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Random Hamiltonians Ergodic in All But One Direction

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Abstract. Let $V_\omega^{(1)}$ and $V_\omega^{(2)}$ be two ergodic random potentials on $\mathbb{R}^d$. We consider the Schrödinger operator $H_\omega = H_0 + V_\omega$, with $H_0 = -\Delta$ and for $x = (x_1, \ldots, x_d)$

$$V_\omega(x) = \begin{cases} V_\omega^{(1)}(x) & \text{if} \quad x_1 < 0 \\ V_\omega^{(2)}(x) & \text{if} \quad x_1 \geqq 0 \end{cases}.$$

We prove certain ergodic properties of the spectrum for this model, and express the integrated density of states in terms of the density of states of the stationary potentials $V_\omega^{(1)}$ and $V_\omega^{(2)}$. Finally we prove the existence of the density of surface states for H_ω.

1. Introduction

In this paper we consider Schrödinger operators $H_\omega = H_0 + V_\omega$ with random potential V_ω on $L^2(\mathbb{R}^d)$. The random potential V_ω we consider has different behavior in the left and right half space. More precisely, there are two ergodic random fields V_ω^+ and V_ω^- on $\mathbb{R}^d$ such that V_ω agrees with V_ω^+ in one half space and with V_ω^- in the complementary half space. To be specific we assume $V_\omega(x) = V_\omega^+$ for $x_1 \geqq 0$ and $V_\omega(x) = V_\omega^-(x)$ for $x_1 < 0$.

Thus V_ω is not an ergodic potential (unless $V_\omega^\pm$ happen to agree). Consequently, the general theory of ergodic potentials (see e.g. [4, 2, 10] and references therein) does not apply. For example, a priori the spectrum $\sigma(H_\omega)$ may depend on ω. In fact, Molcanov and Seidel [15] consider the one dimensional case in detail. They prove that, in their special case, the spectrum $\sigma(H_\omega)$ consists of the half line $[0, \infty)$ plus an additional isolated negative eigenvalue. This eigenvalue depends on the random parameters.

We will prove in the next section that in the higher dimensional case ($d > 1$) the spectrum is non-random under very mild assumptions. The main difference between $d = 1$ and $d > 1$ lies in the "ergodicity" of the potential under shifts parallel to the surface of the half space, which clearly does not apply to the one dimensional case.

Carmona [3] also considers the one dimensional case. He looks at the measure theoretic nature of the spectrum. Carmona proved the remarkable fact that, under suitable assumptions, $H_\omega = H_0 + V_\omega$ has absolutely continuous resp. p.p. spectrum if H_ω^+ has ac. resp. p.p. spectrum near E and $E \notin \sigma(H_\omega^-)$.

The only paper about the multidimensional case we are aware of is the paper [5] by Davies and Simon. While they treat only periodic $V_\omega^\pm$ this paper was one of our main motivations.

Our paper is organized as follows: In Sect. 2 we give some basic results about the spectrum of H_ω. We prove that $\sigma(H_\omega)$ is non-random and contains the spectra $\sigma(H_\omega^+) \cup \sigma(H_\omega^-)$. In general, however, $\sigma(H_\omega)$ is bigger than $\sigma(H_\omega^+) \cup \sigma(H_\omega^-)$ and we give a class of examples for this phenomenon. We call the energies in $\sigma(H_\omega^+) \cup \sigma(H_\omega^-)$ the bulk spectrum and the other energies in $\sigma(H_\omega)$ surface spectrum. This notation is justified by proving that points in the surface spectrum correspond to Weyl sequences concentrated near the surface $\{x_1 = 0\}$.

Section 3 discusses the density of states for H_ω. We show that the integrated density of states for H_ω is nothing but the arithmetic mean of the density of states of H_ω^+ and H_ω^-. Therefore the density of states is unable to detect the surface states. It is rather straightforward to conjecture that this is due to the fact that we normalize by a volume in the density of states while we should normalize by a surface term to grasp the surface states. This conjecture is proven in Sect. 3 and 4. In fact, we prove that there is a density of surface state which exists as a measure in the gaps of the bulk spectrum. Inside the bulk spectrum, the density of surface states exists in the sense of a next order correction to the (bulk) density of state. In this case, however, we can only prove existence in the sense of a (Schwarz) distribution.

The result about the density of surface states was already obtained for the Anderson model by two of the authors [7]. See also [8] and references therein for the consideration of special cases. Our results have been announced in [6].

In Sect. 5 we discuss some extensions and modifications of our results.

