

# Integrated Density of States of Random Schrödinger Operators with Alloy-Type Potential



## Bachelorarbeit

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### **Erklärung**

Hiermit versichere ich, dass ich diese Bachelorarbeit selbstständig verfasst und keine anderen als die angegebenen Quellen und Hilfsmittel verwendet habe.

München, den 23.01.2013

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## 0 Overview

In the first part of this thesis I will introduce three important topics that provide a solid mathematical basis for the discussions in the main part. Firstly, a short introduction to the theory of quadratic forms shall be given in order to treat the Schrödinger operators properly. Secondly, the notion of ergodicity and the two important ergodic theorems used later will be introduced. Thirdly, I will give an overview of the topic of functional integration, providing an important tool, the Feynman-Kac formula, used in the last chapter of this thesis.

In the main part some basic definitions and facts on Schrödinger operators with an alloy-type-potential will be provided. After a short discussion of their spectral properties, the theory of quadratic forms is applied to handle Schrödinger operators on finite subsets properly and prove important inequalities used later. The last section is devoted to the integrated density of states (ids). First of all, the ids will be defined via Dirichlet-Neumann-bracketing and then via the trace of an abstract projection. Using the methods of functional integration we will observe that these definitions coincide.

## 1 Preface on Quadratic Forms

The following self-contained discussion on quadratic forms is mainly based on [Sch12, Tes09, RS78]. Let  $\mathcal{H}$  be a complex Hilbert space. A *quadratic form*  $q$  defined on a dense subspace  $\mathcal{D}(q)$  is a map  $q : \mathcal{D}(q) \rightarrow \mathbb{C}$  corresponding to a *sesquilinear form*  $q' : \mathcal{D}(q) \times \mathcal{D}(q) \rightarrow \mathbb{C}$  satisfying  $q'(\phi, \psi) = \overline{q'(\psi, \phi)}$  such that  $q(\psi) = q'(\psi, \psi)$ . Since  $q'$  can be recovered from  $q$  by the polarization identity both will be used synonymously in the following.  $q$  is called *hermitian* if  $q$  is real valued or equivalently  $q'$  is symmetric (polarization identity) and *semi-bounded* if  $q(\psi) \geq \gamma \|\psi\|^2$  for some  $\gamma \in \mathbb{R}$ . It is called closed if its domain  $\mathcal{D}(q)$  is closed with respect to the norm  $\|\cdot\|_q$  induced by the scalar product

$$\langle \phi, \psi \rangle_q := q'(\phi, \psi) + (1 - \gamma) \langle \phi, \psi \rangle \quad (1)$$

or equivalently its graph is a closed subset of  $\mathcal{H} \times \mathbb{C}$ .

For a semi-bounded operator  $A$  (meaning  $\langle \psi, A\psi \rangle \geq \gamma \|\psi\|^2$ ) defined on its dense domain  $\mathcal{D}(A)$

$$q_A : \mathcal{D}(A) \rightarrow \mathbb{C}, \quad \psi \rightarrow \langle \psi, A\psi \rangle \quad (2)$$

clearly is a hermitian semi-bounded quadratic form which might not be closed. In the subsequent paragraph the existence and a characterization of the closure shall be established.

The map  $(\phi, \psi) \rightarrow \langle \phi, (A - \gamma)\psi \rangle$  is a scalar product which might not be compatible with the original scalar product. Therefore it will be useful to define the scalar product

$$\langle \phi, \psi \rangle_A := \langle \phi, (A - \gamma + 1)\psi \rangle \quad (3)$$

(in agreement with  $\langle \cdot, \cdot \rangle_q$  since for the quadratic form  $q_A(\psi) = \langle \psi, A\psi \rangle$ ,  $\langle \cdot, \cdot \rangle_{q_A} = \langle \cdot, \cdot \rangle_A$ ) which satisfies  $\|\psi\| \leq \|\psi\|_A$ . Hence a Cauchy sequence  $\psi_n$  in  $\mathcal{D}(A)$  with respect to  $\|\cdot\|_A$  is also Cauchy in  $\mathcal{H}$  with respect to the original norm and converges to  $\psi \in \mathcal{H}$ . Since for a Cauchy sequence  $\psi_n$  in  $(\mathcal{D}(A), \|\cdot\|_A)$  such that  $\|\psi_n\| \rightarrow 0$

$$\|\psi_n\|_A^2 = \langle \psi_n, \psi_n - \psi_m \rangle_A + \langle \psi_n, \psi_m \rangle_A \leq \|\psi_n\|_A \|\psi_n - \psi_m\|_A + \|\psi_n\| \|(A - \gamma + 1)\psi_m\| \xrightarrow{n, m \rightarrow \infty} 0$$

the representation of the completion as being embedded  $\overline{\mathcal{D}(A)}^{\|\cdot\|_A} \subseteq \mathcal{H}$  is unique and the map  $\langle \cdot, \cdot \rangle_A$  extends to  $\overline{\mathcal{D}(A)}^{\|\cdot\|_A}$ . By setting

$$q_A(\psi) = \|\psi\|_A^2 - (1 - \gamma)\|\psi\|^2$$

the quadratic form  $\langle \psi, A\psi \rangle$  associated with  $A$  also extends to  $\mathcal{D}(q_A) := \overline{\mathcal{D}(A)}^{\|\cdot\|_A}$ .

It is actually possible to obtain a more concrete expression of  $\mathcal{D}(q_A)$  through the spectral theorem. By the spectral theorem there exists a unitary map  $U$  to  $\bigoplus_{k=1}^N L^2(\mathbb{R}, \mu_k)$  such that the unitary transform of  $A$  is the multiplication by  $x$  on these spaces. Therefore it's possible to define the associated quadratic  $q_A : \mathcal{H} \rightarrow \mathbb{C}$  form on the domain

$$\mathcal{D}(q_A) = \mathcal{D}((A - \gamma)^{1/2}) = U^{-1} \{ (\psi_k)_{k=1}^N \subseteq \bigoplus_{k=1}^N L^2(\mathbb{R}, \mu_k) \mid \sum_{k=1}^N \int |x| |\psi(x)_k|^2 d\mu_k(x) < \infty \}$$

by

$$q_A(\psi) = \sum_{k=1}^N \int x \overline{\psi_k(x)} \psi_k(x) d\mu_k(x).$$

For  $\psi \in \mathcal{D}(A)$  this can be expressed as  $q_A(\psi) = \langle \psi, A\psi \rangle$  but in general  $\mathcal{D}(A) \subsetneq \mathcal{D}(q_A)$ .

In order to see that the quadratic form  $q_A$  from the spectral definition is also closed, note that the norms  $\|\cdot\|_{q_A}$  and  $\|\cdot\|_{(A-\gamma)^{1/2}}$  are equivalent and hence the closedness of the operator  $(A - \gamma)^{1/2}$  implies also the closedness of the associated form.

The reverse relationship between hermitian semi-bounded quadratic forms and self-adjoint operators is characterized by the following important theorem.

**Theorem 1.1.** *To every hermitian semi-bounded quadratic  $q$  form there corresponds a unique self-adjoint operator  $A$  such that  $q(\psi) = q_{A_q}(\psi) = \|\psi\|_{A_q}^2 - (1 - \gamma)\|\psi\|^2$  for all  $\psi \in \mathcal{D}(q) = \overline{\mathcal{D}(A_q)}^{\|\cdot\|_{A_q}}$  given by*

$$\mathcal{D}(A_q) = \{ \psi \in \mathcal{D}(q) \mid \exists \tilde{\psi} \in \mathcal{H} : q'(\phi, \psi) = \langle \phi, \tilde{\psi} \rangle \ \forall \phi \in \mathcal{D}(q) \}, \quad A_q \psi = \tilde{\psi} - (1 - \gamma)\psi.$$

*Proof.* Since  $\mathcal{D}(q)$  is dense,  $A_q$  is well defined. There is no loss in generality in assuming  $q \geq 1$  (since  $A_{q+\lambda} = A_q + \lambda$  for any  $\lambda \in \mathbb{R}$ ) and therefore the choice  $\gamma = 1$  yields  $\langle \cdot, \cdot \rangle_q = q'(\cdot, \cdot)$ . For any  $\tilde{\psi} \in \mathcal{H}$  the map  $\phi \rightarrow \langle \phi, \tilde{\psi} \rangle$  is a linear functional on  $(\mathcal{D}(q), \langle \cdot, \cdot \rangle_q)$  bounded by 1. Therefore by Riesz' representation theorem, there exists  $\psi \in \mathcal{D}(q)$  such that  $\langle \cdot, \tilde{\psi} \rangle = \langle \cdot, \psi \rangle_q = q'(\cdot, \psi)$  implying

$A_q\psi = \tilde{\psi}$  which proves that  $A_q$  is onto. Since for any  $\xi \in \mathcal{D}(A_q^*)$  there exists  $\eta \in \mathcal{D}(A_q)$  such that  $A_q\eta = A_q^*\xi$

$$\langle \xi, A_q\phi \rangle = \langle A_q^*\xi, \phi \rangle = \langle A_q\eta, \phi \rangle = q'(\eta, \phi) = \overline{q'(\phi, \eta)} = \overline{\langle A_q\phi, \eta \rangle} = \langle \eta, A_q\phi \rangle$$

holds for all  $\phi \in \mathcal{D}(A)$  proving  $\xi = \eta \in \mathcal{D}(A_q)$  and hence  $A_q$  being self-adjoint. Assuming there exists  $\xi = A_q\psi \in \mathcal{D}(A_q)^\perp$  (using surjectivity again) with respect to  $\langle \cdot, \cdot \rangle_q$  yields  $\|\xi\|^2 = \langle \xi, A_q\psi \rangle = s(\xi, \psi) = \langle \xi, \psi \rangle_q = 0$  and therefore proves that  $\mathcal{D}(A_q)$  is dense. It's clear that for all  $\psi \in \mathcal{D}(A_q)$ ,  $q(\psi) = q_{A_q}(\psi)$ . Uniqueness follows from the fact that self-adjoint operators are maximal.  $\square$

This important result also allows to define self-adjoint completions of symmetric operators.

**Corollary 1.2** (Friedrichs Extension). *Any semi-bounded symmetric densely defined operator  $A$  has a self-adjoint extension with the same lower bound.*

*Proof.* The associated form  $q_A(\cdot) = \langle \cdot, A \cdot \rangle$  can be closed owing to the preceding discussion to  $q_A = \|\psi\|_A^2 - (1 - \gamma)\|\psi\|^2$  on  $\overline{\mathcal{D}(A)}^{\|\cdot\|_A} = \overline{\mathcal{D}(A)}^{\|\cdot\|_{q_A}}$ . The operator  $A_{q_A}$  given by theorem 1.1 is self-adjoint and extends  $A$ . Since  $A \geq \gamma$  also  $q_A \geq \gamma$  and hence  $A_{q_A} \geq \gamma$ .  $\square$

## 1.1 Definition of Laplacians Using Quadratic Forms

Using theorem 1.1 it is now possible to define various Laplacians via quadratic forms. In the following the Sobolev Space  $H^1(\Lambda) := \{\psi \in L^2(\Lambda) \mid \nabla\psi \in L^2(\Lambda)\}$  with the scalar product  $\langle \psi, \phi \rangle_{H^1(\Lambda)} := \langle \psi, \phi \rangle + \langle \nabla\psi, \nabla\phi \rangle$  and the Sobolev Space  $H_0^1(\Lambda) := \overline{C_0^\infty(\Lambda)}^{\|\cdot\|_{H^1(\Lambda)}}$  with the restricted scalar product will be used.

