in\mathbf{Z}^d} \eta_E^{\pm}(n)) = 0,$$

(see also Section 13.2) For $\epsilon > 0$, the Chebyshev inequality yields

$$\begin{aligned}P_E = P\{E^{-d/\alpha}|S_E^{\pm} - \mathbf{E}(S_E^{\pm})| > \epsilon\} &\le \frac{E^{-2dk/\alpha}\mathbf{E}((S_E^{\pm} - \mathbf{E}(S_E^{\pm}))^{2k})}{\epsilon^{2k}} \\ &\le C\frac{E^{-dk/\alpha}}{\epsilon^{2k}}.\end{aligned}$$

If $dk/\alpha > 1$, $\sum_{E=4d+1}^{\infty} P_E < \infty$ (remember, E was an integer), and Borel-Cantelli Lemma yields (11.12).

Chapter 12: Taming the Animals

This chapter is devoted to A. Gordon's proof of Theorem 10.3.

We start by introducing the continuous analog of the (10.3). If Ω is a region in $\mathbf{R}^d$, the Dirichlet Laplacian $-\Delta_D^\Omega$ is the unique self-adjoint operator whose quadratic form is given by the closure of

$$D(u) = \int_\Omega |\nabla u|^2 \, dx$$

on $C_0^\infty(\Omega)$. In the sequel we will suppose that all regions under consideration have a piecewise smooth boundary. If $|\Omega|$, the Lebesgue measure of Ω, is finite, $-\Delta_D^\Omega$ has a compact resolvent, and its smallest eigenvalue is given by

$$\Lambda(\Omega) = \inf_{\substack{u \in C_0^\infty(\Omega) \\ \|u\|=1}} D(u). \tag{12.1}$$

The corresponding eigenfunction u is a $C^\infty(\Omega)$ function satisfying

$$-\Delta u(x) = \Lambda(\Omega) u(x) \quad \text{for } x \in \Omega, \qquad u(x) = 0 \quad \text{if } x \in \partial\Omega.$$

It is also known that $u(x) > 0$ for $x \in \Omega$. For positive r let

$$\lambda_r = \inf\{\Lambda(\Omega) : |\Omega| = r\}. \tag{12.2}$$

The infimum in (12.2) is achieved when Ω is a ball of volume r [CH], $\lambda_1 = \lambda_D$ and $\lambda_r = \lambda_D / r$. For notational simplicity, in the sequel we will suppose that $d = 2$. We will prove

Lemma 12.1.

$$a_k \le \frac{\lambda_D}{k} \cdot \left(1 + O(1/\sqrt{k})\right).$$

Lemma 12.2.

$$a_k \ge \frac{\lambda_D}{k} \cdot \frac{1 + O(1/\sqrt{k})}{1 + 3 \cdot \#\partial A_{T,k}/k}.$$

Lemma 12.3. If $A_{T,k}$, $k \geq 1$ is a sequence of tamed k-animals, we have

$$\lim_{k\to\infty} \frac{\#\partial A_k}{k} = 0.$$

Theorem 10.3 is an immediate consequence of the above three lemmas. Their proofs are somewhat subtle and we devote to each a separate section.

12.1. Proof of Lemma 12.1

To avoid confusion, throughout the chapter we use Latin letters to denote elements of $L^2(\mathbf{R}^d)$, and Greek letters for elements of $l^2(\mathbf{Z}^d)$. By $\|\cdot\|_\infty$ we denote the norm on $\mathbf{R}^2$ given by $\|(\varepsilon_1,\varepsilon_2)\|_\infty = \max\{|\varepsilon_1|,|\varepsilon_2|\}$. To any subset X of $\mathbf{Z}^2$ we correspond a region X_a in $\mathbf{R}^2$ whose closure is given by

$$\overline{X}_a = \{x \in \mathbf{R}^2 : \sup_{y\in X} \|x-y\|_\infty \leq a\}. \tag{12.3}$$

If A_k is an arbitrary animal, $A_{k,1/2}$ is the region given by (12.3) with $a = 1/2$. For $\Lambda(A_{k,1/2})$ given by (12.1), we denote the corresponding eigenfunction by u and set $u(x) = 0$ if $x \notin A_{k,1/2}$. To every $x \in F = \{x \in \mathbf{R}^2 : \|x\|_\infty < 1/2\}$, we associate a function ϕ_x on $\mathbf{Z}^2$ so that

$$\phi_x(n) = u(n+x), \qquad n \in \mathbf{Z}^2.$$

Obviously, $\phi_x(n) \neq 0$ iff $n \notin A_k$. Furthermore,

$$\int_F \|\phi_x\|^2 dx = \int_F \sum_n u(n+x)^2\, dx = \sum_n \int_F u(n+x)^2\, dx = \|u\|. \tag{12.4}$$

Let $e_1 = (1,0)$, $e_2 = (0,1)$. We have for $i = 1,2$

$$\begin{aligned}\int_F \sum_n (\phi_x(n+e_i) - \phi_x(n))^2\,dx &= \sum_n \int_F (u(n+x+e_i) - u(n+x))^2\,dx \\ &= \sum_n \int_F \left(\int_0^1 \frac{\partial u(n+x+te_i)}{\partial x_i} dt \right)^2 dx \\ &\leq \int_0^1 \sum_n \int_F \left(\frac{\partial u(n+x+te_i)}{\partial x_i} \right)^2 dt\,dx \\ &= \int_{\mathbf{R}^2} \left(\frac{\partial u(x)}{\partial x_i} \right)^2 dx.\end{aligned}$$

Summing over i we obtain

$$\int_F \mathcal{D}(\phi_x)dx \leq D(u), \tag{12.5}$$

and consequently there exists at least one $x_0 \in F$ such that

$$\mathcal{D}(\phi_{x_0}) \leq D(u) = \Lambda(A_{k,1/2})\|u\|^2 = \Lambda(A_{k,1/2})\|\phi_{x_0}\|^2.$$