2. Basic Definitions and Results

Throughout this paper, we take $d \geqq 2$. Let $V_\omega(x)$, $x \in \mathbb{R}^d$ be a random field on a probability space $(\Omega, \mathbb{F}, P)$. V_ω is called $\mathbb{R}^d$-stationary (respectively $\mathbb{Z}^d$-stationary) if there is a family $\{T_i\}_{i \in I}$ of measure-preserving transformations on $(\Omega, \mathscr{F}, P)$ with index set $I = \mathbb{R}^d$ (respectively $\mathbb{Z}^d$), such that $V_{T_i\omega}(x) = V_\omega(x - i)$. We call a random field stationary if it is $\mathbb{R}^d$-stationary or $\mathbb{Z}^d$-stationary. V_ω is called ergodic (respectively $\mathbb{R}^d$-ergodic, respectively $\mathbb{Z}^d$-ergodic) if the corresponding measure preserving transformations are ergodic, i.e. if any set $A \in \mathscr{F}$ invariant under all T_i has probability zero or one. There is an easy procedure, the "suspension technique," to transfer results from the $\mathbb{R}^d$-ergodic case to the $\mathbb{Z}^d$-ergodic case almost automatically (see [9]). We will use suspension freely in what follows.

The general situation we consider in this paper is the following: V_ω^+ and V_ω^- are two ergodic random fields on $\mathbb{R}^d$, independent of each other. We set for

$x=(x_1,\ldots,x_d)\in\mathbb{R}^d$:

$$V_\omega(x)=\begin{cases}V_\omega^+(x) & \text{for} \quad x_1\geqq 0\\ V_\omega^-(x) & \text{for} \quad x_1<0\end{cases}. \tag{2.1}$$

V_ω is obviously not an ergodic potential. In fact, it is not even stationary. However, it is stationary with respect to those T_i with $i_1=0$, i.e. for shifts perpendicular to the x_1-axis. While some of our results below remain true in a more general situation, we will suppose a further condition on the ergodic potentials $V_\omega^\pm$ which roughly speaking, ensures that no direction in space is distinguished by the process.

Definition. We call a family $\{T_i\}_{i\in I}$ ($I=\mathbb{Z}^d$ or $\mathbb{R}^d$) isotropically ergodic, if the families $T_{\Pi_\nu i}$ for $\nu=1,\ldots,d$ are ergodic, where Π_ν is the projection onto the ν^{th} coordinate axis.

Remark. It is easy to see that any mixing family is isotropically ergodic.

Examples. 1. Any periodic potential is an isotropic $\mathbb{Z}^d$-ergodic process (on a finite probability space).
2. Suppose that g_i are i.i.d. random variables and that

$$f\in l^1(L^2):=\left\{\varphi\,\middle|\,\sum_{i\in\mathbb{Z}_d}\left(\int_{C_0}|\varphi(x-i)|^2dx\right)^{1/2}<\infty\right\}$$

(where $C_0=\{x\in\mathbb{R}^d\,|\,-1/2\leqq x_\nu\leqq 1/2,\ \nu=1,\ldots,d\}$). Then the alloy-type potential

$$V_\omega(x)=\sum g_i(\omega)f(x-i)$$

is isotropically $\mathbb{Z}^d$-ergodic.
3. A homogeneous Gaussian process with correlation function vanishing at infinitely is isotropically ergodic.

Henceforth we assume $d\geqq 2$ and that $V^\pm$ are isotropically ergodic.

Theorem 1. *The spectrum $\sigma(H_\omega)$ of H_ω is a non-random set (i.e. there is a set $\Sigma\subset\mathbb{R}$, s.t. $\Sigma=\sigma(H_\omega)$ P-a.s.). The same is true for the pure point, singular continuous, and absolutely continuous part of the spectrum. The discrete spectrum of H_ω is a.s. empty.*

The proof is a not too difficult adjustment of the proof in [11] (see also Pastur [17] and Kunz-Souillard [14]). Another consequence of the ergodicity is the following result. Let us denote by $\Sigma^\pm$ the (a.s. constant) spectra of $H_\omega^\pm$. Set $\Sigma_0=\Sigma^+\cup\Sigma^-$.

Theorem 2. *The spectrum, Σ, of H_ω contains Σ_0.*

Proof. Suppose $E\in\Sigma^+$. Then there is a Weyl sequence ψ_n, $\|\psi_n\|=1$, ($\|H_\omega^+-E)\psi_n\|\to 0$ and $\psi_n\in C_0^\infty(\mathbb{R}^d)$. Take $\varepsilon>0$ arbitrary. Denote by K_n the compact support of ψ_n. Consider the set

$$\Omega_{n,\varepsilon}=\left\{\omega\,\middle|\,\left(\int_{K_n}|V_\omega(x)-V_\omega(x+(i,0))|^2dx\right)^{1/2}<\varepsilon \text{ for infinitely many } i\geqq 0\right\}.$$

By Poincaré's recurrence theorem this event has probability one. Thus for P-almost all ω there exist $\tilde{\psi}_n(x)=\psi_n(x+i)$ such that $\operatorname{supp}\tilde{\psi}_n\subset\{x_1>0\}$, $\|\tilde{\psi}_n\|=1$ and

$(H_\omega^+ - E)\tilde{\psi}_n \to 0$. Consequently $\tilde{\psi}_n$ is a Weyl sequence for H_ω and E, i.e. $E \in \sigma(H_\omega)$. □

This result, of course, raises the question whether Σ_0 is already all of Σ. The question was considered in [5] for the special case of periodic $V_\omega^\pm$. These authors found, in fact, additional spectrum in general. They called the corresponding states surface states, a notion we adopt. We call the corresponding energies in $\Sigma \backslash \Sigma_0$ the "surface energies," while we sometimes refer to Σ_0 as the "bulk spectrum."