**Definition 1.3.** *The Laplacian  $-\Delta$  is the unique self-adjoint operator on  $L^2(\mathbb{R}^n)$  corresponding to the form  $q : H^1(\mathbb{R}^n) \rightarrow \mathbb{C}$  mapping  $\psi \rightarrow \langle \nabla\psi, \nabla\psi \rangle$ . For Laplacians defined on subsets of  $\mathbb{R}^n$  let  $\Lambda \subseteq \mathbb{R}^n$  open*

- (i) *The Dirichlet Laplacian  $-\Delta_D^\Lambda$  is the unique self-adjoint operator on  $L^2(\Lambda)$  corresponding to the form  $q : H_0^1(\Lambda) \rightarrow \mathbb{C}$  mapping  $\psi \rightarrow \langle \nabla\psi, \nabla\psi \rangle$ .*
- (ii) *Analogously, the Neumann Laplacian  $-\Delta_N^\Lambda$  is the unique self-adjoint operator on  $L^2(\Lambda)$  corresponding to the form  $q : H^1(\Lambda) \rightarrow \mathbb{C}$  mapping  $\psi \rightarrow \langle \nabla\psi, \nabla\psi \rangle$ .*

**Remark 1.4.** In order to use theorem 1.1 in this definition, it is necessary that the form  $q$  is hermitian, semi-bounded and closed. Hermiticity follows from the fact that  $q$  is real, semi-boundedness is clear since  $q(\psi) = \|\nabla\psi\|^2 \geq 0$ . For closedness with respect to the form norm note that

$$\|\psi\|_q^2 = q(\psi) + \|\psi\|^2 = \|\psi\|_{H_0^1(\Lambda)}^2$$

and that the Sobolev Space  $H_0^1(\Lambda)$  is a Hilbert space and analogously with  $H^1(\Lambda)$  for the Neumann Laplacian and  $H^1(\mathbb{R}^n)$  for the Laplacian in the whole space.

## 1.2 Results form Perturbation Theory

However this thesis is mainly concerned with Schrödinger operators in the form of  $-\Delta + V$  with  $V$  being the multiplication operator with some equally named potential. Although the domains of both operators will be dense it may occur that their intersection is empty. Therefore it is generally not possible to define this operator sum pointwise, but rather as the sum of their associated forms. This will also allow us to study the spectra of the Schrödinger operators as perturbations of the Laplacians.

The form  $q_V$  associated with  $V$  is clearly hermitian and closed on  $\mathcal{D}(q_V)$ . It is called relatively bounded with respect to the quadratic form  $q$  associated with the Laplacian if  $\mathcal{D}(q) \subseteq \mathcal{D}(q_V)$  and  $|q(\psi)| \leq aq(\psi) + b\|\psi\|_2^2$  for constants  $a, b \geq 0$  where  $a$  is called relative bound. The case of actual interest will be  $a < 1$  since then by  $q_V(\psi) + q(\psi) \geq (1 - a)q(\psi) - b\|\psi\|_2^2 \geq -b\|\psi\|_2^2$  the form sum is again semi-bounded. Moreover since  $q(\psi) \leq \frac{1}{1-a}(q_V(\psi) + q(\psi) + b\|\psi\|_2^2)$ , the norms  $\|\cdot\|_{q+q_V}$  and  $\|\cdot\|_q$  are equivalent and therefore  $q_V + q$  is also closed on it's domain  $\mathcal{D}(q)$ . By theorem 1.1 a unique self-adjoint operator corresponds to this form sum, which will be denoted by  $-\Delta + V$ . The preceding argument for general  $\gamma$  is known as the following theorem named after Kato, Lions, Lax, Milgram and Nelson.

**Theorem 1.5** (KLMN). *For a semi-bounded closed quadratic form  $q$  and a relative bounded quadratic form  $\tilde{q}$  with bound less than 1 the form sum  $q + \tilde{q}$  is again a semi-bounded closed form and hence gives rise to a semi-bounded self-adjoint operator.*

The following Lemma gives a sufficient condition on  $V$  such that  $q_V$  has relative bound less than 1 and therefore  $-\Delta + V$  can be defined as a form sum.

**Lemma 1.6.** *Let  $V \in L^p(\Lambda)$  for  $\Lambda \subseteq \mathbb{R}^n$  with  $p = 1$  for  $n = 1$ ,  $p > 1$  for  $n = 2$  and  $p \geq \frac{n}{2}$  for  $n \geq 3$ . Then for all  $\epsilon > 0$  there exists  $b(\epsilon, V)$  just depending on these quantities such that for all  $\psi \in H^1(\Lambda)$*

$$|\langle \psi, V\psi \rangle| \leq \epsilon \|\nabla \psi\|_2^2 + b(\epsilon, V) \|\psi\|_2^2$$

*Proof.* Since by dominated convergence  $\int_\Lambda |V \mathbb{1}_{|\psi| < N}|^p \xrightarrow{N \rightarrow \infty} \|V\|_p^p$  it is possible to split  $V = V_\infty + V_p$  where  $V_\infty \in L^\infty(\Lambda)$  and  $V_p \in L^p(\Lambda)$  such that  $\|V_p\|_p \leq \tilde{\epsilon}$  for any  $\tilde{\epsilon} > 0$ . Hence

$$|\langle \psi, V\psi \rangle| \leq |\langle \psi, V_\infty \psi \rangle| + |\langle \psi, V_p \psi \rangle| \leq \|V_\infty\|_\infty \|\psi\|_2^2 + \|V_p\|_p \|\psi\|_{2q}^2$$

by Hölder's inequality with  $\frac{1}{2q} = \frac{1}{2} - \frac{1}{2p} \geq \frac{1}{2} - \frac{1}{n}$ . Thus the standard Sobolev inequality is applicable and yields

$$|\langle \psi, V\psi \rangle| \leq \tilde{\epsilon} c \|\nabla \psi\|_2^2 + \|V_\infty\|_\infty \|\psi\|_2^2 = \epsilon q(\psi) + b(\epsilon, V) \|\psi\|_2^2.$$

□

## 2 Preface on Ergodicity

Let  $(\Omega, \tilde{\mathcal{F}}, \tilde{P})$  be some probability space. A stochastic process is a family of random variables on  $(X_i)_{i \in I}$  mapping  $X_i : \Omega \rightarrow \mathbb{R}$  with some index set  $I$  (mostly  $I = \mathbb{N}$ ,  $I = \mathbb{R}$  or as in the case needed later  $I = \mathbb{Z}^n$ ).

### 2.1 Canonical Probability Space

Since the only important characteristic of the  $X_i$  is their probability distribution and not the underlying probability space  $\Omega$  itself, one can freely choose a more natural space. For all  $i \in I$  the probability distribution  $P_{X_i}(B) = \tilde{P}(\{\omega \in \Omega \mid X_i(\omega) \in B\})$  is a measure on  $(\mathbb{R}, \mathcal{B}(\mathbb{R}))$ . Therefore, the map  $\tilde{X}_i : (\mathbb{R}, \mathcal{B}(\mathbb{R}), P_{X_i}) \rightarrow \mathbb{R}$ ,  $\tilde{X}_i(\omega) = \omega$  defines a random variable with the same distribution. Since their distributions coincide  $X_i$  and  $\tilde{X}_i$  can be used synonymously. In order to extend this method to the joint distribution on the canonical probability space  $\mathbb{R}^I := \{\omega : I \rightarrow \mathbb{R}\}$ , we will define the system  $\mathcal{F}_0$  of the so called cylinder sets  $M = \{\omega \in \mathbb{R}^I \mid (\omega(i_1), \dots, \omega(i_d)) \in B\}$  for some  $B \in \mathcal{B}(\mathbb{R}^d)$  and  $d \in \mathbb{N}$ . On  $\mathcal{F}_0$  one can define the canonical probability measure

$$P(\{\omega \in \mathbb{R}^I \mid (\omega(i_1), \dots, \omega(i_d)) \in B\}) := \tilde{P}(\{\omega \in \Omega \mid (X_{i_1}(\omega), \dots, X_{i_d}(\omega)) \in B\}).$$

The smallest  $\sigma$ -algebra  $\mathcal{F} = \sigma(\mathcal{F}_0)$  containing  $\mathcal{F}_0$  completes our definition of the canonical space  $(\mathbb{R}^I, \mathcal{F}, P)$ . The equally named stochastic process in the new space is then simply given by

$$X_i(\omega) = \omega(i). \quad (4)$$

The preceding paragraph shows that there is no loss of generality in assuming that all stochastic processes are in the form of eq. (4).

### 2.2 Stationarity and Ergodicity

**Definition 2.1.** A stochastic process  $(X_i)_{i \in I}$  with an index set  $I$  closed under addition is called stationary if<sup>1</sup>  $\mathcal{L}[(X_i)_{i \in I}] = \mathcal{L}[(X_{i+j})_{i \in I}]$  for any  $j \in I$ .

In the setting of the canonical probability space, we define a group of shifts  $(T_i)_{i \in I}$  by  $T_i : \mathbb{R}^I \rightarrow \mathbb{R}^I$ ,  $T_i \omega = \omega(\cdot - i)$ . Using this, we can rephrase the stationarity of a stochastic process as follows.  $(X_i)_{i \in I}$  is stationary if and only if the shifts  $T_j$  are measure-preserving for all  $j \in I$  in the sense that  $P(A) = P(T_j^{-1}A)$ .

**Definition 2.2.** The stochastic process  $(X_i)_{i \in I}$  is called ergodic if  $\mathcal{I}$ , the  $\sigma$ -algebra of  $(T_i)_{i \in I}$ -invariant sets defined by

$$\mathcal{I} = \{A \in \mathcal{F} \mid T_i^{-1}A = A \text{ for all } i \in I\}.$$

---

<sup>1</sup>For a random variable or a stochastic process  $\mathcal{L}[\cdot]$  denotes the distribution.



is  $P$ -trivial, that is all sets  $A \in \mathcal{I}$  have  $P(A) = 0$  or  $1$ .

The following easy proposition states an equivalent definition of ergodicity which will turn out useful later.

**Proposition 2.3.**  *$(X_i)_{i \in I}$  is ergodic if and only if any invariant random variable  $Y$  in the sense that  $Y(T_i \omega) = Y(\omega)$  for all  $i \in I$  is constant<sup>2</sup>.*

*Proof.* Assume first that  $(X_i)_{i \in I}$  is ergodic and let  $Y : \Omega \rightarrow \mathbb{R}$  be an invariant random variable altered on a set of measure 0 such that  $Y(T_i \omega) = Y(\omega)$  for all  $i \in I$  and  $\omega \in \Omega$ . Then for all  $i \in I$ ,  $T_i^{-1}\{f > t\} = \{f \circ T_i > t\} = \{f > t\}$  and then by ergodicity  $P(\{f > t\}) = 0$  or  $1$  for all  $t \in \mathbb{R}$ . That is  $Y$  is a.e. constant.

Now assume the contrary and let  $A \in \mathcal{F}$  an invariant set. Then  $\mathbb{1}_A \circ T_i = \mathbb{1}_{T_i^{-1}(A)} = \mathbb{1}_A$  is invariant and a.e. 0 or 1 by assumption. Thus  $P(A) = 0$  or  $1$ .  $\square$

One of the earliest and deepest results on ergodic theory is due to Birkhoff and will be of great importance in the later discussions. The theorem is adapted and only stated for the case  $I = \mathbb{Z}^n$  without proof.