It is immediate that

$$a_k \leq \Lambda(A_k) \leq \Lambda(A_{k,1/2}).$$

Let $a > 1/\sqrt{2}$ be arbitrary, and denote by $B(r)$ the ball of radius r centered at 0. For k large enough let $S = B(\sqrt{k/\pi} - a) \cap \mathbf{Z}^2$. We have

$$\#S = |S_{1/2}| \leq |B(\sqrt{k/\pi} - a + 1/\sqrt{2})| < |B(\sqrt{k/\pi})| = k, \tag{12.6}$$

and so there exists a k-animal A_k that contains S. We have

$$A_{k,1/2} \supset S_{1/2} \supset B(\sqrt{k/\pi} - a - 1/\sqrt{2}),$$

and consequently,

$$\begin{aligned} a_k \le \Lambda(A_{k,1/2}) &\le \Lambda(B(\sqrt{k/\pi} - a - 1/\sqrt{2})) \\ &= \frac{\lambda_D}{\pi(\sqrt{k/\pi} - a - 1/\sqrt{2})^2} \\ &= \frac{\lambda_D}{k}(1 + O(1/\sqrt{k})). \end{aligned}$$

The lemma follows.

12.2. Proof of Lemma 12.2

Let $A_k \subset \mathbf{Z}^2$ be an arbitrary animal, and let ϕ be the normalized eigenfunction corresponding to $\Lambda(A_k)$. We extend ϕ to a continuous function $u : \mathbf{R}^2 \to \mathbf{R}$ in the following way: $u(k) = \phi(k)$ if $k \in \mathbf{Z}^2$, and on each quadrant $Q_{ij} = \{(x_1, x_2) : i \le x_1 \le i+1,\ j \le x_2 \le j+1\}$, u is of the form

$$u(x_1, x_2) = a_{ij} + b_{ij}x_1 + c_{ij}x_2 + d_{ij}x_1x_2.$$

Such extension exists and is unique. We divide the rest of the argument into three steps.

`Step 1:` $D(u) \le \mathcal{D}(\phi)$.

The change of variable $\varepsilon_1 = x_1 - i - 1/2$, $\varepsilon_2 = x_2 - j - 1/2$ transforms Q_{ij} into the quadrant $Q = \{(\varepsilon_1, \varepsilon_2) : |\varepsilon_1| \le 1/2, |\varepsilon_2| \le 1/2\}$, and $u(x)$ into the function

$$U(\varepsilon) = h + a\varepsilon_1 + b\varepsilon_2 + c\varepsilon_1\varepsilon_2,$$

for suitable i, j -dependent constants h, a, b, c. We have

$$\int\limits_{Q_{ij}} \left(\frac{\partial u}{\partial x_1}\right)^2 dx = \int\limits_{Q} \left(\frac{\partial U}{\partial \varepsilon_1}\right) d\varepsilon = \int\limits_{Q} (a + c\varepsilon_2)^2 d\varepsilon = a^2 + c^2/12, \tag{12.7}$$

and

$$\frac{1}{2}(u(i+1,j) - u(i,j))^2 + (u(i+1,j+1) - u(i,j+1)^2) =$$
$$= \frac{1}{2}\left((U(1/2,-1/2) - U(-1/2,-1/2))^2 + (U(1/2,1/2) - U(-1/2,1/2))^2\right)$$

$$= \frac{1}{2}((a - c/2)^2 + (a + c/2)^2) = a^2 + c^2/4. \tag{12.8}$$

From (12.7), (12.8) we obtain, summing over i, j,

$$\int_{\mathbf{R}^2} \left(\frac{\partial u}{\partial x_1}\right)^2 dx \le \sum_{i,j} (u(i+1,j) - u(i,j))^2, \tag{12.9}$$

and similarly

$$\int_{\mathbf{R}^2} \left(\frac{\partial u}{\partial x_2}\right)^2 dx \le \sum_{i,j} (u(i,j+1) - u(i,j))^2. \tag{12.10}$$

The result follows by adding (12.9), (12.10).

Step 2: $\|u\|^2 \ge 1 - 3\Lambda(A_k)/4$.

First, note that

$$\begin{aligned}\int_{Q_{i,j}} u(x)^2 dx &= \int_Q (h + a\varepsilon_1 + b\varepsilon_2 + c\varepsilon_1\varepsilon_2)^2 d\varepsilon_1\, d\varepsilon_2 \\ &= h^2 + (a^2 + b^2)/12 + c^2/24 \\ &\ge h^2 = u(i + 1/2, j + 1/2)^2.\end{aligned}$$

Consequently,

$$\|u\|^2 \ge \sum_{i,j} u(i + 1/2, j + 1/2)^2. \tag{12.11}$$

Let $\widehat{\mathbf{Z}}^2$ be a dual lattice of $\mathbf{Z}^2$, obtained by translating $\mathbf{Z}^2$ by the vector $(1/2, 1/2)$. Let $T : l^2(\mathbf{Z}^2) \to l^2(\widehat{\mathbf{Z}}^2)$ be the averaging operator defined as

$$T\psi(i + 1/2, j + 1/2) = \frac{1}{4} \sum_{\pm,\pm} \psi(i + 1/2 \pm 1/2, j + 1/2 \pm 1/2).$$

From its very definition, $u|_{\widehat{\mathbf{Z}}^2} = T\phi$, and

$$\|u\| \ge \|u|_{\widehat{\mathbf{Z}}^2}\| = \|T\phi\|. \tag{12.12}$$

The adjoint $T^* : l^2(\widehat{\mathbf{Z}}^2) \to l^2(\mathbf{Z}^2)$ is given by

$$T^*\eta(i,j) = \frac{1}{4} \sum_{\pm,\pm} \eta(i \pm 1/2, j \pm 1/2),$$

and we have $\|T\| = \|T^*\|$,

$$\|u\| \geq \|T^* T\phi\|. \tag{12.13}$$

Let $B_n(a)$ be a ball of radius a centered at n (in the Euclidean metric), and denote by $B(a)$ the k-independent number of integer points contained in $B_n(a)$. Let K_a : $l^2(\mathbf{Z}^2) \to l^2(\mathbf{Z}^2)$ be defined as

$$K_a u(n) = \frac{1}{B(a)} \sum_{m \in B_n(a)} u(m).$$

For example, $H_0 = 4(K_1 - 1)$. For any k we have $\Lambda(A_k) \leq 4$, $\phi \geq 0$ on A_k, and consequently,

$$K_1 \phi(n) \geq (1 - \Lambda(A_k)/4)\phi(n), \qquad K_1^2 \phi(n) \geq (1 - \Lambda(A_k)/4)^2 \phi(n).$$