To construct additional examples of H_ω with $\Sigma \backslash \Sigma_0 \neq \phi$ we consider more closely the spectrum of H_ω in the case of alloy-type potentials, i.e.:

$$V_\omega^\pm(x) = \sum_{i \in \mathbb{Z}^d} q_i^{(\pm)}(\omega) f^{(\pm)}(x-i). \tag{2.2}$$

We assume that the q_i^+, q_j^- are independent with distributions $P_0^\pm$ and that the measures $P_0^\pm$ have compact support. Moreover, we assume that

$$f^{(\pm)} \in l^1(L^p) = \left\{ f \,\middle|\, \sum_{i \in \mathbb{Z}^d} \left(\int_{C_0} |f(x-i)|^p dx \right)^{1/p} < \infty \right\}$$

with $C_0 = \{x \mid 0 \leqq x_i < 1; i = 1, \ldots, d\}$ and some $p > \max\left(1, \frac{d}{2}\right)$. By $\mathscr{P}$ we denote the class of all potentials W of the form:

$$W_\omega(x) = \begin{cases} \Sigma \lambda_i^- f^-(x-i) & \text{for} \quad x_1 < 0 \\ \Sigma \lambda_i^+ f^+(x-i) & \text{for} \quad x_1 \geqq 0 \end{cases},$$

with $\lambda_i^\pm$ periodic sequences (with some period) and $\lambda_i^\pm \in \operatorname{supp} P_0^\pm$. Following [7] or [12] it is not difficult to show:

Theorem 3.
$$\Sigma = \overline{\bigcup_{W \in \mathscr{P}} \sigma(H_0 + W)}. \tag{2.2}$$

Take now periodic potentials $V^\pm = \Sigma \lambda^\pm f^\pm(x-i)$ and $V(x) = V^\pm(x)$ for $\pm x_1 > 0$, such that $\sigma(H_0 + V) \backslash (\sigma(H^+) \cup \sigma(H^-)) \neq \phi$. Potentials $V^\pm$ with this property can be constructed by the methods in [5]. Now we choose distribution $P_0^\pm$ concentrated close to $\lambda^\pm$ and consider $V_\omega(x)$ as in (2.2) with these distributions. Then, by the above theorem we have $\sigma(H_0 + V) \subset \Sigma (= \sigma(H_\omega))$. But by shrinking $\operatorname{supp} P_0^\pm$ we can make $\sigma(H_\omega^\pm)$ arbitrarily close to $\sigma(H^\pm)$. Thus by taking $\operatorname{supp} P_0^\pm$ small enough we get $\Sigma \backslash (\sigma(H_\omega^+) \cup \sigma(H_\omega^-)) \neq \phi$ (−almost surely).

While we believe the notion of "surface energies" for points in $\Sigma \backslash \Sigma_0$ is rather intuitive, we will "justify" this notion further in various ways in the following. Recall that according to Weyl's criterion (see e.g. [18]) for any $E \in \sigma(H)$ there is a sequence $\psi_n \in L^2(\mathbb{R}^d)$ ("Weyl sequence") with $\|\psi_n\| = 1$ and $H\psi_n - E\psi_n \to 0$. The next result tells us that a Weyl sequence for a surface energy remains close to the surface $\{x_1 = 0\}$. Here we can work in the following general setting: Suppose $V^\pm$ are operator bounded potential (with relative bounds less than 1). Set

$$V(x) = \begin{cases} V^-(x) & \text{for} \quad x_1 < 0 \\ V^+(x) & \text{for} \quad x_1 \geqq 0 \end{cases}$$

and $\Sigma^\pm = \sigma(H_0 + V^\pm)$, $\Sigma_0 = \Sigma^+ \cup \Sigma^-$, $\Sigma = \sigma(H_0 + V)$. Let us, furthermore, denote by χ_R the characteristic function of the set $S_R = \{x \mid |x_1| \leqq R\}$.

Theorem 4. *If $E \in \Sigma \backslash \Sigma_0$ and if $\psi_n \in C_0^\infty$ is a Weyl sequence for $H = H_0 + V$ at energy E, then for any $R > 0$,*

$$\lim_{n\to\infty} \|\chi_R \psi_n\| > 0 .$$

Proof. Suppose the assertion is wrong. By going over to a subsequence, if necessary, we may assume that

$$\chi_R \psi_n \to 0$$

It follows that also $\chi_{\frac{3}{4}R} \nabla \psi_n \to 0$. This can be seen as follows: Take $g \in C^\infty$, $0 \leqq g(x) \leqq 1$ such that Δg is bounded and $g(x) = 1$ for $|x_1| \leqq \frac{3}{4}R$, $g(x) = 0$ for $|x_1| \geqq R$. Integrating by parts we get

$$\begin{aligned} \int g(x)\,|\nabla \psi_n|^2 dx &\leqq \int |\Delta g(x)|\,|\psi_n|^2 dx + \int g(x)\,|\psi_n|\,|\Delta \psi_n| dx \\ &\leqq M \int_{|x_1| \leqq R} |\psi_n(x)|^2 dx + \|\Delta \psi_n\| \left(\int_{|x_1| \leqq R} |\psi_n(x)|^2 dx \right)^{1/2} . \end{aligned}$$