**Theorem 2.4** (Birkhoff's ergodic theorem). *Suppose  $(X_i)_{i \in \mathbb{Z}^n}$  is an ergodic stationary stochastic process and  $X_0 \in L^1(P)$  then*

$$\frac{1}{(2L+1)^n} \sum_{\|i\|_\infty \leq L} X_i \xrightarrow{L \rightarrow \infty} \mathbb{E}[X_0] \text{ } P\text{-almost surely}$$

*Proof.* See e.g. [Kle08].  $\square$

There are various ergodic theorems for sub- and superadditive processes as generalizations of Birkhoff's theorem. The first is due to Kingman, the one discussed here due to Akcoglu and Krengel.

**Definition 2.5.** *Let  $J := \{(a, b) \mid a, b \in \mathbb{Z}^n\}$  the set of open  $n$ -dimensional intervals with integer coordinates. An integrable stochastic process  $(F_\Lambda)_{\Lambda \in J}$  indexed by these intervals is called superadditive if*

- (i)  $F_\Lambda \circ T_i = F_{\Lambda-i}$
- (ii)  $F_\Lambda \geq F_{\Lambda_1} + F_{\Lambda_2}$  if  $\Lambda = \Lambda_1 \cup \Lambda_2$
- (iii)  $\gamma(F) := \sup_{\Lambda \in J} \frac{1}{|\Lambda|} \mathbb{E}[F_\Lambda] < \infty$ .

$F_\Lambda$  is called subadditive if  $-F_\Lambda$  is superadditive.

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<sup>2</sup>Here and in all other cases equalities between random variables are meant  $P$ -almost surely.

**Theorem 2.6** (Akcoglu-Krengel). *Let  $\Lambda_L := (-L, L)^n$ . If the shifts  $T_i$  are ergodic, then under the assumptions of definition 2.5*

$$\lim_{L \rightarrow \infty} \frac{1}{|\Lambda_L|} F_{\Lambda_L} = \gamma(F) \text{ } P\text{-almost surely.}$$

*Proof.* See e.g. [AK81]. □

### 3 Principles of Wiener Measures and Functional Integration

Before addressing the main topic of this thesis, some basic properties of Wiener processes and their connection to quantum mechanics via path integrals shall be established.

#### 3.1 Wiener Measure

In the following, let for any  $a \in \mathbb{R}$ ,  $C_0^a := C_0([0, a], \mathbb{R}^n)$  be the space of continuous functions  $x$  from  $[0, a]$  to  $\mathbb{R}^n$  such that  $x(0) = 0$  (the vector full of zeros). The usual sup-norm  $\|x\|_\infty := \max_{t \in [0, a]} \|x(t)\|$  makes this space to a Banach space. The following discussion based on [JL00] considers the problem of defining a measure  $\mathfrak{m}$  on this space. Since this construction is quite technical, no rigorous proofs will be given.

Let  $\mathcal{I}$  denote the set of *intervals* in  $C_0^a$  of the form

$$I = \{x \in C_0^a \mid \alpha_\nu^j < x_\nu(t_j) \leq \beta_\nu^j \text{ for all } \nu = 1, \dots, n \text{ and } j = 1, \dots, k\}$$

for some  $k \in \mathbb{N}$ ,  $\alpha^1, \dots, \alpha^k, \beta^1, \dots, \beta^k \in (\mathbb{R} \cup \{-\infty, \infty\})^n$  and  $0 < t_0 < \dots < t_k < a$ . Inspired by the Brownian motion<sup>3</sup> one defines  $\mathfrak{m}$  on  $\mathcal{I}$  by

$$\mathfrak{m}(I) := \int_{(\alpha^k, \beta^k]} \dots \int_{(\alpha^1, \beta^1]} \prod_{j=1}^k p(u_j, u_{j-1}, t_j - t_{j-1}) du_1 \dots du_n$$

with the *probability*

$$p(u_j, u_{j-1}, t_j - t_{j-1}) = \frac{1}{(4\pi(t_j - t_{j-1}))^{n/2}} e^{-\frac{(u_j - u_{j-1})^2}{4(t_j - t_{j-1})}}$$

of a  $n$ -dimensional Brownian motion starting at  $u_{j-1}$  at  $t = 0$  and arriving at  $u_j$  at  $t = t_j - t_{j-1}$ . It can be shown that  $\mathcal{I}$  is a semi-algebra and that  $\mathfrak{m}$  is additive on  $\mathcal{I}$ . Thus the Carathéodory extension of  $\mathfrak{m}$  on  $(C_0^a, \sigma(\mathcal{I}))$  exists. Actually it holds that  $\mathcal{B}(C_0^a) = \sigma(\mathcal{I})$  where  $\mathcal{B}(C_0^a)$  is the Borel  $\sigma$ -algebra generated by the norm-open sets.

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<sup>3</sup>As a slight difference in this definition processes with variance  $2(t_j - t_{j-1})$  are used. The reason for that becomes clear in the connection with semi-groups of the Laplacians.

### 3.2 Integration with Respect to the Wiener Measure

Using the just defined measure the Lebesgue theory allows us to define an integration with respect to  $\mathbf{m}$ . Of great importance later on will be the following proposition.

**Proposition 3.1** (Wiener's integration formula). *Let  $f : \mathbb{R}^k \rightarrow \mathbb{R}^n$  Lebesgue measurable. Then*

$$\int_{C_0^a} f(x(t_1), \dots, x(t_k)) d\mathbf{m}(x) = \int_{(\mathbb{R}^n)^k} f(u_1, \dots, u_k) \prod_{j=1}^k p(u_j, u_{j-1}, t_j - t_{j-1}) du_1 \dots du_n$$

with  $t_0 = 0, u_0 = 0$ .

*Proof.* Define  $P_{t_1, \dots, t_k} : C_0^a \rightarrow (\mathbb{R}^n)^k$  by  $P_{t_1, \dots, t_k} x := (x(t_1), \dots, x(t_k))$  which is clearly continuous and therefore Borel-measurable. Hence for any Borel set  $B \in (\mathbb{R}^n)^k$   $\{x \in C_0^a \mid (x(t_1), \dots, x(t_k)) \in B\} = P_{t_1, \dots, t_k}^{-1}(B) \in \mathcal{B}(C_0^a) = \sigma(\mathcal{I})$ . Using this  $\mathbf{m}(P_{t_1, \dots, t_k}^{-1}(B))$  is well defined and clearly satisfies  $\mathbf{m}(P_{t_1, \dots, t_k}^{-1}(B)) = \int_B \prod_{j=1}^k p(u_j, u_{j-1}, t_j - t_{j-1}) du_1 \dots du_n$  since the sets  $(\alpha^j, \beta^j]$  generate  $\mathcal{B}(\mathbb{R}^n)$ . Therefore the image measure  $\mathbf{m} \circ P_{t_1, \dots, t_k}^{-1}$  has density  $\prod_{j=1}^k p(u_j, u_{j-1}, t_j - t_{j-1})$  with respect to the Lebesgue measure on  $(\mathbb{R}^n)^k$ . Then by change of variables

$$\begin{aligned} \int_{C_0^a} f(P_{t_1, \dots, t_k} x) d\mathbf{m}(x) &= \int_{(\mathbb{R}^n)^k} f(u_1, \dots, u_k) d(\mathbf{m} \circ P_{t_1, \dots, t_k}^{-1}) \\ &= \int_{(\mathbb{R}^n)^k} f(u_1, \dots, u_k) \prod_{j=1}^k p(u_j, u_{j-1}, t_j - t_{j-1}) du_1 \dots du_n. \end{aligned}$$

□

The following Lemma shows why the integration with respect to the Wiener measure might be helpful in the analysis of the differential operators defined earlier.

**Lemma 3.2.** *The semi-group generated by the Laplacian  $e^{-t(-\Delta)} = e^{t\Delta}$  has the integral kernel  $\frac{1}{(4\pi t)^{n/2}} e^{-\frac{(x-y)^2}{4t}}$ , i.e. for all  $\psi \in L^2(\mathbb{R}^n)$  and  $t > 0$  it holds that*

$$(e^{t\Delta}\psi)(x) = \frac{1}{(4\pi t)^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{(x-y)^2}{4t}} \psi(y) dy.$$

*Proof.* Let  $\psi \in \mathcal{S}$ , the Schwartz space on which the Fourier transform  $\mathcal{F}$  is a bijection. Then by elementary properties of the Fourier transform

$$\begin{aligned} (e^{t\Delta}\psi)(x) &= \mathcal{F}^{-1} \left[ e^{-t\|\cdot\|^2} (\mathcal{F}\psi)(\cdot) \right] (x) = \frac{1}{(4\pi)^{n/2}} \left[ \mathcal{F}^{-1}(e^{-t\|\cdot\|^2}) * \mathcal{F}^{-1}(\mathcal{F}\psi) \right] (x) \\ &= \frac{1}{(4\pi)^{n/2}} \left[ t^{-n/2} e^{-\frac{\|\cdot\|^2}{4t}} * \psi \right] (x) = \frac{1}{(4\pi t)^{n/2}} \int_{\mathbb{R}^n} e^{-\frac{(x-y)^2}{4t}} \psi(y) dy. \end{aligned}$$

This can be extended to  $L^2(\mathbb{R}^n)$  as follows. Let  $\psi \in L^2(\mathbb{R}^n)$  approximated by  $\psi_n \in \mathcal{S}$ , i.e.  $\|\psi - \psi_n\|_2 \rightarrow 0$ . Then  $f_t(y) := \frac{1}{(4\pi t)^{n/2}} e^{-\frac{y^2}{4t}} \in L^1(\mathbb{R}^n)$  and by Young's inequality  $\|f_t * \psi\|_2 \leq$

$\|f_t\|_1\|\psi\|_2$ . Hence also  $e^{t\Delta}\psi_n \rightarrow e^{t\Delta}\psi$  and  $f_t * \psi_n \rightarrow f_t * \psi$ . Therefore

$$(e^{t\Delta}\psi)(x) = \lim_{n \rightarrow \infty} (e^{t\Delta}\psi_n)(x) = \lim_{n \rightarrow \infty} (f_t * \psi_n)(x) = (f_t * \psi)(x).$$

□

It's not hard to see that the probabilities defined earlier exactly match the integral kernel of  $e^{t\Delta}$  i.e.  $f_{t_j-t_{j-1}}(u_j - u_{j-1}) = p(u_j, u_{j-1}, t_j - t_{j-1})$  which is the actual reason for the slight redefinition mentioned earlier. Therefore it holds for example for  $\xi \in \mathbb{R}^n$  that

$$(e^{t\Delta}\psi)(\xi) = \int_{\mathbb{R}^n} \frac{e^{-\frac{(y-\xi)^2}{4t}}}{(4\pi t)^{n/2}} \psi(y) dy = \int_{\mathbb{R}^n} \psi(y+\xi) p(y, 0, t) dy = \int_{C_0^a} \psi(x(t)+\xi) d\mathbf{m}(x) = \mathbb{E}[\psi(x(t) + \xi)]$$

where the expectation is meant with respect to  $x$ . The question whether it is possible to generalize such an expression to  $H = \Delta + V$  (again as a form sum) is answered by the Feynman-Kac formula.