A direct calculation yields

$$T^* T = \frac{1}{4}\mathbf{1} + \frac{1}{2} K_1 + \frac{1}{4} K_{\sqrt{2}},$$
$$K_{\sqrt{2}} = 2K_1^2 - \frac{1}{2} K_2 - \frac{1}{2}\mathbf{1}.$$

Thus, using (12.12) we obtain

$$\begin{aligned} \|u\| &\geq \|T^* T\phi\| \geq (T^* T\phi, \phi) \\ &\geq \frac{1}{2}(1 - \Lambda(A_k)/4) + \frac{1}{2}(1 - \Lambda(A_k)/4)^2, \end{aligned} \tag{12.14}$$

and consequently,

$$\|u\|^2 \geq 1 - 3\Lambda(A_k)/4.$$

`Step 3:`

$$a_k \geq \frac{\lambda_D}{k} \cdot \frac{1 + O(1/\sqrt{k})}{1 + 3 \cdot \#\partial A_{T,k}/k}.$$

From the above two steps we obtain, if $\Lambda(A_k) \leq 4/3$,

$$\frac{D(u)}{\|u\|} \leq \frac{\mathcal{D}(\phi)}{1 - 3\Lambda(A_k)/4} = \frac{\Lambda(A_k)}{1 - 3\Lambda(A_k)/4}. \tag{12.15}$$

Let $A_{k,1}$ be given by (12.3), with $a = 1$. u belongs to the quadratic form domain of the Dirichlet Laplacian in the region $A_{k,1}$, and from (12.15) we get

$$\Lambda(A_{k,1}) \leq \frac{\Lambda(A_k)}{1 - 3\Lambda(A_k)/4}.$$

Consequently,

$$\begin{aligned}\Lambda(A_k) \geq \frac{\Lambda(A_{k,1})}{(1 + 3\Lambda(A_{k,1})/4)} &\geq \frac{\lambda_D |A_{k,1}|^{-1}}{1 + 3\lambda_D |A_{k,1}|^{-1}/4} \\ &= \lambda_D |A_{k,1}|^{-1}(1 + O(1/k)).\end{aligned} \tag{12.16}$$

(12.16) is trivially satisfied if $\Lambda(A_k) > 4/3$, and so is true for all k. We also have $|A_{k,1}| \leq \#A_k + 3 \cdot \#\partial A_k$, and consequently,

$$\Lambda(A_k) \geq \frac{\lambda_D}{k + 3 \cdot \#\partial A_k} \cdot (1 + O(1/k)) = \frac{\lambda_D}{k} \cdot \frac{1 + O(1/\sqrt{k})}{1 + 3 \cdot \#\partial A_k / k}. \tag{12.17}$$

(12.17) is true for any k-animal, and in particular for any tamed k-animal $A_{T,k}$. The lemma follows.

12.3. Proof of Lemma 12.3

For $n, m \in \mathbf{Z}^d$, a path between n and m is a sequence of sites $n_1, n_2, \dots n_k$ such that $n_1 = n, n_k = m, |n_j - n_{j-1}|_+ = 1$. For $X \subset \mathbf{Z}^2$, denote

$$\partial_n X = \{m \in X : \text{ there exists a path of length } \leq n \text{ starting at } m \text{ and ending at } m' \in \mathbf{Z}^2 \setminus X\}.$$

Obviously, $\partial_1 X = \partial X$. If $A_{T,k}$, $k > 0$, is a chosen sequence of tamed animals, we will prove

$$\lim_{k \to \infty} \frac{\#\partial_n A_{T,k}}{k} = 0. \tag{12.18}$$

The lemma follows by setting $n = 1$ in (12.18). As before, ϕ denotes the normalized eigenfunction corresponding to $a_k = \Lambda(A_{T,k})$. For $X \subset \mathbf{Z}^d$ let

$$\|\phi\|_X = \sum_{n \in X} |\phi(n)|^2.$$

Again, we split the proof into three steps.

Step 1: $\|\phi\|^2_{\partial_n A_{T,k}} = O(a_k) = O(1/k)$.

If $m \in \partial_n A_{T,k}$, there exists a path of length $l \leq n$, $m = m_1, m_2, \ldots, m_l$, $|m_{j-1} - m_j|_+ = 1$, $m_l \notin A_{T,k}$. We have

$$|\phi(m)| \leq \sum_{j=1}^{l} |\phi(m_{j-1}) - \phi(m_j)|^2$$

$$|\phi(m)|^2 \leq n \sum_{j=1}^{l} |\phi(m_{j-1}) - \phi(m_j)|^2.$$

Any couple (m, m'), $|m - m'|_+ = 1$ can belong only to finitely many paths of length n, the number depending only on n, and consequently,there exists a uniform constant C_n so that

$$\sum_{m \in \partial_n A_{T,k}} \phi(k)^2 \leq C_n \sum_{\substack{\langle m', m\rangle \\ |m' - m|_+ = 1}} |\phi(m') - \phi(m)|^2 = C_n \cdot a_k = O(1/k).$$

Step 2: Denote $O_k^n = A_{T,k} \setminus \partial_n A_{T,k}$, and let $\psi(m) = \max\{0, \phi(m) - b/\sqrt{k}\}$ for $0 < b < 1$. Then

(a) $\mathcal{D}(\psi) \leq \mathcal{D}(\phi)$.

(b) $\|\psi\| \geq 1 - b$.

(c) If $Z_k^n = O_k^n \cup \{m \in A_{T,k} : \psi(m) > 0\}$ then $\#(Z_k^n \setminus O_k^n) = O(1)$ as $k \to \infty$.