Choose now a C^∞-function ϱ, $0 \leqq \varrho \leqq 1$ with $\varrho(x) = 1$ for $|x_1| \geqq \frac{3}{4}R$ and $\varrho(x) = 0$ for $|x_1| \leqq \frac{R}{2}$, such that $\Delta \varrho$ and $\nabla \varrho$ are bounded. Then

$$\|(H-E)\varrho\psi_n\| \leqq \|(H-E)\psi_n\| + 2\|\nabla\varrho \nabla \psi_n\| + \|(\Delta\varrho)\psi_n\| . \tag{2.3}$$

Since both $\nabla\varrho$ and $\Delta\varrho$ have support in $S_R = \{x \mid |x_1| \leqq R\}$, the right side of (2.3) goes to zero. Consequently $\varrho\psi_n$ gives a Weyl sequence for H^+ or H^- associated to E, hence $E \in \Sigma_0$ in contrast to our assumption. □

Corollary. *For any $\varepsilon > 0$ there is an $R > 0$ such that*

$$\lim \|\chi_R \psi_n\| \geqq 1 - \varepsilon .$$

Remark. Intuitively speaking, this corollary means that "surface states" are localized around the surface $x_1 = 0$.

Proof. Suppose the corollary is wrong for an $\varepsilon > 0$, then (by going over to a subsequence) eventually

$$\|(1-\chi_n)\psi_n\| > \varepsilon$$

for all n. Let g be a C^∞-function on $\mathbb{R}$, such that $0 \leqq g(t) \leqq 1$, $g(1) = 1$ for $t \geqq 1$, $g(t) = 0$ for $t \leqq 1/2$ and set $\varrho(x) = g(x_1)$, $\varrho_n(x) = \varrho\left(\frac{x}{n}\right)$. Then $\|(1-\varrho_n)\psi_n\| \geqq \varepsilon > 0$ for all n and

$$\|(H-E)(1-\varrho_n)\psi_n\| \leqq \|(1-\varrho_n)(H-E)\psi_n\| + 2\|\nabla\varrho_n \nabla\psi_n\| + \|(\Delta\varrho_n)\psi_n\| . \tag{2.4}$$

Since both $\nabla\varrho_n$ and $\Delta\varrho_n$ go to zero in sup-norm the right-hand side of (2.4) goes to zero, hence $(1-\varrho_n)\psi_n$ is a Weyl sequence.

3. The Density of Surface States

There are two equivalent ways to define the (integrated) density of states for an ergodic quantum mechanical disordered system. Let H_ω be a random Hamiltonian, with ergodic potential $V_{\omega \Lambda_L}$ a cube of side length $2L$ centered at the origin.

We denote by $(H_\omega)^D_{\Lambda_L}$ respectively $(H_\omega)^N_{\Lambda_L}$ the operator H_ω restricted to $L^2(\Lambda_L)$ with Dirichlet, respectively Neumann boundary conditions. It is easy to see that the functional

$$f \mapsto \frac{1}{|\Lambda_L|} \operatorname{tr} f((H_\omega)^D_{\Lambda_L}) \quad \text{for} \quad f \in C_0(\mathbb{R})$$

on the continuous functions of compact support defines a Borel measure ν^D_L on $\mathbb{R}$. Under mild assumptions on the potential V_ω it can be shown that ν^D_L converges vaguely to a measure ν as $L \to \infty$. Moreover, if we define ν^N_L in the same way replacing Dirichlet with Neumann boundary conditions, ν^N_L converges to the same limit. The measure ν is called the density of state measure for H_ω.

The other method to define the density of states starts from the measures $\tilde{\nu}_L$ given by

$$f \mapsto \frac{1}{|\Lambda_L|} \operatorname{tr}(\chi_{\Lambda_L} f(H_\omega)).$$

Again, it can be shown that $\tilde{\nu}_L$ converges vaguely as $L \to \infty$ and the limit is ν. As one might expect from physical intuition the support, $\operatorname{supp}\nu$, of the density of states measure coincides with the spectrum $\Sigma(=\sigma(H_\omega))$. For technical details we refer to [16, 1, 2, 13, 4].

To be specific, we will assume throughout that for all $t > 0$,

$$\mathbb{E}\left(\int_{C_0} e^{-tV^\pm_\omega(x)} dx\right) < \infty .$$

This ensures the existence of the density of states measures $\nu^\pm$ of $H^\pm_\omega$.

It is remarkably easy to prove the existence of the density of states ν also for the operator $H_\omega = H_0 + V_\omega$, with V_ω given by (2.1) and to express it in terms of ν^+ and ν^-.