**Theorem 3.3** (Feynman-Kac). *Let  $V : \mathbb{R}^n \rightarrow \mathbb{R}$  relative bounded with respect to  $-\Delta$  with bound less than 1. Then for  $H = -\Delta + V$  and all  $\xi \in \mathbb{R}^n$ ,  $\psi \in L^2(\mathbb{R}^n)$*

$$(e^{-tH}\psi)(\xi) = \int_{C_0^t} e^{-\int_0^t V(x(s)+\xi) ds} \psi(x(t) + \xi) d\mathbf{m}(x) = \mathbb{E} \left[ e^{-\int_0^t V(x(s)+\xi) ds} \psi(x(t) + \xi) \right]. \quad (5)$$

Before giving an idea of the proof the central technical tool needed shall be stated.

**Theorem 3.4** (Trotter product formula as in [Nel64]). *If  $A$  is self-adjoint and  $B$  is symmetric and a small perturbation with  $A$ -bound less than 1, then the self-adjoint operator  $C = A + B$  defined in the sense of forms satisfies*

$$e^{-tC}\psi = \lim_{k \rightarrow \infty} (e^{-\frac{t}{k}A} e^{-\frac{t}{k}B})^k \psi$$

for all  $\psi \in \mathcal{H}$ .

*Idea of the proof of theorem 3.3.* The proof in full technical details is quite tedious, hence only the basic idea will be given. By the remark earlier it becomes clear that  $(e^{t\Delta} e^{-tV}\psi)(\xi) = \int_{\mathbb{R}^n} f_t(u - \xi) e^{-tV(u)} du$  and similarly for the  $k$ th Trotter product

$$[(e^{\frac{t}{k}\Delta} e^{-\frac{t}{k}V})^k \psi](\xi) = \int_{\mathbb{R}^n} \cdots \int_{\mathbb{R}^n} \prod_{j=1}^k f_{t/k}(u_j - u_{j-1}) e^{-(t/k) \sum_{j=1}^k V(u_j)} \psi(u_k) du_k \cdots du_1$$

where  $u_0 := \xi$ . Hence by variable transform  $v_j = u_j - \xi$

$$\begin{aligned} [(e^{\frac{t}{k}\Delta} e^{-\frac{t}{k}V})^k \psi](\xi) &= \int_{\mathbb{R}^n} \cdots \int_{\mathbb{R}^n} \prod_{j=1}^k f_{t/k}(v_j - v_{j-1}) e^{-(t/k) \sum_{j=1}^k V(v_j + \xi)} \psi(v_k) dv_k \dots dv_1 \\ &= \int_{C_0^t} e^{-(t/k) \sum_{j=1}^k V(x(jt/k) + \xi)} \psi(x(t) + \xi) d\mathbf{m}(x) \end{aligned} \quad (6)$$

where the last equality follows from proposition 3.1. Then taking the limit  $k \rightarrow \infty$  on both sides of eq. (6) proves the claim for continuous bounded potentials since by Riemann sums  $\frac{t}{k} \sum_{j=1}^k V(x(\frac{jt}{k}) + \xi) \rightarrow \int_0^t V(x(s) + \xi) ds$ . The general claim is proved by approximation of general potentials  $V$  by continuous ones. For full details see [JL00].  $\square$

Similarly to the above procedure one defines the conditional Wiener measure  $\mathbf{m}_{0,x}^{a,b}$  on the space  $C_{0,a}^{t,b}$  with the slight modification that one requires paths to start in  $a$  at time 0 end in  $b$  at time  $t$ . With this notation the integral kernel of  $e^{-tH}$  is given by

$$e^{-tH}(a, b) = \int_{C_{0,a}^{t,b}} e^{-\int_0^t V(x(s)) ds} d\mathbf{m}_{0,a}^{t,b}(x). \quad (7)$$

Since we are not only interested in Hamiltonians in the form of  $-\Delta + V$  but also in Hamiltonians with Dirichlet or Neumann Laplacians on finite subsets  $\Lambda \subseteq \mathbb{R}^n$  we have to introduce a version of the Feynman-Kac-formula in this setting.

The Feynman-Kac-Formula for Dirichlet Hamiltonians on  $\Lambda = (-\frac{L}{2}, \frac{L}{2})^n$  [BR03] is

$$(e^{-tH_\Lambda^D} \psi)(\xi) = \int_{C_0^t} e^{-\int_0^t V(x(s) + \xi) ds} \psi(x(t) + \xi) \mathbf{1}_{\Omega_\Lambda^t} d\mathbf{m}(x) \quad (8)$$

with  $\Omega_\Lambda^t = \{x \in C_0^t \mid x(s) \in \Lambda \text{ for } 0 \leq s \leq t\}$ . Similarly for the Neumann Laplacian [KM99] one has

$$(e^{-tH_\Lambda^N} \psi)(\xi) = \sum_{u \in \epsilon^{-1}(\xi)} \int_{C_0^t} e^{-\int_0^t V(\epsilon(x(s) + \xi)) ds} \psi(x(t) + \xi) d\mathbf{m} \quad (9)$$

where  $\epsilon : \mathbb{R}^n \rightarrow \Lambda$  with

$$\epsilon_i(x) = \begin{cases} \epsilon_i(x) = x_i - kL & \text{if } (2k - \frac{1}{2})L \leq x_i \leq (2k + \frac{1}{2})L \\ \epsilon_i(x) = (2k + 1)L - x_i & \text{if } (2k + \frac{1}{2})L \leq x_i \leq (2k + \frac{3}{2})L \end{cases}$$

Their integral kernels are computed in an analogue manner as in eq. (7).

## 4 Introduction to Random Schrödinger Operators

This section shall be a short introduction to the topic of random Schrödinger operators, especially their spectral properties. The material is largely taken from [Kir89]. Schrödinger operators with a random potential can be used as a model for disordered quantum systems like amorphous solids or liquids. The specific form to be discussed here is named alloy-type potential.

**Definition 4.1.** *Let  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  measurable such that  $\sum_{i \in \mathbb{Z}^n} |f(\cdot - i)| \in L^p(\mathbb{R}^n)$  with  $p = 1$  for  $n = 1$ ,  $p > 1$  for  $n = 2$  and  $p \geq \frac{n}{2}$  for  $n \geq 3$  and  $(\mathbb{R}^{\mathbb{Z}^n}, \mathcal{F}, P)$  a canonical probability space and  $(q_i(\omega))_{i \in \mathbb{Z}^n} = (\omega(i))_{i \in \mathbb{Z}^n}$  an ergodic stochastic process bounded by some  $M > 0$ , that is the shifts  $T_j$  are ergodic in the sense that  $T_j^{-1}A = A$  for  $A \in \mathcal{F}$  only if  $P(A) = 0$  or 1. Then the potential*

$$V_\omega(x) = \sum_{i \in \mathbb{Z}^n} q_i(\omega) f(x - i) \quad (10)$$

*is called alloy-type-potential. The corresponding Schrödinger operator is named  $H_\omega = -\Delta + V_\omega$  where the sum is in the sense of quadratic forms.*

$H_\omega$  could be a model for a crystal with various atoms on a cubic lattice with  $q_i$  interpreted as charges. The definition includes the possibility of  $q_i$  being independent equally distributed random variables. The reason for the choice of  $p$  becomes clear in view of lemma 1.6 since by boundedness of  $q_i$ ,  $|V_\omega| \leq M \sum_{i \in \mathbb{Z}^n} |f(\cdot - i)| \in L^p(\mathbb{R}^n)$  and therefore  $H_\omega$  is self-adjoint. The unitary operators  $(U_i)_{i \in \mathbb{Z}^n}$  on  $L^2(\mathbb{R}^n)$  defined by  $U_i \psi = \psi(\cdot - i)$  satisfy

$$H_{T_i \omega} = U_i H_\omega U_i^* \quad (11)$$

since  $U_i H_\omega U_i^* \psi = U_i H_\omega U_{-i} \psi = U_i H_\omega \psi(\cdot + i) = U_i (-\Delta \psi(\cdot + i) + V_\omega \psi(\cdot + i)) = H_{T_i \omega} \psi$ .

### 4.1 Measurability

By the form of  $V_\omega$  it is clear that  $V_\omega(x)$  is jointly measurable in  $\omega$  and  $x$ . The concept of measurability can be transferred to operators as follows:

**Definition 4.2.** (i) *A family of bounded operator  $A_\omega$  on  $\mathcal{H}$  is called weakly measurable if  $\langle \psi, A_\omega \phi \rangle$  is measurable in  $\omega$  for all  $\psi, \phi \in \mathcal{H}$ .*

(ii) *A family of self-adjoint operators is called measurable if for any bounded Borel-function  $f : \mathbb{C} \rightarrow \mathbb{C}$  the family  $f(A_\omega)$  is weakly measurable.*

The condition in (ii) might be complicated to check. Luckily the following proposition gives an equivalent condition.

**Proposition 4.3.** *If  $\omega \rightarrow e^{itA_\omega}$  is weakly measurable for all  $t \in \mathbb{R}$  or  $\omega \rightarrow (A_\omega - z)^{-1}$  is weakly measurable for  $z \in \mathbb{C} \setminus \mathbb{R}$ , then the family of self-adjoint operators  $A_\omega$  is measurable.*

*Proof.* Since

$$\mp \int_0^\infty i e^{\mp it(\lambda - z)} dt = \left[ \frac{-1}{\lambda - z} e^{\mp it(\lambda - \Re(z)) \mp t \Im(z)} \right]_0^\infty$$

choosing  $\mp$  according to the sign of  $\Im(z)$  such that the right hand side equals  $\frac{1}{\lambda - z}$ . By the functional calculus

$$\langle \psi, (A_\omega - z)^{-1} \phi \rangle = \mp \int_0^\infty e^{\pm itz} \langle \psi, e^{\mp it A_\omega} \phi \rangle dt$$

the measurability of  $(z - A_\omega)^{-1}$  follows from the measurability of  $e^{itA_\omega}$ . Let any  $a < b \in \mathbb{R}$  and  $\epsilon > 0$  and define the integral

$$I_{a,b}(\epsilon) := \frac{1}{2\pi i} \int_a^b \left( \frac{1}{t - \lambda - i\epsilon} - \frac{1}{t - \lambda + i\epsilon} \right) dt = \int_{a-\lambda}^{b-\lambda} \frac{\epsilon}{(t^2 + \epsilon^2)\pi} dt = \frac{\arctan \frac{b-\lambda}{\epsilon} - \arctan \frac{a-\lambda}{\epsilon}}{\pi}.$$

It's clear that  $\lim_{\epsilon \searrow 0} I_{a,b}(\epsilon) = \frac{1}{2} \mathbb{1}_{[a,b]} + \frac{1}{2} \mathbb{1}_{(a,b)}$  and hence  $\lim_{\delta \searrow 0} \lim_{\epsilon \searrow 0} I_{a-\delta, b+\delta}(\epsilon) = \mathbb{1}_{[a,b]}$ . By the functional calculus also

$$\langle \psi, \mathbb{1}_{[a,b]}(A_\omega) \phi \rangle = \lim_{\delta \searrow 0} \lim_{\epsilon \searrow 0} \frac{1}{2\pi i} \int_{a-\delta}^{b+\delta} \langle \psi, [(t - i\epsilon - A_\omega)^{-1} - (t + i\epsilon - A_\omega)^{-1}] \phi \rangle dt.$$

By approximating any bounded Borel function  $f$  with simple functions of the form  $\sum \alpha_i \mathbb{1}_{(a_i, b_i)}$  it is established that  $\langle \psi, f(A_\omega) \phi \rangle$  is measurable for any Borel function  $f$  and  $\psi, \phi \in \mathcal{H}$ .  $\square$

Actually the Trotter product formula stated above (theorem 3.4) can be used to prove that  $e^{itH_\omega}$  is weakly measurable. Since by lemma 1.6  $V_\omega$  is measurable in  $\omega$  and a small perturbation of  $-\Delta$  this shows that  $H_\omega$  is measurable as the limit of measurable operators.