The part (a) is trivial. To prove (b), let $\widehat{\phi}(m) = \max\{\phi(m), b/\sqrt{k}\}$. Then

$$\|\widehat{\phi}\|^2_{A_{T,k}} = \sum_{m \in A_{T,k}} |\widehat{\phi}(m)|^2 \leq \|\phi\|^2 = 1, \qquad \psi(m) = \widehat{\phi}(m) - b/\sqrt{k},$$

and the Minkowski inequality yields

$$\|\psi\| \geq \|\widehat{\phi}\|_{A_{T,k}} - \left(\sum_{m \in A_{T,k}} b^2/k \right)^{1/2} \geq 1 - b.$$

To prove (c), note that from Step 1 we have

$$\#\{m \in \partial_n A_{T,k} : \phi(m) > b/\sqrt{k}\} = O(1).$$

On the other hand, $\psi(m) > 0$ iff $\phi(m) > b/\sqrt{k}$ and (c) follows.

`Step 3:` If $\alpha_n = \limsup_{k\to\infty}(\#\partial_n A_{T,k})/k$, then $\lim_{n\to\infty}\alpha_n = 0$.

We first remark that $0 \le \alpha_1 \le \alpha_2 \le \ldots \le 1$, and consequently, $\lim_{n\to\infty}\alpha_n = \alpha$ exists. Let $\theta = 1-\alpha$ and suppose that $\theta < 1$. Let $\rho \in (\theta, 1)$ be arbitrary, and denote

$$\theta_n = \liminf_{k\to\infty} \frac{\#Z_k^n}{k}.$$

From Step 2 we have that

$$\frac{\#Z_k^n}{k} = \frac{O(1)}{k} + 1 - \frac{\#\partial_n A_{T,k}}{k}, \tag{12.19}$$

and consequently, $\theta_n = 1-\alpha_n \le \rho$ for n large enough. Step 2 also implies that for any $b > 0$ and any $k_0 \in \aleph$, there exist k, m, $k > k_0$, $m < \rho k$, so that $\#A_k^n = m$ and

$$\Lambda(Z_k^n) \le a_k/(1-b)^2. \tag{12.20}$$

First, (12.20) implies that $\theta \ge 1/4$. Otherwise, we can choose $\rho < 1/4$ and derive from (12.17), (12.20)

$$\begin{aligned}\frac{\lambda_D}{4m}\cdot(1+O(1/m)) &\le a_m \le \Lambda(Z_k^n)\\ &\le \frac{a_k}{(1-b)^2} \le \frac{\lambda_D}{k(1-b)^2}\cdot(1+O(1/\sqrt{k})).\end{aligned} \tag{12.21}$$

$m/k < \rho$, and so when $k\to\infty$, $m\to\infty$ as well, and we obtain $1/4 \le \rho(1-b)^2$ for all $b > 0$, which contradicts the choice $\rho < 1/4$.

Let $0 < \varepsilon < 1$ be chosen in such a way that $\rho/\theta < 1/(1-\varepsilon)$. For n large enough, $\theta_n < \rho$ and consequently, $\theta/\theta_n \ge 1-\varepsilon$. There exists a sequence $k_j \to \infty$ so that

$$\lim_{j\to\infty} \frac{\#\partial_n A_{T,k_j}}{k_j} = \alpha_n.$$

On the other hand, from (12.19) we derive

$$\limsup_{j\to\infty} \frac{\#\partial_{n+1} A_{T,k_j}}{k_j} \le \alpha_{n+1} < 1,$$

$$\lim_{j\to\infty} \frac{\#O_n^{k_j}}{k_j} = \theta_n, \qquad \liminf_{j\to\infty} \frac{\#O_{n+1}^{k_j}}{k_j} \ge \theta_{n+1} \ge \theta.$$

Because $\partial O_k^n = O_k^n \setminus O_{k+1}^n$, we have

$$\limsup_{j\to\infty} \frac{\#\partial O_{k_j}^n}{\#O_{k_j}^n} \le \frac{\theta_n - \theta}{\theta_n} < \varepsilon.$$

Again, Step 2 (c) yields

$$\limsup_{j\to\infty} \frac{\#\partial Z_{k_j}^n}{\#Z_{k_j}^n} < \varepsilon.$$

For j large enough, to any k_j we correspond m_j with $m_j < \rho k_j$ so that $\#Z_{k_j}^n = m_j$ and (12.20) is true. It follows from (12.17) that for any $\delta > 0$ and large enough j,

$$\Lambda(Z_{k_j}^n) \ge \frac{\lambda_D(1-\delta)}{m_j(1 + 3\cdot \#\partial Z_{k_j}^n/m_j)} \ge \frac{\lambda_D(1-\delta)}{\rho k_j(1+3\varepsilon)}.$$

On the other hand, from (12.21) and Lemma 12.1 we obtain

$$\Lambda(Z_{k_j}^n) \le \frac{a_{k_j}}{(1-b)^2} \le \frac{\lambda_D}{k_j(1-b)^2}\cdot(1 + O(1/\sqrt{k_j})),$$

and consequently, for a large j we have

$$\rho \ge (1-b)^2 \frac{1-\delta}{(1+3\varepsilon)(1+\delta)}.$$

The numbers b, ε, δ can be chosen to be arbitrarily small and so $\rho \ge 1$, which contradicts the choice of ρ, namely, that $\theta < \rho < 1$. So, $\theta = 1$, and for all n, $\alpha_n = 0$. The lemma follows.