Theorem 5. *The density of state measure* ν *of* $H_\omega = H_0 + V_\omega$,

$$V_\omega(x) = \begin{cases} V^+_\omega(x) & \text{for} \quad x_1 < 0 \\ V^-_\omega(x) & \text{for} \quad x_1 \geqq 0 \end{cases}$$

exists and is given by $\nu = \frac{1}{2}\nu^+ + \frac{1}{2}\nu^-$.

Proof. Let us set $\Lambda^+_L = \{x \in \Lambda_L;\ x_1 \geqq 0\} \Lambda^-_L = \{x \in \Lambda_L;\ x_1 < 0\}$. By Dirichlet-Neumann bracketing (see [20, 13]) we have

$$(H_\omega)^D_{\Lambda_L} \leqq (H_\omega)^D_{\Lambda^-_L} + (H_\omega)^D_{\Lambda^+_L} = (H^-_\omega)^D_{\Lambda^-_L} + (H^+_\omega)^D_{\Lambda^+_L}$$

and

$$(H_\omega)^N_{\Lambda_L} \geqq (H^-_\omega)^N_{\Lambda^-_L} + (H^+_\omega)^N_{\Lambda^+_L}.$$

Consequently, the distribution functions $N^D_{\Lambda_L}$, $N^N_{\Lambda_L}$ of ν^D_L and ν^N_L admit the estimate ($|A|$ denotes the Lebesgue measure of the set A):

$$\begin{aligned} \frac{1}{|\Lambda_L|} N^D_{\Lambda_L}(\lambda) &:= \frac{1}{L^d} \operatorname{tr} \chi_{(-\infty,\lambda)}((H_\omega)^D_{\Lambda_L}) \\ &\leqq \frac{1}{2}\left\{\frac{1}{|\Lambda^-_L|} \operatorname{tr} \chi_{(-\infty,\lambda)}((H^-_\omega)^D_{\Lambda^-_L}) + \frac{1}{|\Lambda^+_L|} \operatorname{tr} \chi_{(-\infty,\lambda)}((H^+_\omega)^D_{\Lambda^+_L}\right\}, \end{aligned} \quad (3.1)$$

and similarly

$$\frac{1}{|\Lambda_L|} N^N_{\Lambda_L}(\lambda) \geqq \frac{1}{2}\left\{\frac{1}{|\Lambda_L|} \operatorname{tr}\chi_{(-\infty,\lambda)}((H^-_\omega)^N_{\Lambda_L^-}) + \frac{1}{|\Lambda_L^+|} \operatorname{tr}\chi_{(-\infty,\lambda)}((H^+_\omega)^N_{\Lambda_L^-})\right\}. \tag{3.2}$$

The right-hand side of (3.1) and (3.2) both converge to $\frac{1}{2}\left(\int_{-\infty}^{\lambda} d\nu_L^+ + \int_{-\infty}^{\lambda} d\nu_L^-\right)$ at all continuity points of the latter function; thus both $N^N_{\Lambda_L}(\lambda)$ and $N^D_{\Lambda_L}(\lambda)$ converge to this limit. It is well known that the vague convergence of the measure follows from the convergence of the distribution functions (at all continuity points of the limit). □

The above result has as an immediate consequence that $\mathrm{supp}(\nu) = \Sigma_0$ which is (strictly) smaller than Σ in general. This should not be too surprising from a physical point of view. It only tells us that the density of state is too rough a quantity to "see" the surface states. In fact, for an energy interval, I, to have non-trivial density of states measure, it is necessary that the number of states with energy in I grows like the volume of the sample. For surface states it is however intuitively clear that their number should grow like a surface term.

Thus, instead of normalizing by the volume term $|\Lambda_L| = (2L)^d$ we should rather normalize by a surface term $(2L)^{d-1}$ which is just the area of the (hyper-)surface $\{x_1 = 0\}$ inside Λ_L. This is precisely how we define the density of surface states in $\Sigma\backslash\Sigma_0$. Obviously, for an interval $I \subset \Sigma_0$ the measures $\frac{|\Lambda_L|}{(2L)^{d-1}} \tilde{\nu}_L$ cannot converge since $\tilde{\nu}_L$ converges to a nonzero limit. Therefore, inside the bulk spectrum, Σ_0, we define the density of surface states as the order L^{d-1} correction to the bulk density of states (see below).

Definition. For a bounded function of compact support we set

$$\nu^S_L(f) := \frac{1}{(2L)^{d-1}} \operatorname{tr}\{\chi_{\Lambda_L^+}(f(H_\omega) - f(H^+_\omega)) + \chi_{\Lambda_L^-}(f(H_\omega) - f(H^-_\omega))\}.$$

In other words ν^S_L just measures the deviation of $f(H_\omega)$ on Λ_L from the direct sum of $f(H^+_\omega)$ on Λ_L^+ and $f(H^-_\omega)$ on Λ_L^-.