## 4.2 Spectral properties of $H_\omega$

The following proposition establishes that eq. (11) carries over to the functional calculus

**Proposition 4.4.** *For any bounded measurable function it holds that  $f(H_{T_i\omega}) = U_i f(H_\omega) U_i^*$  and hence  $f(H_\omega)$  is ergodic too.*

*Proof.* By the spectral theorem  $H_\omega = \int \lambda dP_\omega$  with the associated spectral resolution  $P_\omega$ . Then  $\tilde{P}_\omega := U_i P_\omega U_i^*$  is also a spectral resolution satisfying  $H_{T_i\omega} = \int \lambda d\tilde{P}_\omega$  and therefore by uniqueness of the spectral resolution  $\tilde{P}_\omega = P_{T_i\omega}$ . Hence for all Borel sets  $A$ ,  $\mathbb{1}_A(H_\omega) = P_\omega(A) = U_i P_{T_i\omega}(A) U_i^* = U_i \mathbb{1}_A(H_{T_i\omega}) U_i^*$ . If  $f$  is a bounded measurable function this proves  $f(H_{T_i\omega}) = \int f(\lambda) dP_{T_i\omega} = U_i f(H_\omega) U_i^*$ .  $\square$

As seen in the proof for an ergodic family of operators  $H_\omega$ , the family of associated projection operators  $P_\omega$  is also ergodic since  $P_{T_i\omega} = U_i P_\omega U_i^*$ . The next lemma is the key ingredient for the main result of this section.

**Lemma 4.5.** *The projection operators  $P_\omega$  satisfy  $\dim \text{Ran } P_\omega$  is  $P$ -almost surely constant.*

*Proof.* Define  $f : \Omega \rightarrow \mathbb{N}_0 \cup \{\infty\}$  by  $f(\omega) = \dim \text{Ran } P_\omega$  which is invariant since  $f(T_i\omega) = \dim \text{Ran } P_{T_i\omega} = \dim \text{Ran } U_i P_\omega U_i^* = \dim \text{Ran } P_\omega$  where the last equality follows from unitarity of  $U_i$ . To see that  $f$  is measurable choose any orthonormal basis  $e_i$  and note  $f(\omega) = \text{tr}(P_\omega) = \sum \langle e_i, P_\omega e_i \rangle$ . Therefore by proposition 2.3  $f$  is constant.  $\square$

Now we are in position to state the main result of this section

**Theorem 4.6** (due to Pastur [Pas80]). *There is a set  $\Sigma \subset \mathbb{R}$  such that*

$$P(\sigma(H_\omega) = \Sigma) = 1.$$

*Proof.* It's clear that  $\lambda \in \sigma(H_\omega)$  if and only if  $\dim \text{Ran } P_\omega((p, q)) \neq 0$  for all  $p, q \in \mathbb{Q}$  such that  $p < \lambda < q$ . By lemma 4.5 there exist  $\Omega_{p,q}$  of probability 1 such that for  $\omega \in \Omega_{p,q}$ ,  $\dim \text{Ran } P_\omega((p, q))$  is constant and hence  $\lambda \in \sigma(H_{\omega_1})$  if and only if  $\lambda \in \sigma(H_{\omega_2})$  for all  $\omega_1, \omega_2 \in \bigcap_{p,q \in \mathbb{Q}, p < \lambda < q} \Omega_{p,q}$ .  $\square$

Actually as in [Kir89] a few stronger statements about the spectral properties of random Schrödinger operators hold true. As these are not needed in the further discussions they shall be stated here without proof.

**Proposition 4.7.** *Under the assumptions of lemma 4.5  $\dim \text{Ran } P_\omega = \infty$  or 0  $P$ -almost surely.*

**Theorem 4.8.** *Under the assumptions of theorem 4.6 there exist  $\Sigma_c, \Sigma_{ac} \subseteq \mathbb{R}$  such that  $\sigma_c(H_\omega) = \Sigma_c$  and  $\sigma_{ac}(H_\omega) = \Sigma_{ac}$  almost surely. Furthermore  $\sigma_{pp}(H_\omega) = \emptyset$  almost surely.*

The concept of the integrated density of states involves counting the eigenvalues of an operator below a certain threshold. Since Schrödinger operators defined on  $\mathbb{R}^n$  seem to have continuous spectrum this can't be applied directly. The next chapter shall introduce the Schrödinger operators restricted on finite subsets of  $\mathbb{R}^n$  which as seen there have purely discrete spectra.

## 5 Dirichlet-Neumann-Bracketing

This section shall introduce some properties of Dirichlet and Neumann Laplacians defined as form sums. The inequalities between their quadratic forms will be of great importance to establish the existence of the integrated density of states.

### 5.1 Spectrum of the Dirichlet and Neumann Laplacians

In this section the spectral properties of both Laplacians shall be studied. The following lemma taken from [Sch12] is an important tool for the proof that booth Laplacians under certain assumptions on the domain have purely discrete spectrum.



**Lemma 5.1.** *Suppose  $q \geq \gamma$  is a semi-bounded closed form and denote the corresponding operator (theorem 1.1) by  $A_q$ . If the canonical embedding  $(\mathcal{D}(q), \|\cdot\|_q) \rightarrow (\mathcal{H}, \|\cdot\|)$  is compact then the resolvent  $R_\lambda(A_q)$  is compact for all  $\lambda \in \rho(A_q)$  and  $A_q$  has purely discrete spectrum with no accumulation points.*

*Remark 5.2.* As in [Sch12] this assertion is actually an if and only if, but only this direction will be needed.

*Proof.* Let any  $\tilde{\gamma} < \gamma$  and denote by  $\|\cdot\|_q$  the form norm with respect to the constant  $\gamma$ . By the functional calculus it's clear that  $\|(A_q - \tilde{\gamma})^{1/2}\psi\| \geq (\gamma - \tilde{\gamma})^{1/2}\|\psi\|$  and hence  $\|\cdot\|'_{q_A} := \|(A_q - \gamma)^{1/2}\cdot\|$  is a norm on  $\mathcal{D}(q_A)$  equivalent to  $\|\cdot\|_{q_A}$  and it holds that  $\|(A_q - \tilde{\gamma})^{-1/2}\psi\|'_{q_A} = \|\psi\|$ . By the norm equality for  $M \subseteq \mathcal{H}$  bounded  $(A_q - \tilde{\gamma})^{-1/2}M$  is bounded in  $(\mathcal{D}(q_A), \|\cdot\|_{q_A})$  and hence relative compact by the assumption that the embedding is compact proving  $(A_q - \tilde{\gamma})^{-1/2}$  is also compact which is the case if and only if  $(A_q - \tilde{\gamma})^{-1}$  is compact. Due to the resolvent identity

$$R_\lambda(A_q) - R_{\tilde{\gamma}}(A_q) = (\lambda - \tilde{\gamma})R_\lambda(A_q)R_{\tilde{\gamma}}(A_q)$$

$R_\lambda(A_q)$  is therefore compact for all  $\lambda$  in  $\rho(A_q)$ . In order to study the spectrum of  $A_q$  we'd like to show that for any  $\lambda_0 \in \rho(A_q)$

$$\rho(A_q) = \{\lambda_0\} \cup \{\lambda \in \mathbb{C} \mid \lambda \neq \lambda_0, (\lambda - \lambda_0)^{-1} \in \rho(R_{\lambda_0}(A_q))\}. \quad (12)$$

To see this define  $B = A - \lambda_0$ , then it holds that  $R_{\lambda_0} = B^{-1}$  and

$$\lambda \in \rho(A_q) \iff \lambda - \lambda_0 \in \rho(B).$$

Let any  $0 \neq \lambda \in \rho(B)$ , then  $S := BR_\lambda(B)$  is bounded and  $(B^{-1} - \lambda^{-1})S = \lambda^{-1}$  proving that  $B^{-1} - \lambda^{-1}$  is onto. But since  $(B^{-1} - \lambda^{-1})\psi = 0$  implies  $B\psi = \lambda\psi$  and  $\lambda$  is no eigenvalue this implies that  $B^{-1} - \lambda^{-1}$  is invertible and  $(B^{-1} - \lambda^{-1})^{-1} = -\lambda S$  is bounded, therefore  $\lambda^{-1} \in \rho(B^{-1})$ . Analogously it holds that for  $0 \neq \lambda \in \rho(B^{-1})$ ,  $\lambda \in \rho(B)$ , thus eq. (12) is shown. By eq. (12)  $\sigma(A_q)$  is at most countable with no finite accumulation points since it is well known that the compact operator  $R_{\lambda_0}(A_q)$  has at most countable spectrum only accumulating around 0.  $\square$

The question whether the Laplacians have discrete spectra is therefore reduced to two important theorems on compact embeddings which shall be stated here without proof.

**Theorem 5.3** (Rellich's embedding theorem). *(i) For any bounded open  $\Lambda \subset \mathbb{R}^n$  the embedding  $H_0^1(\Lambda) \rightarrow L^2(\Lambda)$  is compact.*

*(ii) If in addition  $\Lambda$  has Lipschitz boundary which is that  $\partial\Lambda$  can be covered by  $\Lambda_1, \dots, \Lambda_n$  such that for each  $k$  in some euclidean coordinate system  $\partial\Lambda \cap \Lambda_k$  is graph of some lipschitz-continuous function, then the embedding  $H^1(\Lambda) \rightarrow L^2(\Lambda)$  is also compact.*

*Proof.* See e.g. [Alt06]. □

For the case needed later of  $\Lambda$  being finite open boxes theorem 5.3 can clearly be applied since boxes have Lipschitz boundary with constant 1. But since in this case it is even possible to construct eigenfunctions with eigenvalues diverging to  $\infty$  the discreteness of the spectra could also be proved more directly. Nevertheless the author chose the presented way since it applies to a much larger class of domains.

## 5.2 Schrödinger Operators on Finite Subsets

In the previous section the spectral properties of the Laplacians  $-\Delta_N^\Lambda$  and  $-\Delta_D^\Lambda$  were studied. We have seen, that the corresponding Hamiltonians can be treated as small perturbations of these Laplacians. For the analysis of the spectral properties of the Neumann and Dirichlet Hamiltonians the important min-max-theorem will turn out to be very useful, which shall be stated here without proof.

**Theorem 5.4** (Min-max). *Let  $A$  be a self-adjoint operator on  $\mathcal{H}$  and define*

$$\mu_n(A) = \sup_{\psi_1, \dots, \psi_{n-1} \in \mathcal{H}} \inf_{\psi \in \mathcal{D}(q_A), \|\psi\|=1, \psi \perp \psi_1, \dots, \psi_{n-1}} q_A(\psi).$$

*Then it holds that  $\sup_{n \in \mathbb{N}} \mu_n(A) = \inf \sigma_{\text{ess}}(A)$ .*

*Proof.* See e.g. Theorem 4.10 in [Tes09]. □

Now the Hamiltonians with potentials as in lemma 1.6 can be defined as form sums  $H_D^\Lambda = -\Delta_D^\Lambda + V$  and  $H_N^\Lambda = -\Delta_N^\Lambda + V$  as above with form domains  $H_0^1(\Lambda)$  or respectively  $H^1(\Lambda)$ . Since by the previous discussion it is already known that the Laplacians have empty essential spectrum by the min-max-theorem  $\mu_n(-\Delta_D^\Lambda) \rightarrow \infty$  and therefore also  $\mu_n(H_D^\Lambda) \geq (1-a)\mu_n(-\Delta_D^\Lambda) - b \rightarrow \infty$ , which by the min-max-theorem again implies that  $H_D^\Lambda$  and analogously  $H_N^\Lambda$  have discrete spectra.