Chapter 13: Continuous Model

In this chapter we study the continuous analog of the model (10.1), namely, the random Schrödinger operators $H_\omega = -\Delta + V_\omega(x)$, acting on $L^2(\mathbf{R}^d)$, where

$$V_\omega(x) = \xi_n(\omega)(1+|n|^\alpha) \qquad \text{for } x \in I_n. \tag{13.1}$$

In (13.1), I_n are unit cubes centered at integers, $\mathbf{R}^d = \cup_{n\in\mathbf{Z}^d} I_n$, and ξ_n are as in (10.1). It certainly does not come as a surprise that, suitably modifed, the results of the previous chapters remain valid for H_ω. The continuous analog of the k-animals, for which we reserve the same name, are the connected regions consisting of k cubes from $\{I_n\}$. For a k-animal A_k, $\Lambda(A_k)$stands for the lowest eigenvalue of a Dirichlet Laplacian $-\Delta_D^{A_k}$. We set again

$$a_k = \inf_{A_k} \Lambda(A_k).$$

$B(p,q)$ stands for the Beta function,

$$B(p,q) = \int_0^1 x^{p-1}(1-x)^{q-1}dx, \qquad p>0,\ q>0.$$

Theorem 13.1. H_ω has discrete spectrum P-a.s. if and only if $\alpha > d$. For $\alpha > d$ and for a. e. ω,

$$N_\omega(E) \sim \frac{d}{\alpha-d}\frac{(\tau_d)^2}{(2\pi)^d} B\left(\frac{d}{\alpha}, \frac{d}{2}+1\right) E^{d/2+d/\alpha}. \tag{13.2}$$

Theorem 13.2. If $d/k \geq \alpha > d/(k+1)$, we have for a. e. ω

a) $\sigma_{\text{ess}}(H_\omega) = [a_k, \infty)$.

b) $\sigma_{\text{ac}}(H_\omega) = \emptyset$.

Theorem 13.3. With λ_D as in Theorem 10.3,

$$a_k \sim k^{-d/2} \cdot \lambda_D.$$

The probabilistic part of the proofs coincides with the one from the discrete case (and so does the intuition where the above results come from), while the rest of the argument suffers mostly minor technical changes. The remarkable difference is that in contrast to the discrete case, the proof of Theorem 13.3 is trivial (!). Naturally, that does not mean that model (13.1) is simpler to study than (10.1). For example, proving the absence of a singular continuous spectrum for operators (13.1) seems to be beyond the reach of existing techniques (the problem is not in the decay of the resolvent kernel but in the Simon-Wolff theorem). Such problems remain to be studied in the future.

We finally remark that while in the discrete model the proofs trivially accommodate the case when ξ_n are uniformily distributed on $[-1, 1]$, in the continuous model a new class of phenomena emerges. Already for $\alpha > 2$, it is not clear at all that operators H_ω are essentially self-adjoint on $C_0^\infty(\mathbf{R}^d)$. In the one-dimensional case, that question was answered in [GMO], where furthermore it was shown that for $0 < \alpha < 2$ $\sigma(H_\omega) = \sigma_{\text{pp}}(H_\omega) = (-\infty, \infty)$, while for $\alpha > 2$ the spectrum is discrete (!). To prove essential self-adjointness in a dimension larger than one (we believe that operators are essentialy self-adjoint on $C_0^\infty(\mathbf{R}^d)$) is a much harder problem. Also, we believe that in a dimension larger than one and for all α, one has $\sigma(H_\omega) = (-\infty, \infty)$, which should be quite easy to prove, providing self-adjointness questions are answered. The models where ξ_n has a negative component also remain to be studied in the future.

13.1. Proof of Theorem 13.1

For $\alpha > d$, $V_\omega(x) \to \infty$ P–a.s. when $|x| \to \infty$, by the argument of Section 11.1. Thus, for $\alpha > d$, H_ω certainly has a discrete spectrum. We give details of the eigenvalue asymptotics calculation since we will consider some generalizations in the next section. Again, note that monotonicity of the function $N_\omega(E)$ implies that it is enough to consider the case when $E \to \infty$ as an integer. To simplify notation, we replace $1+|n|^\alpha$ with $|n|^\alpha$, observing that by the min-max principle such change cannot alter the result. For E fixed, denote by $Q_E(\omega)$ a cube centered at the origin whose edges are parallel to the axes, such that $V_\omega(x) > E$ for $x \notin Q_E(\omega)$. For $\alpha > d$, $|Q_E(\omega)| < \infty$ P-a.s, and as in Section 11.4, $\mathbf{E}(|Q_E(\omega)|^k) < CE^{dk/\alpha}$, where C is a uniform constant. Without loss of generality, we can assume that $|Q_E(\omega)|$ is an integer. Denote by $N^\pm_{n,\omega}(E)$ the number of eigenvalues that are less than E of the operator $-\Delta + \xi_n|n|^\alpha$ in the cube I_n, subject to the Dirichlet and Neumann boundary conditions, respectively. Dirichlet-Neumann bracketing implies (note that $H_\omega > E$ outside Q_E)

$$\sum_{n\in\mathbf{Z}^d} N^+_{n,\omega}(E) \le N_\omega(E) \le \sum_{n\in\mathbf{Z}^d} N^-_{n,\omega}(E).$$

Denote $(\,\cdot\,)_+ = \max\{\,\cdot\,,0\}$. Weyl's law for cubes [RS4] gives

$$N^\pm_{n,\omega}(E) = \frac{\tau_d}{(2\pi)^d}\left((E-\xi_n(\omega)|n|^\alpha)_+\right)^{d/2} + r^\pm_n(E)$$

where $|r^\pm_n(E)| \le C\cdot E^{(d-1)/2}$ for a uniform constant C. After summing over n, a simple calculation yields

$$\sum_{n\in\mathbf{Z}^d} \frac{N^\pm_\omega(E)}{E^{d/2+d/\alpha}} = \frac{\tau_d}{(2\pi)^d}\sum_{n\in\mathbf{Z}^d}\frac{1}{E^{d/\alpha}}\left(\left(1-\xi_n(\omega)\left|\frac{n}{E^{1/\alpha}}\right|^\alpha\right)_+\right)^{d/2} + r^\pm(E), \tag{13.3}$$

where $r^\pm(E) \to 0$ as $E \to \infty$ (or more precisely, $|r^\pm(E)| \le D\cdot E^{-1/2}$ for a uniform constant D). Denote

$$\varsigma^\pm_n(\omega,E) = \left(\left(1-\xi_n(\omega)\left|\frac{n}{E^{1/\alpha}}\right|^\alpha\right)_+\right)^{d/2}$$

and let

$$\eta^\pm_n(\omega,E) = \varsigma^\pm_n(\omega,E) - \mathbf{E}(\,\varsigma^\pm_n(\omega,E)).$$