We state our main result about the density of surface states:

Theorem 6. *Suppose $f \in C^3(\mathbb{R})$ and $f(x) = 0(e^{-a|x|})$ for some $\alpha > 0$. Then the limit*

$$\nu^S(f) = \lim_{L\to\infty} \nu^S_L(f)$$

exists P-almost surely and is non-random. ν^S is a distribution of order (at most) 3.

The above defined ν^S is called the density of surface states (distribution). Before we begin the proof of Theorem 6 we turn to the behavior of ν^S in the "gaps" of Σ^0.

Corollary 7. *ν^S restricted to $\mathbb{R}\backslash\Sigma_0$ is a positive measure which is finite on any compact subset of $\mathbb{R}\backslash\Sigma_0$.*

Remarks. 1. Because, as is intuitively clear, Dirichlet and Neumann boundary conditions introduce surface terms, we cannot use Dirichlet-Neumann breaketing to define a surface density of states.

2. Sometimes we will apply ν_L^S to functions of non-compact support, provided they decay sufficiently rapidly at infinity. We use this extension of the definition without further comment.

It is reasonable to call the limit of ν_L^S the density of surface states, provided this limit exists. In fact, below we will prove the existence of the limits ν_L^S (as $L\to\infty$) for functions f that are sufficiently smooth. Therefore, we do not know whether the limit is a measure; we know, it is a distribution (of a certain order). We will however prove that it is a measure if restricted to the complement of Σ_0. We have no clear intuition whether this limitation is a drawback of our proof or whether ν^S is really not a measure. Let us, however, remark that ν^S certainly is not a positive measure, in general. In fact, it is not difficult to construct, in the spirit of Theorem 3, examples where $\nu^S(f)$ is negative for certain positive f. This is to be expected from physical reasoning and we might speak of "surface holes" in this case instead of surface states.

Proof (of the Corollary given the Theorem):
Take $f\in C^3$, $\operatorname{supp} f\subset \mathbb{R}\backslash\Sigma_0$ compact, $f\geqq 0$. Then

$$\begin{aligned}\nu_L^S(f)&=\frac{1}{(2L)^{d-1}}\operatorname{tr}\{\chi_{\Lambda_L}f(H_\omega)-\chi_{\Lambda_L^+}f(H_\omega^+)-\chi_{\Lambda_L^-}f(H_\omega^-)\}\\&=\frac{1}{(2L)^{d-1}}\operatorname{tr}\{\chi_{\Lambda_L}f(H_\omega)\}\geqq 0\,. \qquad \text{(a.s.)}\end{aligned}$$

Observe that $f(H_\omega^\pm)=0$ since $\sigma(H_\omega^\pm)\cap\operatorname{supp} f=\phi$. Therefore the functional ν_L^S is positive and so is ν^S. But, a positive functional on $C_0^3(\mathbb{R})$ is in fact (the integral) with respect to a positive measure by the Riesz representation theorem (and an inspection of its proof). □

The rest of this section is devoted to the proof of Theorem 6 modulo an essentially deterministic result (Theorem 7 below) which is proven in the next section. To prove Theorem 6, we may restrict ourselves to the "right" part of $\nu_L^S(f)$, i.e. to prove the convergence of

$$\nu_L^{S,+}:=\frac{1}{(2L)^{d-1}}\operatorname{tr}\{\chi_{\Lambda_L^+}(f(H_\omega)-f(H_\omega^+))\}\,. \tag{3.3}$$

The other part can be handled in precisely the same way. Equation (3.3) can be written as a sum in the following way:

$$\frac{1}{(2L)^{d-1}}\sum_{j=0}^{L-1}\sum_{i\in\Lambda_L^1\cap\mathbb{Z}^{d-1}}\operatorname{tr}\{\chi_{C_{(j,i)}}(f(H_\omega)-f(H_\omega^+))\}\,,$$

where

$$\Lambda_L^1 = \{y \in \mathbb{R}^{d-1} \mid (x,y) \in \Lambda_L \text{ for some } x \in \mathbb{R}\}$$

(recall that $C_{(j,i)} = \{x \mid j \leqq x_1 \leqq j+1,\ i_\nu \leqq x_\nu < i_\nu + 1 \text{ for } \nu = 2, \ldots, d\}$). To shorten notation, we introduce

$$\xi_{(j,i)} = \xi_{(j,i)}(f) = \operatorname{tr}\{\chi_{C_{(j,i)}}(f(H_\omega) - f(H_\omega^+))\}.$$

In the next section we will show that:

Theorem 7. $E(|\xi_{(j,i)}|) \leqq \dfrac{C}{1+j^2}$.

The constant C depends on f.