## 5.3 Inequalities between Laplacians

In the following an order relation  $\geq$  for self-adjoint operators by comparing their forms shall be defined. For semi-bounded self-adjoint operators  $A, B$  defined on dense subsets of  $\mathcal{H}$  one can define  $A \leq B$  if  $\mathcal{D}(q_B) \subseteq \mathcal{D}(q_A)$  and  $q_A(\psi) \leq q_B(\psi)$  for all  $\psi \in \mathcal{D}(q_B)$ . The following theorem characterizes important order relations between Neumann and Dirichlet Hamiltonian.

**Theorem 5.5.** (i) *If  $\Lambda \subseteq \Lambda'$ , then  $H_D^{\Lambda'} \leq H_D^\Lambda$*

(ii) *For any  $\Lambda$ ,  $H_N^\Lambda \leq H_D^\Lambda$*

(iii) *If  $\Lambda = \overline{\bigcup_{k=1}^N \Lambda_k}^\circ$  with pairwise disjoint open sets  $\Lambda_k$ , then  $H_D^\Lambda \leq \bigoplus_{k=1}^N H_D^{\Lambda_k}$ .*

(iv) *If  $\Lambda = \overline{\bigcup_{k=1}^N \Lambda_k}^\circ$  with pairwise disjoint open sets  $\Lambda_k$  such that  $\Lambda \setminus \bigcup_{k=1}^N \Lambda_k$  is of measure 0, then  $H_N^\Lambda \geq \bigoplus_{k=1}^N H_N^{\Lambda_k}$ .*

*Proof.* (i) Clearly  $H_0^1(\Lambda) \subseteq H_0^1(\Lambda')$  and  $q_{H_D^\Lambda}(\psi) = q_{H_N^{\Lambda'}}(\psi)$  for all  $\psi \in H_0^1(\Lambda)$ .

(ii) Similarly  $H_0^1(\Lambda) \subseteq H^1(\Lambda)$  and  $q_{H_N^\Lambda}|_{H_0^1(\Lambda)} = q_{H_D^\Lambda}$ .

(iii) Special case of (i) since  $\bigcup_{k=1}^N \Lambda_k \subseteq \Lambda$  and  $H_D^\Lambda \leq H_D^{\Lambda_1 \cup \dots \cup \Lambda_N} = \bigoplus_{k=1}^N H_D^{\Lambda_k}$ .

(iv) Since for  $\psi \in H^1(\Lambda)$ ,  $\psi|_{\Lambda_1} \oplus \dots \oplus \psi|_{\Lambda_N} \in \bigoplus_{k=1}^N H^1(\Lambda_k)$  it is clear that  $\bigoplus_{k=1}^N H^1(\Lambda_k) \subseteq H^1(\Lambda)$ . Moreover since  $\Lambda \setminus \bigcup_{k=1}^N \Lambda_k$  is of measure 0

$$\sum_{k=1}^N q_{H_N^{\Lambda_k}}(\psi|_{\Lambda_k}) = q_{H_N^{\Lambda_1 \cup \dots \cup \Lambda_N}}(\psi) = q_{H_N^\Lambda}(\psi).$$

□

*Remark 5.6.* Clearly these inequalities carry over to  $\mu_n$  from the min-max-theorem.

The main application of the just proved inequalities is the partitioning of  $\Lambda$  in disjoint subsets. Then the inequalities together with the min-max-theorem show that the eigenvalues go up by partitioning in the case of Dirichlet boundary conditions and go down in case of Neumann boundary conditions. Morally speaking this makes sense since adding a *Dirichlet surface* enforces a further requirement on the wave functions (they must vanish on the boundary) whereas removing a *Neumann surface* enforces the wave functions to be more *smooth* on the removed surface.

## 6 Density of States

The integrated density of states measures the *number* of energy levels per unit volume below a given energy. Since the spectrum of the Laplacian and therefore also of the Schrödinger operators on  $\mathbb{R}^n$  is continuous the integrated density of states has to be obtained by a limiting procedure. As seen in section 5.2 the operators  $H_{\omega,\Lambda}^D$  and  $H_{\omega,\Lambda}^N$  with alloy-type potential have discrete spectra if  $\Lambda$  is bounded with Lipschitz boundary. Therefore it makes sense to define the microscopic density of states still dependent on the realization  $\omega$  for any Borel set  $A$  by

$$\nu_{\omega,\Lambda}^D(A) := \#\{n \in \mathbb{N} \mid \mu_n(H_{\omega,\Lambda}^D) \in A\} = \text{tr}(\mathbb{1}_A(H_{\omega,\Lambda}^D)) \quad (13a)$$

$$\nu_{\omega,\Lambda}^N(A) := \#\{n \in \mathbb{N} \mid \mu_n(H_{\omega,\Lambda}^N) \in A\} = \text{tr}(\mathbb{1}_A(H_{\omega,\Lambda}^N)) \quad (13b)$$

where  $\mathbb{1}_A(H)$  is the spectral projection to  $A$  corresponding to the operator  $H$ . For the random point measure concentrated in the discrete spectrum of  $H$  the second equality follows since the trace of a projection is the dimension of its range i.e. the number of eigenfunctions. The corresponding distribution functions are defined by

$$N_{\omega,\Lambda}^D(E) := \nu_{\omega,\Lambda}^D((-\infty, E]) \quad (14a)$$

$$N_{\omega,\Lambda}^N(E) := \nu_{\omega,\Lambda}^N((-\infty, E]). \quad (14b)$$

In the following we want to consider limits of the form<sup>4</sup>  $\frac{\nu_{\omega,\Lambda}^X}{|\Lambda|}$  as  $\Lambda$  fills  $\mathbb{R}^n$ . In fact we shall see now that the limit exists and is macroscopic in the sense that it does not depend on  $\omega$  anymore.

**Theorem 6.1.** *The stochastic processes  $(N_{\omega,\Lambda}^X(E))_{\Lambda \in J}$  are super-/subadditive ergodic processes for  $X = N, D$  and all  $E \in \mathbb{R}$  and hence the limits exist and satisfy*

$$\lim_{L \rightarrow \infty} \frac{N_{\omega,\Lambda_L}^D(E)}{|\Lambda_L|} = \sup_{L \in \mathbb{N}} \frac{\mathbb{E}[N_{\omega,\Lambda_L}^D(E)]}{|\Lambda_L|} =: N^D(E) \text{ } P\text{-almost surely} \quad (15a)$$

$$\lim_{L \rightarrow \infty} \frac{N_{\omega,\Lambda_L}^N(E)}{|\Lambda_L|} = \inf_{L \in \mathbb{N}} \frac{\mathbb{E}[N_{\omega,\Lambda_L}^N(E)]}{|\Lambda_L|} =: N^N(E) \text{ } P\text{-almost surely} \quad (15b)$$

*Proof.* Condition (i) of definition 2.5 is clear by definition. Condition (ii) follows from theorem 5.5 and the fact stated in remark 5.6 that the inequalities carry over to  $\mu_n$  and hence also to  $N_{\omega,\Lambda}^X$ . In order to check condition (iii) let any  $\Lambda \in J$  which can be partitioned in  $|\Lambda|$  cubes of length 1 of the form  $(i, i+1)$  for  $i \in \mathbb{Z}^n$  in the sense that  $\overline{\cup_i (i, i+1)}^\circ = \Lambda$ . Using the inequalities again yields  $N_{\omega,\Lambda}^D(E) \leq N_{\omega,\Lambda}^N(E) \leq \sum N_{\omega,(i,i+1)}^N(E)$  which stays true for the expectations, i.e.  $\mathbb{E}[N_{\omega,\Lambda}^D(E)] \leq \mathbb{E}[N_{\omega,\Lambda}^N(E)] \leq |\Lambda| \mathbb{E}[N_{\omega,(0,1)^n}^N(E)]$ . Therefore it's enough to check that  $\mathbb{E}[N_{\omega,(0,1)^n}^N(E)] < \infty$ . This is true since by the assumption on the uniform boundedness of the  $q_i$ ,  $|V_\omega| \leq |\tilde{V}|$  for some non-random  $\tilde{V} \in L^p(\mathbb{R}^n)$ . Then by lemma 1.6

$$|\langle \psi, V_\omega \psi \rangle| \leq \left| \langle \psi, \tilde{V} \psi \rangle \right| \leq \epsilon \|\nabla \psi\|_2^2 + b(\epsilon, \tilde{V}) \|\psi\|_2^2$$

and therefore

$$\mu_n(H_{\omega,(0,1)^n}^N) \geq (1 - \epsilon) \mu_n(-\Delta_N^{(0,1)^n}) - b(\epsilon, \tilde{V}).$$

Counting the eigenvalues then yields

$$N_{\omega,(0,1)^n}^N(E) \leq \# \left\{ n \in \mathbb{N} \mid \mu_n(-\Delta_N^{(0,1)^n}) \leq \frac{E + b(\epsilon, \tilde{V})}{1 - \epsilon} \right\}$$

which is finite since it was proven in section 5.2 that the eigenvalues of the Neumann-Laplacian on bounded domains with Lipschitz boundary are discrete and converge to infinity. Since the right-hand side is non-random condition (iii) is fulfilled.

Hence theorem 2.6 is applicable and proves the limits claimed. The  $\inf_{L \in \mathbb{N}}$  is due to the fact that in the Neumann case the process is subadditive.  $\square$

*Remark 6.2.* Actually the assumption on the uniform boundedness of the  $q_i$  is not necessary.

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<sup>4</sup>for notational purposes  $X$  can stand for  $D$  and  $N$ .

Instead as proved in [Kir89] it is sufficient to assume

$$\mathbb{E} \left[ \left( \int_{(0,1)} |V_\omega(x)|^p dx \right)^{\frac{n}{2p-n}} \right] < \infty.$$

**Corollary 6.3.** *From the just proved theorem it becomes clear that for any  $\Lambda \in J$*

$$\frac{1}{|\Lambda|} \mathbb{E} [N_{\omega, \Lambda}^D(E)] \leq N^D(E) \leq N^N(E) \leq \frac{1}{|\Lambda|} \mathbb{E} [N_{\omega, \Lambda}^N(E)].$$

The following argument is taken from [Mil12]. The theorem just proved shows that for any *fixed* energy  $E \in \mathbb{R}$  there exists a set  $\Omega_E \subseteq \Omega$  of measure  $P(\Omega_E) = 1$  such that for all  $\omega \in \Omega_E$

$$\lim_{L \rightarrow \infty} \frac{N_{\omega, \Lambda_L}^X(E)}{|\Lambda_L|} = N^X(E). \quad (16)$$

This immediately generalizes to countable sets  $S \subseteq \mathbb{R}$  since  $P(\cap_{\omega \in S} \Omega_E) = 1$ .