Rewrite the right-hand side of (13.3) as

$$\frac{\tau_d}{(2\pi)^d}E^{-d/\alpha}\sum_{n\in\mathbf{Z}^d}\mathbf{E}(\,\varsigma^\pm_n(\omega,E)) + \frac{\tau_d}{(2\pi)^d}E^{-d/\alpha}\sum_{n\in\mathbf{Z}^d}\eta^\pm_n(\omega,E) + r^\pm(E). \tag{13.4}$$

The first sum of (2.2) approaches

$$\mathbf{E}\int_{\mathbf{R}^d}((1-\xi_0(\omega)|x|^\alpha)_+)^{d/2}\,dx=\frac{\tau_d}{\alpha-d}\frac{(\tau_d)^2}{(2\pi)^d}B\left(\frac{d}{\alpha},\frac{d}{2}+1\right) \tag{13.5}$$

when $E\to\infty$. It remains to estimate the second sum. Note that $\eta_n^\pm(\omega,E)$ are independent random variables that satisfy

$$\mathbf{E}(\eta_n^\pm)=0, \qquad |\eta_n^\pm|\leq 2. \tag{13.6}$$

The rest of the argument is identical to that in Section 11.4. Let $M=|Q_E(\omega)|$, and consider (after relabelling)

$$\begin{aligned}\mathbf{E}\left(\sum_{n\in\mathbf{Z}^d}\eta_n^\pm(\omega,E)^{2k}\right)&=\mathbf{E}\sum_{\substack{k_i\geq 0\\k_1+\cdots+k_M=2k}}\prod_{i=1}^M(\eta_i^\pm(\omega))^{k_i})((2k)!)\Big/\prod_{i=1}^M k_i!\\&=\mathbf{E}\sum_{\substack{k_i\neq 1\\k_1+\cdots+k_M=2k}}\prod_{i=1}^M(\eta_i^\pm(\omega))^{k_i})((2k)!)\Big/\prod_{i=1}^M k_i!,\\&\leq C|Q_E(\omega)|^k\end{aligned}$$

where C is a uniform constant. The above estimates follow from elementary combinatorics and (13.6). Chebyshev's inequality yields

$$\begin{aligned}P_E=P\Big\{\Big|E^{-d/\alpha}(\sum_{n\in\mathbf{Z}^d}\eta_n^\pm)\Big|>\epsilon\Big\}&\leq P\Big\{E^{-2dk/\alpha}(\sum_{n\in\mathbf{Z}^d}\eta_n^\pm)^{2k}>\epsilon^{2k}\Big\}\\&\leq\frac{C}{E^{dk/\alpha}\epsilon^{2k}}.\end{aligned} \tag{13.7}$$

If $dk/\alpha>1$, $\sum_{E=1}^\infty P_E<\infty$ and the Borel-Cantelli lemma implies that

$$E^{-d/\alpha}\sum_{n\in\mathbf{Z}^d}\eta_n^\pm(\omega,E)\to 0\quad P\text{–a.s.}\qquad \text{as } E\to\infty.$$

(13.2) follows.

Let now $\alpha\leq d$. As in Section 11.1, we obtain that for a. e. ω, within infinitely many cubes $I_{n_i}(\omega)$ we have $V_\omega(x)<1$. If $-\Delta_D$ is the Laplacian with Dirichlet boundary condition along the boundary of such cubes, we have

$$\inf \sigma_{\text{ess}}(-\Delta + V_\omega(x)) \le \inf \sigma_{\text{ess}}(-\Delta_D + V_\omega(x)) \le a_1 + 1.$$

Thus, H_ω cannot have discrete spectrum for $\alpha \le d$.

13.2. More on the Eigenvalue Asymptotics

The proof of (13.2) can be extended to cover one interesting example which, to the best of our knowledge, has not been studied before. It involves the case where the random variables ξ_n are no longer independent. Let H_ω be a random Schrodinger operator of the form

$$H_\omega = -\Delta + \xi(x,\omega)|x|^\alpha,$$

where $\xi(x,\omega)$ is a stationary random field on some probability space (Ω, F, P). On the random field we impose the following conditions: $\xi(x,\omega)$ is φ-mixing with $\varphi(x) < C \ln^{-(1+\delta)}(2+|x|)$ and $0 < c_1 \le \xi(x,\omega) \le c_2$ P-a.s.. We recall

Definition: For $\Gamma \subset \mathbf{R}^d$, denote by $\mathcal{F}_\Gamma$ the sigma algebra generated by $\{\xi(x,\omega) : x \in \Gamma\}$ and by $d(\Gamma_1, \Gamma_2)$, the distance between Γ_1 and Γ_2. A stationary random field $\xi(x,\omega)$ is φ-mixing if there exists a function $\varphi : \mathbf{R}^+ \to \mathbf{R}^+$, $\lim_{x\to\infty} \varphi(x) = 0$, such that for $A \in \mathcal{F}_{\Gamma_1}$, $B \in \mathcal{F}_{\Gamma_2}$

$$|P(A \cap B) - P(A)P(B)| \le \varphi(d(\Gamma_1, \Gamma_2))P(A).$$

The operator H_ω certainly has a discrete spectrum and its eigenvalue asymptotics is given by the following

Theorem 13.4. Let us suppose that in addition to the above conditions one of the following is true:

a) $\xi(x,\omega) = \xi_n(\omega)$ for $x \in I_n$

b) $|\xi(x,\omega)-\xi(y,\omega)| \le M|x-y|$ P–a.s., for non-random constant M. Then

$$N_\omega(E) \sim \frac{d}{\alpha}\frac{(\tau_d)^2}{(2\pi)^d} B\left(\frac{d}{\alpha}, \frac{d}{2}+1\right) \mathbf{E}(\xi(0,\omega)^{-d/\alpha}) E^{d/2+d/\alpha}.$$

`Remark 1:` Consider for a moment the averaged Schrödinger operator

$$\bar{H} = -\Delta + \mathbf{E}(\xi(0,\omega))|x|^\alpha.$$

Its eigenvalue distribution is given by

$$\bar{N}(E) \sim \frac{d}{\alpha}\frac{(\tau_d)^2}{(2\pi)^d} B\left(\frac{d}{\alpha}, \frac{d}{2}+1\right) (\mathbf{E}(\xi(0,\omega)))^{-d/\alpha} E^{d/2+d/\alpha}.$$

The Jensen inequality implies that for $\alpha < d$, randomness pulls the eigenvalues down, while for $\alpha > d$ it pulls them up. The critical value is $\alpha = d$, when the asymptotics of the two distributions coincide.