Proof of Theorem 6. Given Theorem 7, we may write $v_L^{S,+}$ as:

$$v_L^{S,+} = \frac{1}{L^{d-1}} \sum_{i \in \Lambda_L^1 \cap \mathbb{Z}^{d-1}} \left(\sum_{j=0}^{\infty} \xi_{(j,i)} \right) - \frac{1}{L^{d-1}} \sum_{i \in \Lambda_L^1 \cap \mathbb{Z}^{d-1}} \left(\sum_{j=L}^{\infty} \xi_{(j,i)} \right).$$

Let us set $\eta_i = \sum_{j=0}^{\infty} \xi_{(j,i)}$. By Theorem 7 the random variable η_i exists and is integrable. Moreover η_i is invariant under the shifts $T_i^1 = T_{(0,i)}$. Consequently

$$\frac{1}{L^{d-1}} \sum_{i \in \Lambda_L^1 \cap \mathbb{Z}^{d-1}} \eta_i;$$

the first summand above, converges by Birkhoff's ergodic theorem. The second summand admits the estimate

$$\mathbb{E}\left(\left| \frac{1}{L^{d-1}} \sum_{i \in \Lambda_L^1 \cap \mathbb{Z}^{d-1}} \left(\sum_{j=L}^{\infty} \xi_{(j,i)} \right) \right| \right) \leqq \sum_{j=L}^{\infty} \mathbb{E}(|\xi_{j,i}|) \to 0 \quad \text{as} \quad L \to \infty.$$

It follows from this and the Birkhoff theorem again that this term goes pointwise to zero (P-a.s.) as L goes to infinity. This finishes the proof of Theorem 6 modulo Theorem 7.

4. Proof of Theorem 7

In this section we will prove Theorem 7 in a somewhat more general setting.

Suppose that $V^\pm$ are two potentials on $\mathbb{R}^d$ in the Kato class K_d (see e.g. [21] or [4]). We set

$$V(x) = \begin{cases} V^-(x) & \text{for} \quad x_1 < 0 \\ V^+(x) & \text{for} \quad x_1 \geqq 0 \end{cases}$$

and define $H^\pm = H_0 + V^\pm$ and $H = H_0 + V$. As above we denote by $C_{(j,i)}$ for $j \in \mathbb{Z}$, $i \in \mathbb{Z}^{d-1}$ the cube

$$C_{(j,i)} = \{x \mid 0 \leqq x_1 - j < 1,\ 0 \leqq x_\nu - i_{\nu-1} < 1,\ \nu = 2, \ldots, d\}.$$

We define $\xi_{(j,i)}(f)=\operatorname{tr}\{\chi_{C_{(j,i)}}(f(H)-f(H^+)\}$ for $j\geqq 0$ and with H^+ replaced by H^- for $j<0$.

Theorem 7′. *For any $f\in C^3(\mathbb{R})$ with $f^{(l)}(x)=0(e^{-ax})$ (with $a>0$ and $l=0,1,2,3$) as $x\to\infty$, there is a constant C (depending only on f and the K_d-norms of V^+) such that*

$$|\xi_{(j,i)}(f)|\leqq \frac{C}{1+j^2}.$$

We start the proof of Theorem 7′ by investigating the special case $f(x)=e^{-tx}$ for some $t>0$. Since $H^\pm$ and H are bounded below we may assume that $H^\pm\geqq 1$ and $H\geqq 1$ by adding a constant. In the rest of the proof we restrict ourselves to the case $j\geqq 0$, the other one being similar.

Proposition 1. *For some C, α, $\beta>0$,*

$$|\xi_{(j,i)}(e^{-tx})|\leqq Ce^{-\alpha j}e^{-\beta t}.$$

Proof. Set $\varphi(t):=\xi_{(j,i)}(e^{-tx})$. Since $e^{-tH}\leqq e^{-t}$, we have for $t\geqq j$,

$$|\varphi(t)|=|\operatorname{tr}\chi_{C(j,i)}(e^{-tH}-e^{-tH^+})|\leqq 2e^{-\frac{1}{2}t}e^{-\frac{1}{2}j}|\operatorname{tr}(\chi_{C(j,i)}e^{-\frac{t}{3}H})|\leqq ce^{-\frac{1}{2}t}e^{-\frac{1}{2}j}.$$

For $t<j$ we rely on a Feymann-Kac argument,

$$|\varphi(t)|=|\operatorname{tr}\chi_{C_{(j,i)}}(e^{-tH}-e^{-tH^+}))|\leqq \int_{C_{(j,i)}}\mathbb{E}^{t,0}_{0,0}\left\{\left|e^{-\int_0^t V(b(s)+x)ds}-e^{-\int_0^t V^+(b(s)+x)ds}\right|\right\}dx,$$

where $\mathbb{E}^{t,y}_{0,x}$ denotes expectation over the Brownian bridge starting at time zero in x and ending at time t in y (see [21] for more information). Unless the path reaches the negative half space the exponentials cancel so

$$|\varphi(t)|\leqq \int_{C_{(j,i)}}\mathbb{E}^{1,0}_{0,0}\left\{\left(e^{-\int_0^t V(b(s)+x)ds}-e^{-\int_0^t V^+(b(s)+x)ds}\right)\chi\left\{b\,\Big|\sup_{0\leqq s\leqq t}|b_1(s)|>j\right\}\right\}ds.$$