Since  $N_{\omega, \Lambda_L}^X(E)$  are non-decreasing in  $E$  the same holds for  $N^X(E)$ . Therefore the following proposition shows that  $N^X(E)$  has at most countably discontinuities.

**Proposition 6.4.** *If  $f : \mathbb{R} \rightarrow \mathbb{R}$  is non-decreasing, then it has at most countably many discontinuities.*

*Proof.* There is a bijection between the discontinuities and disjoint open sets not in the range of  $f$ . Since these are disjoint they are in bijection with a subset of the rationals and therefore countable.  $\square$

Choosing any countable dense set  $\mathcal{D} \subseteq \mathbb{R}$  one defines the countable set  $S = \mathcal{D} \cup A$  with  $A$  being the discontinuities of  $N^X(E)$ . By the preceding paragraph the limit in eq. (16) holds for all  $E \in S$ .

**Lemma 6.5.** *If a sequence of non-decreasing functions  $f_k : \mathbb{R} \rightarrow \mathbb{R}$  converges pointwise to a piecewise continuous function  $f : \mathbb{R} \rightarrow \mathbb{R}$  on a dense subset  $S \subseteq \mathbb{R}$  including the discontinuities of  $f$ , then the convergence holds everywhere.*

*Proof.* Let any  $x \in S^c$  and choose  $\alpha_n \nearrow x$  and  $\beta_n \searrow x$  with  $\alpha_n, \beta_n \in S$ . Then  $\limsup_k f_k(x) \leq \limsup_k f_k(\beta_n) = \lim_{k \rightarrow \infty} f_k(\beta_n) = f(\beta_n) \xrightarrow{n \rightarrow \infty} f(x)$ . Similarly  $\liminf_k f_k(x) \geq f(x)$ .  $\square$

Applying this lemma to  $N^X(E)$  the following proposition is proved.

**Proposition 6.6.** *Under the assumptions of theorem 6.1 there is an subset  $\tilde{\Omega} \subseteq \Omega$  such that for all  $\omega \in \tilde{\Omega}$  and all  $E \in \mathbb{R}$*

$$\lim_{L \rightarrow \infty} \frac{N_{\omega, \Lambda_L}^D(E)}{|\Lambda_L|} = \sup_{L \in \mathbb{N}} \frac{\mathbb{E} [N_{\omega, \Lambda_L}^D(E)]}{|\Lambda_L|} =: N^D(E) \quad (17a)$$

$$\lim_{L \rightarrow \infty} \frac{N_{\omega, \Lambda_L}^N(E)}{|\Lambda_L|} = \inf_{L \in \mathbb{N}} \frac{\mathbb{E}[N_{\omega, \Lambda_L}^N(E)]}{|\Lambda_L|} =: N^N(E). \quad (17b)$$

Since the boundary conditions are artificially imposed and not properties of the physical system one would hope that  $N^D$  and  $N^N$  coincide. In the next section an alternative approach to the integrated density of states shall be introduced and afterwards it will be proved that all three definitions are more or less the same.

## 6.1 Alternative Approach to the Integrated Density of States

Inspired by eq. (13) one might define the integrated density of states as follows. Let  $\mathbb{1}_\Lambda$  denote the multiplication operator of the set  $\Lambda$ .

**Proposition 6.7.** *For any  $\phi \in C^\infty(\mathbb{R})$  (continuous bounded functions  $\mathbb{R} \rightarrow \mathbb{R}$ )*

$$\lim_{L \rightarrow \infty} \frac{1}{|(-L, L)^n|} \text{tr}(\phi(H_\omega) \mathbb{1}_{(-L, L)^n}) = \mathbb{E}[\text{tr}(\phi(H_\omega) \mathbb{1}_{(0,1)^n})] \text{ } P\text{-almost surely.}$$

*Proof.* The sequence  $(X_i)_{i \in \mathbb{Z}^n}$  defined by  $X_i = \text{tr}(\phi(H_\omega) \mathbb{1}_{(i, i+1)^n})$  is clearly ergodic. Hence Birkhoff's ergodic theorem (theorem 2.4) implies

$$\lim_{L \rightarrow \infty} \frac{1}{|(-L, L)^n|} \text{tr}(\phi(H_\omega) \mathbb{1}_{(-L, L)^n}) = \lim_{L \rightarrow \infty} \frac{1}{|(-L, L)^n|} \sum_{i \in \mathbb{Z}^n \cap [-L, L-1]^n} X_i = \mathbb{E}[\text{tr}(\phi(H_\omega) \mathbb{1}_{(0,1)^n})]$$

$P$ -almost surely. □

$\frac{1}{|(-L, L)^n|} \text{tr}(\phi(H_\omega) \mathbb{1}_{(-L, L)^n})$  and  $\mathbb{E}[\text{tr}(\phi(H_\omega) \mathbb{1}_{(0,1)^n})]$  are positive linear functionals on  $C^\infty(\mathbb{R})$  and by the Riesz-Markov-Theorem define measures  $\nu_L$  and  $\nu$  such that

$$\int \phi \, d\nu_L = \frac{1}{|(-L, L)^n|} \text{tr}(\phi(H_\omega) \mathbb{1}_{(-L, L)^n}) \quad (18a)$$

$$\int \phi \, d\nu = \mathbb{E}[\text{tr}(\phi(H_\omega) \mathbb{1}_{(0,1)^n})]. \quad (18b)$$

It will be seen that the measures  $\nu_L$  converge to  $\nu$  in the following sense<sup>5</sup>.

**Definition 6.8.** *We say a sequence of measure  $\nu_n$  converges to  $\nu$  vaguely if for any  $f \in C_c(\mathbb{R})$*

$$\int f \, d\mu_n \rightarrow \int f \, d\mu \text{ as } n \rightarrow \infty$$

For any  $\phi \in C_c(\mathbb{R})$  the convergence  $\int \phi \, d\nu_L \rightarrow \int \phi \, d\nu$  holds for  $\omega \in \Omega_\phi$  for a set of full measure. Choosing a countable dense set  $S \subseteq C_c(\mathbb{R})$  and approximating  $\phi \in C_c$  by  $\phi_n \in S$

$$\int \phi \, d\nu_L \rightarrow \int \phi \, d\nu$$

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<sup>5</sup>Actually the measures are said to converge weakly since the convergence holds for any bounded continuous function, but the notion of vague convergence is sufficient and will be used later again.

for  $\omega \in \bigcap_{\theta \in S} \Omega_\theta$  of full measure. This argument proves

**Proposition 6.9.** *The measures  $\nu_L$  converge to  $\nu$  vaguely  $P$ -almost surely.*

The corresponding distribution functions  $N_L(E) = \nu_L((-\infty, E])$  converge to  $N(E) = \nu((-\infty, E])$  in all points of continuity of the latter  $P$ -almost surely by the following proposition.

**Proposition 6.10.** *A sequence  $\mu_n$  of Borel measures on  $\mathbb{R}$  converge  $\mu_n \rightarrow \mu$  vaguely if and only if the normalized distribution function converges everywhere pointwise except points of continuity.*

*Proof as in [Tes09].* Let any open interval  $(a, b) \subseteq \mathbb{R}$ , then for all  $f, g \in C_c(\mathbb{R})$  such that  $f \leq \mathbb{1}_{(a, b)} \leq g$

$$\mu((a, b)) - \mu_n((a, b)) \leq \int (g - f) d\mu + \left| \int f d\mu - \int f d\mu_n \right|$$

and similarly for  $-(\mu((a, b)) - \mu_n((a, b)))$ . Hence

$$|\mu((a, b)) - \mu_n((a, b))| \leq \int (g - f) d\mu + \left| \int f d\mu - \int f d\mu_n \right| + \left| \int g d\mu - \int g d\mu_n \right|.$$

Choosing  $f, g$  such that  $g - f$  approximates  $\mathbb{1}_{\{a\}} + \mathbb{1}_{\{b\}}$  yields (by dominated convergence)  $\limsup_{n \rightarrow \infty} \leq \mu(\{a\}) + \mu(\{b\})$  and therefore proves convergence at every point where  $\mu(\{a\}) = 0$ , i.e. every point of continuity.

Now assume that convergence of distribution is pointwise at every point of continuity. Let any  $f \in C_c(\mathbb{R})$  and  $\epsilon > 0$ , then by uniform continuity there exists  $\delta > 0$  such that  $|x - y| < \delta \implies |f(x) - f(y)| < \epsilon$ . Fix points of continuity  $x_0 < \dots < x_k$  of  $\mu$  such that  $\text{supp } f \subseteq (x_0, x_k)$  and  $x_j - x_{j-1} < \delta$ . Then

$$\begin{aligned} \left| \int f d\mu_n - \int f d\mu \right| &\leq \sum_{j=1}^k \left[ \int_{(x_{j-1}, x_j)} |f(x) - f(x_j)| d\mu_n + |f(x_j)| |\mu((x_{j-1}, x_j)) - \mu_n((x_{j-1}, x_j))| \right] \\ &\quad \sum_{j=1}^k \int_{(x_{j-1}, x_j)} |f(x) - f(x_j)| d\mu(x) \end{aligned}$$

shows the claim since the terms on the right can be estimated in terms of  $\epsilon$ .  $\square$

This shows that there exists  $\tilde{\Omega} \subseteq \Omega$  of measure 1 such that  $N_L(E) \xrightarrow{L \rightarrow \infty} N(E)$  for all  $\omega \in \tilde{\Omega}$  and all points of continuity  $E$ . To see that in the present case the convergence holds indeed everywhere note that  $N(E)$  has again at most countable many discontinuities  $S$  and the convergence holds for any fixed  $E \in S$  for a set  $\Omega_E$ . Hence  $\Omega_0 = \tilde{\Omega} \cap (\bigcap_{E \in S} \Omega_E)$  still has full measure and the convergence for  $\omega \in \Omega_0$  holds everywhere.

## 6.2 Feynman-Kac-Representation

The concluding section of this thesis shall be devoted to the proof that the quantities  $N, N^D, N^N$  do indeed agree. It follows [KM07, Kir89, CL90] closely. The idea of the proof will be to show

that their Laplace transforms coincide and therefore by the uniqueness of the Laplace transform  $N, N^D, N^N$  do so as well.

**Definition 6.11.** *The Laplace-Stieltjes transform of a probability distribution  $N$  is defined by*

$$\tilde{N}(t) = \int e^{-t\lambda} dN(\lambda). \quad (19)$$

The laplace transform is linear and unique (see e.g. [Fel71]).