`Remark 2:` The result (and the proof) extend to the case when

$$V_\omega(x) = \xi(x,\omega)|x|^\alpha\, a(x),$$

where $a(x) = a(x/|x|)$ is a strictly positive continuous function on the unit sphere S^d. Let $g_\omega(x) = \max\{\,(1-\xi_0(\omega)|x|^\alpha\, a(x)), 0\,\}$. The asymptotic has the form

$$\lim_{E\to\infty} \frac{N_\omega(E)}{E^{d/2+d/\alpha}} = \mathbf{E}\int_{\mathbf{R}^d} (g_\omega(x))^{d/2}\, dx.$$

Proof :

a) First note that cube Q_E can be chosen now in an ω-independent way. The construction of the previous section carries through, and the estimate (13.6) remains true, but because of the dependence of $\eta_n^\pm(\omega,E)$, some additional argument is needed to establish that

$$S_E^\pm(\omega) = |Q_E|^{-1} \sum_{n\in Q_E} \eta_n^\pm(\omega,\epsilon) \to 0 \quad P\text{–a.s.} \qquad \text{as } E\to\infty. \tag{13.8}$$

We drop $\pm$ in the sequel. For $E > 1$,

$$\begin{aligned}\mathrm{Var}(S_E) &\le |Q_E|^{-2} \sum_{n,n+m\in Q_E} |\mathrm{Cov}(\eta_n, \eta_{n+m})| \\ &\le 4C|Q_E|^{-2} \sum_{n,n+m\in Q_E} \ln^{-(1+\delta)}(2+|m|) \\ &\le D\ln^{-(1+\delta)}(E)\end{aligned}$$

for a uniform constant D. We used $|\mathrm{Cov}(\eta_n, \eta_{n+m})| \le 4\varphi(m)$ (see, e.g., Billingsley [BIL]).

Let $\gamma > 0$ be fixed and consider a subsequence S_{E_k} for $E_k = [(1+\gamma)^k] + 1$. Chebyshev's inequality yields

$$P_{E_k} = P\{|S_{E_k}| > \epsilon\} \le \frac{\mathrm{Var}(S_{E_k})}{\epsilon^2} < \frac{C}{\epsilon^2 k^{1+\delta}}.$$

The series $\sum_{k=1}^{\infty} P_{E_k}$ converges and the Borel-Cantelli lemma gives $S_{E_k} \to 0$, as $k \to \infty$ $P-$ a.s. To pass to the general case, note that for every E there exists an E_k such that $E_k < E \le E_{k+1}$, and consequently,

$$\limsup_{E\to\infty} |S_E(\omega)| < L\gamma \qquad P\text{–a.s.}$$

for a uniform constant L. Taking $\gamma \to 0$, we get (13.8) and part a) follows.

b) Approximate ξ by a piecewise constant field for a net of cubes of volume ϵ. Applying part a) we get an upper and a lower bound on $N_\omega(E)$. Then let $\epsilon \to 0$. ∎

13.3. Proofs of Theorems 13.2 and 13.3

The main role in our argument is played by the following

Theorem 13.5. Let $\{C_n\}_{n=1}^{\infty}$ be a sequence of disjoint balls in $\mathbf{R}^d$ of diameter l_n, and let

$$d_n = \min\{\, |x - x'| \,:\, x \in C_n,\ x' \in C_m \text{ for some } n \ne m\}.$$

Let $\{C'_n\}_{n=1}^{\infty}$ be a sequence of balls such that C'_n has the same center as C_n and has a diameter $l_n + d_n$. Let V be in $L^1_{\text{loc}}(\mathbf{R}^d)$, bounded below, and satisfying

$$V(x) \geq 0 \text{ if } x \notin \bigcup_n C_n, \qquad V(x) \geq d_n \text{ if } x \in C'_n \setminus C_n.$$

Then, if for every $\epsilon > 0$

$$\sum_n (1 + l_n^d) \exp(-\epsilon d_n) < \infty,$$

we have

$$\sigma_{\text{ac}}(-\Delta + V) \cap (-\infty, 0) = \emptyset. \tag{13.9}$$

Remark: Think about C_n as potential wells. In comparison to Theorem 11.2, it is the distance-size ratio of the wells *together* with the potential walls surrounding them that prevents tunneling at negative energies. From the technical point of view, that makes life much easier.

Proof : We will give a somewhat sketchy argument. Let D_n, D'_n be balls of diameters $l_n + d_n/3$, $l_n + 2d_n/3$ and with the same center as C_n. Denote $S = \cup_n D_n$ and let $-\Delta_D$ be Laplacian with the Dirichlet boundary condition along ∂S, the boundary of S. Denote $H = -\Delta + V$, $H_D = -\Delta_D + V$. The theorem will follow if we show that

$$K = \exp(-H) - \exp(-H_D)$$

is a trace class operator, since then (see, e.g., [RS3]) $\sigma_{\text{ac}}(H) = \sigma_{\text{ac}}(H_D)$, and it is obvious that $\sigma_{\text{ac}}(H_D) \cap (-\infty, 0) = \emptyset$. K is a positive operator, and trace norm is just a trace. One can show, following the argument of Theorem 9.2 and Theorem 21.1 in [SIM1], that

$$\text{Tr}(K) = \int_{\mathbf{R}^d} dx \int_P \exp\left(-\int_0^1 V(\omega(s))ds\right) d\mu_{0,x,x,1}(\omega),$$

where $\mu_{0,x,x,1}$ is a Wiener measure (time $t = 1$) conditioned at point (x, x), and

$$P = \{\omega \, : \, \omega(s) \in \partial S \text{ for some } 0 \leq s \leq 1\}.$$