We start to compute

$$\begin{aligned} \tilde{N}_{\omega, \Lambda_L}^D(t) &= \sum_{\lambda \in \sigma(H_{\omega, \Lambda}^D)} e^{-t\lambda} = \text{tr}(e^{-tH_{\omega, \Lambda_L}^D}) = \sum_n \langle \psi_n, e^{-tH_{\omega, \Lambda_L}^D} \psi_n \rangle \\ &= \int_{\mathbb{R}^n} \sum_n \psi_n(u) \int_{\mathbb{R}^n} e^{-tH_{\omega, \Lambda_L}^D}(x, y) \overline{\psi_n(v)} dv du = \int_{\mathbb{R}^n} e^{-tH_{\omega, \Lambda_L}^D}(u, u) du \\ &= \int_{\Lambda_L} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_{\omega}(x(s)) ds} \mathbb{1}_{\Omega_{\Lambda_L}^t} d\mathbf{m}_{0,u}^{t,u}(x) du \end{aligned}$$

Intuitively the factor  $\mathbb{1}_{\Omega_{\Lambda}^t}$  should get less important as  $\Lambda_L$  fills  $\mathbb{R}^n$  since the Wiener process gets less probable to reach the boundary. Rigorously this can be seen as follows

$$\begin{aligned} \frac{1}{|\Lambda_L|} \int_{\Lambda_L} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_{\omega}(x(s)) ds} \mathbb{1}_{\Omega_{\Lambda_L}^t} d\mathbf{m}_{0,u}^{t,u}(x) du &= \underbrace{\frac{1}{|\Lambda_L|} \int_{\Lambda_L} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_{\omega}(x(s)) ds} d\mathbf{m}_{0,u}^{t,u}(x) du}_{:= A_L} \\ &\quad - \underbrace{\frac{1}{|\Lambda_L|} \int_{\Lambda_L} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_{\omega}(x(s)) ds} (1 - \mathbb{1}_{\Omega_{\Lambda_L}^t}) d\mathbf{m}_{0,u}^{t,u}(x) du}_{:= B_L} \end{aligned}$$

Writing  $A_L$  in the form

$$\frac{1}{|\Lambda_L|} \sum_{i \in \mathbb{Z}^n \cap [-L, L-1]^n} \int_{[i, i+1)} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_{\omega}(x(s)) ds} d\mathbf{m}_{0,u}^{t,u}(x) du =: \frac{1}{|\Lambda_L|} \sum_{i \in \mathbb{Z}^n \cap [-L, L-1]^n} X_i(\omega)$$

with  $(X_i)_{i \in \mathbb{Z}^n}$  ergodic and stationary since  $\mathcal{L}[(X_i)_{i \in \mathbb{Z}^n}] = \mathcal{L}[(X_{i+j})_{i \in \mathbb{Z}^n}]$  (by the ergodicity assumptions on  $V_{\omega}$ ) satisfies the requirements of Birkhoff's ergodic theorem and therefore

$$A_L \xrightarrow{L \rightarrow \infty} \mathbb{E}[X_0] = \mathbb{E} \left[ \int_{[0,1)^n} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_{\omega}(x(s)) ds} d\mathbf{m}_{0,u}^{t,u}(x) du \right]$$

$P$ -almost surely where  $\mathbb{E}[\cdot]$  is meant with respect to  $\omega$ .



To prove that  $B_L \rightarrow 0$  note that by Hölder's inequality with  $1 < q < \infty$

$$B_L \leq \underbrace{\left( \frac{1}{|\Lambda_L|} \int_{\Lambda_L} \int_{C_{0,u}^{t,u}} e^{-q \int_0^t V_\omega(x(s)) ds} d\mathbf{m}_{0,u}^{t,u} du \right)^{\frac{1}{q}}}_{:=C_L} \cdot \underbrace{\left( \frac{1}{|\Lambda_L|} \int_{\Lambda_L} \int_{C_{0,u}^{t,u}} (1 - \mathbb{1}_{\Omega_{\Lambda_L}^t}) d\mathbf{m}_{0,u}^{t,u} du \right)^{\frac{q}{q-1}}}_{:=D_L}$$

$C_L$  can be treated in the same way as  $A_L$  proving that

$$C_L \rightarrow \mathbb{E} \left[ \int_{[0,1]^n} \int_{C_{0,u}^{t,u}} e^{-q \int_0^t V_\omega(x(s)) ds} d\mathbf{m}_{0,u}^{t,u}(x) du \right]^{\frac{1}{q}}$$

$P$ -almost surely. For  $D_L$  note that  $(1 - \mathbb{1}_{\Omega_{\Lambda_L}^t}) = 1$  if and only if  $x(s) \notin \Lambda_L$  for some  $0 < s < t$ . By Fubini's theorem

$$D_L = \left( \int_{C_{0,u}^{t,u}} \int_{\Lambda_L} \frac{1 - \mathbb{1}_{\Omega_{\Lambda_L}^t}}{|\Lambda_L|} du d\mathbf{m}_{0,u}^{t,u} \right)^{\frac{q}{q-1}}$$

where the integrand  $\int_{\Lambda_L} \frac{1}{|\Lambda_L|} (1 - \mathbb{1}_{\Omega_{\Lambda_L}^t}) du$  is bounded by 1 uniform in  $x \in C_{0,u}^{t,u}$  and converges to 0 for any fixed path  $x$ . Thus by dominated convergence  $D_L \xrightarrow{L \rightarrow \infty} 0$   $P$ -almost surely. Altogether we have proven:

**Theorem 6.12.** *Under the assumption*

$$\mathbb{E} \left[ \int_{[0,1]^n} \int_{C_{0,u}^{t,u}} e^{-q \int_0^t V_\omega(x(s)) ds} d\mathbf{m}_{0,u}^{t,u}(x) du \right] < \infty$$

for some  $1 < q < \infty$  the Laplace transform of  $N^D$  is given by

$$\tilde{N}^D(t) = \mathbb{E} \left[ \int_{[0,1]^n} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_\omega(x(s)) ds} d\mathbf{m}_{0,u}^{t,u}(x) du \right] = \text{tr}(e^{-tH_\omega} \mathbb{1}_{[0,1]^n}).$$

The computation of the Laplace transform of  $N$  works in a similar manner. The analog computation yields

$$\begin{aligned} \tilde{N}_L(t) &= \int e^{-\lambda t} d\nu_L = \frac{1}{|\Lambda_L|} \text{tr}(e^{-tH_\omega} \mathbb{1}_{\Lambda_L}) = \frac{1}{|\Lambda_L|} \int_{\Lambda_L} e^{-tH_\omega}(u, u) du \\ &= \frac{1}{|\Lambda_L|} \int_{\Lambda_L} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_\omega(x(s)) ds} d\mathbf{m}_{0,u}^{t,u}(x) du \xrightarrow{L \rightarrow \infty} \mathbb{E} \left[ \int_{[0,1]^n} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_\omega(x(s)) ds} d\mathbf{m}_{0,u}^{t,u}(x) du \right] \end{aligned}$$

$P$ -almost surely and therefore proves:

**Theorem 6.13.** *The Laplace transform of  $N$  is given by*

$$\tilde{N}(t) = \mathbb{E} \left[ \int_{[0,1]^n} \int_{C_{0,u}^{t,u}} e^{-\int_0^t V_\omega(x(s)) ds} d\mathbf{m}_{0,u}^{t,u}(x) du \right] = \text{tr}(e^{-tH_\omega} \mathbb{1}_{[0,1]^n}).$$

To see that the same result also holds for  $N^N$  a similar computation is necessary which shall not be stated here (see [KM99]). By the uniqueness of the Laplace transform we have proven that all three concepts of the integrated density of states actually coincide under rather weak conditions.

**Corollary 6.14.** *Under the condition of theorem 6.12 we have  $N(E) = N^D(E) = N^N(E)$  at all continuity points.*

*Proof.* We have seen that  $\tilde{N}(t) = \tilde{N}^D(t) = \tilde{N}^N(t)$ . As in VIII.1 from [Fel71] the Laplace transform of a distribution function does not depend on the behaviour in the discontinuities and is unique modulo the behaviour at the discontinuities. Therefore  $N(E) = N^D(E) = N^N(E)$  at all points of continuity.  $\square$

Combining the above results it just remains to pick the correct behaviour at the discontinuities to prove everywhere pointwise convergence. Therefore a small lemma is needed.

**Lemma 6.15.** (i) *The supremum of sequence of left-continuous non-decreasing functions  $f_k : \mathbb{R} \rightarrow \mathbb{R}$ ,  $f(x) := \sup_k f_k(x)$  is also left-continuous wherever it is finite.*

(ii) *Analogously the infimum of right-continuous non-decreasing functions is right-continuous wherever it is finite.*

*Proof.* Let any  $x \in \mathbb{R}$  be a point of discontinuity of  $f$  and choose a sequence  $x_n \nearrow x$ . Then  $f(x_n) \leq f(x)$  for any  $n \in \mathbb{N}$ . Now fix any  $\epsilon > 0$  and choose  $k_0$  such that  $f(x) \leq f_{k_0}(x) + \frac{\epsilon}{2}$  and  $n_0$  such that  $f_{k_0}(x) \leq f_{k_0}(x_{n_0}) + \frac{\epsilon}{2}$ . Then  $f(x) \leq f_{k_0}(x) + \frac{\epsilon}{2} \leq f_{k_0}(x_{n_0}) + \epsilon \leq \sup_k f_k(x_{n_0}) + \epsilon = f(x_{n_0}) + \epsilon$  and the claim follows since  $\epsilon$  was arbitrary. The proof of (ii) is similar.  $\square$

Redefining the Dirichlet density of states by

$$N_{\omega, \Lambda}^D(E) := \nu_{\omega, \Lambda}^D((-\infty, E)), \quad N^D(E) := \sup_{L \in \mathbb{N}} \frac{N_{\omega, \Lambda_L}^D(E)}{|\Lambda_L|}$$

makes it a left-continuous function (by lemma 6.15) agreeing with the density of states defined earlier in points of continuity. Analogously the Neumann density of states as defined earlier is right-continuous. Altogether we have the following theorem.

**Theorem 6.16.** *There exists a set  $\tilde{\Omega} \subseteq \Omega$  of measure 1 such that*

$$\lim_{L \rightarrow \infty} \frac{N_{\omega, \Lambda_L}^D(E)}{|\Lambda_L|} = \sup_{L \in \mathbb{N}} \frac{\mathbb{E}[N_{\omega, \Lambda_L}^D(E)]}{|\Lambda_L|} = \nu((-\infty, E)) = \mathbb{E}[\text{tr}(\mathbb{1}_{(-\infty, E)}(H_\omega) \mathbb{1}_{(-L, L)^n})] \quad (20a)$$

$$\lim_{L \rightarrow \infty} \frac{N_{\omega, \Lambda_L}^N(E)}{|\Lambda_L|} = \inf_{L \in \mathbb{N}} \frac{\mathbb{E}[N_{\omega, \Lambda_L}^N(E)]}{|\Lambda_L|} = \nu((-\infty, E]) = \mathbb{E}[\text{tr}(\mathbb{1}_{(-\infty, E]}(H_\omega) \mathbb{1}_{(-L, L)^n})] \quad (20b)$$

for all  $E \in \mathbb{R}$  and  $\omega \in \tilde{\Omega}$ . Furthermore the right-continuous density of states measure  $\nu((-\infty, E])$  can be approximated on any  $n$ -dimensional interval  $\Lambda \in J$  by

$$\frac{1}{|\Lambda|} \mathbb{E}[N_{\omega, \Lambda}^D(E)] \leq N^D(E) \leq \nu((-\infty, E]) = N^N(E) \leq \frac{1}{|\Lambda|} \mathbb{E}[N_{\omega, \Lambda}^N(E)]$$

and analogously the left-continuous density of states measure  $\nu((-\infty, E))$  can be approximated on any  $n$ -dimensional interval  $\Lambda \in J$  by

$$\frac{1}{|\Lambda|} \mathbb{E} [N_{\omega, \Lambda}^D(E)] \leq N^D(E) = \nu((-\infty, E)) \leq N^N(E) \leq \frac{1}{|\Lambda|} \mathbb{E} [N_{\omega, \Lambda}^N(E)] .$$

*Proof.* After the above argument it just remains to mention that the expectations on the right hand side of eq. (20) have exactly the desired behaviour in the discontinuities. The second claim follows immediately from corollary 6.3.  $\square$

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