If $x \in \mathbf{R}^d \setminus \cup_n D'_n$, one can easily estimate (see [SIM1], Lemma 21.3)

$$\int_P \exp\left(-\int_0^1 V(\omega(s))ds\right) d\mu_{0,x,x,1}(\omega) \leq C\exp(-\mathrm{dist}(x,\partial S))/2,$$

where C can be chosen as $\exp(-a)/(2\pi)^{d/2}$ if $V \geq a$. So,

$$\int_{\mathbf{R}^d\setminus\cup D'_n} dx \int_P \exp\left(-\int_0^1 V(\omega(s))ds\right) d\mu_{0,x,x,1}(\omega) \leq C' \sum_n \int_{t>d_n/6} \exp(-t/4)dt$$
$$\leq C' \sum_n \exp(-d_n/24) < \infty.$$

It remains to estimate

$$\sum_n \int_{D'_n} dx \int_P \exp\left(-\int_0^1 V(\omega(s))ds\right) d\mu_{0,x,x,1}(\omega).$$

As in [SIM1], we denote by b a $d-$dimensional Brownian motion, with a probability space $(B, \mathcal{B}, db)$. $E(f)$ stands for mathematical expectation of a function f, and $E(A)$ for a $db-$ measure of a set A. For $x \in D'_n$, denote

$$A_{x,d_n} = \{\omega : \max_{0\leq s\leq 1} |\omega(s) - x| \geq d_n/6\}.$$

We have

$$\begin{aligned}\mu_{0,x,x,1}(A_{x,d_n}) &= \mu_{0,0,0,1}\{\omega : \max_{0\leq s\leq 1} |\omega(s)| \geq d_n/6\}\\ &\leq E(\max_{0\leq s\leq 1} |b(s)| \geq d_n/6)\\ &\leq 2 \cdot E(|b(1)| \geq d_n/6)\\ &\leq C\exp(-d_n/6),\end{aligned}$$

where C is a uniform constant. In the above, we used the Levy and Chebyshev inequality [SIM1], and the fact that Gaussian random variables have exponential momentum. Since for some $s_0, 0 \leq s_0 \leq 1$, $\omega(s_0) \in \partial S$, we conclude that $\omega \in P \setminus A_{x,d_n}$ in the time interval $[0,1]$ never leaves $C'_n \setminus C_n$ (or belongs to a set of $\mu_{0,x,x,1}$-measure 0), and we have

$$\int_0^1 V(\omega(s))ds > d_n.$$

Thus, if $x \in D'_n$,

$$\int_P d\mu_{0,x,x,1}(\omega) \exp\left(-\int_0^1 V(\omega(s))ds\right) \leq C(\exp(-d_n/6) + \exp(-d_n)),$$

and finally, for suitable constant C,

$$\int_{D'_n} dx \int_P \exp\left(-\int_0^1 V(\omega(s))ds\right) d\mu_{0,x,x,1}(\omega) \leq C(l_n + d_n)^d \exp(-d_n/6).$$

Since

$$\sum_n (l_n + d_n)^d \exp(-d_n/6) < \infty,$$

the theorem follows. ∎

Again, it is an immediate consequence of Theorem 13.5 that if in addition

$$\lim_{\substack{x \to \infty \\ x \notin \cup_n C_n}} V(x) = \infty, \tag{13.10}$$

we have

$$\sigma_{\mathrm{ac}}(-\Delta + V) = \emptyset.$$

We now deduce part b) of Theorem 13.5 as in Section 11.2. Let C_n be the ω-dependent balls chosen as in (11.9). One certainly can choose balls C'_n so that the conditions of Theorem 13.5 are satisfied. Since 13.10 is also valid, we deduce part b) of Theorem 13.2.

For the above choice of C_n, C'_n, let $H_{\omega,D}$ be the operator H_ω with the Dirichlet boundary condition along ∂S, as in the proof of Theorem 13.5, and let $\widehat{H}_{\omega,D}$ be the operator $H_{\omega,D}$ with an additional Dirichlet boundary condition along boundaries of $G^{(i)}$−s (recall their definition in Section 11.2). We certainly have

$$0 \leq \exp(-H_\omega) - \exp(-\widehat{H}_{\omega,D}) \leq \exp(-H_\omega) - \exp(-H_{\omega,D}),$$

and so $\exp(-H) - \exp(-\widehat{H}_D)$ is a trace-class operator. In particular, we have

$$\sigma_{\text{ess}}(H_\omega) = \sigma_{\text{ess}}(\widehat{H}_{\omega,D}).$$

Thus, it immediately follows that $\inf \sigma_{\text{ess}}(\widehat{H}_{\omega,D}) \geq a_k$, and one shows that

$$\sigma_{\text{ess}}(\widehat{H}_{\omega,D}) \subset [a_k, \infty),$$

following line by line the Weil-sequence argument of Section 11.2. Part a) of Theorem 13.2 follows.

For simplicity of writing, we again prove Theorem 13.3 only in the case $d = 2$. If A_k is an arbitrary k-animal, and if B is a ball of volume k in $\mathbf{R}^2$, we have

$$\Lambda(A_k) \geq \Lambda(B) = \frac{\lambda_D}{k},$$

and so $a_k \geq \lambda_k$. On the other hand, as in (12.6), for large k and any $a > 1/\sqrt{2}$, there exists a k-animal A_k which contains the ball $B(\sqrt{k/\pi} - a - 1/\sqrt{2})$ of radius $\sqrt{k/\pi} - a - 1/\sqrt{2}$, and so

$$a_k \leq \frac{\lambda_D}{k}(1 + O(1/\sqrt{k})).$$

Theorem 13.3 follows.

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