By the Schwarz inequality:

$$|\varphi(0)|\leqq 2\int_{C_{(j,i)}}\mathbb{E}^{t,0}_{0,0}\left\{e^{-\int_0^t V(b(s)+x)ds}+e^{-2\int_0^t V^+(b(s)+x)ds}\right)^{1/2}dx$$

$$\mathbb{P}^{t,0}_{0,0}\left(\sup_{0\leqq s\leqq t}\{|b_1(s)|>j\}\right)^{1/2}.$$

The first factor in the above formula is bounded since V, $V^+\in K_d$ by assumption. The second part can be estimated by:

$$\mathbb{P}^{t,0}_{0,0}\left(\sup_{0\leqq s\leqq t}\{|b_1(s)|>j\}\right\}\leqq Me^{-\gamma\frac{j^2}{t}}\leqq Me^{-\gamma j}\leqq Me^{-\frac{\gamma}{2}j}e^{-\frac{\gamma}{2}t}.\quad\square$$

The idea will be to analytically continue the estimates in t and then use the Fourier transform. So, we consider the function

$$\psi(z)=e^{\beta z}\xi_{(j,i)}(e^{-z\cdot})$$

as a function of the complex variable $z(\operatorname{Re}z\geqq 0)$.

Proposition 2.

$$|\psi(t+is)| \leqq C e^{-\alpha j \arctan \frac{t}{|s|}}.$$

Proof. ψ is analytic for $t = \mathrm{Re}\, z > 0$ and $|\psi(z)| \leqq C_2$ for $\mathrm{Re}\, z \geqq 0$.

Moreover, from Proposition 1 we learn that

$$|\psi(t+is)| \leqq C e^{-\alpha j}.$$

From this we infer the assertion of the proposition by complex interpolation as follows: The transformation $\xi \mapsto e^{\xi}$ maps the strip $\{ | 0 \leqq \mathrm{im}\, \xi \leqq \pi/2\}$ into $\{z \mid \mathrm{Re}\, z \geqq 0, \mathrm{Im}\, z \geqq 0, z \neq 0\}$. By setting $\chi(\xi) = \psi(e^{\xi})$. We define a function χ analytic in the above strip. We have

$$|\chi(\xi)| \leqq C_1 e^{-\alpha j} \quad \text{for} \quad \mathrm{Im}\, v = 0,$$

$$|\chi(\xi)| \leqq C_2 \quad \text{for} \quad \mathrm{Im}\, \xi = \pi/2.$$

Thus Hadamard's three line theorem (see e.g. [19]) implies that:

$$|\chi(\xi)| \leqq C_1^{\mathrm{Im}\, \xi} C_2^{\pi/2 - \mathrm{Im}\, \xi} e^{-\alpha j(\pi/2 - \mathrm{Im}\, \xi)}.$$

Since for $z = e^{\xi}$ we have that $\mathrm{Im}\, \xi = \arg z$, we get

$$|\psi(\xi)| \leqq C_1^{\arg z} C_2^{\pi/2 - \arg z} e^{-\alpha j(\pi/2 - \arg z)}$$
$$\leqq C e^{-\alpha j(\pi/2 - \arg z)}.$$

For $z = t + is$ we have $\arg z = \arctan \frac{s}{t}$. Thus, we obtain the result for $s \geqq 0$. The argument for $s \leqq 0$ is the same.

The above result tells us that

$$|\xi_{(j,i)}(e^{-(t+is)})| \leqq C e^{-\beta t} e^{-\alpha j \arctan \frac{t}{|s|}}.$$

We come to the proof for arbitrary $f \in C^3(\mathbb{R})$ with $f(x) = 0(e^{-ax})$ as $x \to \infty$ $(a > 0)$. Such a function can be written as

$$f(x) = \frac{1}{x^2} g(x) \quad \text{for} \quad x > 1/2 \text{ (say)},$$

where g is of the same type. Let g be the Fourier transition of g normalized by

$$g(x) = \int \tilde{g}(s) e^{-isx} ds.$$

Then

$$f(H) - f(H^+) = H^{-2} g(H) - (H^+)^{-2} g(H^+)$$
$$= \int_{-\infty}^{+\infty} (H^{-2} e^{-isH} - H_+^{-2} e^{-isH^+}) \tilde{g}(s) ds$$
$$= \int_{-\infty}^{+\infty} \tilde{g}(s) \int_0^{\infty} t(e^{-(t+is)H} - e^{-(t+is)H^+}) dt\, ds.$$

Consequently

$$\begin{aligned}|\xi_{(j,k)}(f)| &= |\operatorname{tr}\{\chi_{(j,k)}(f(H)-f(H^+))\}| \\ &= \left|\int_{-\infty}^{+\infty} \tilde{g}(s) \int_0^\infty t\operatorname{tr}\{\chi_{C_{(j,i)}}(e^{-(t+is)H}-e^{-(t+is)H^+})\}dt\,ds\right. \\ &\leqq \int_{-\infty}^{+\infty} \tilde{g}(s) \int_0^\infty t|\xi_{(j,i)}((e^{-(t+is)x})|dt\,ds \\ &\leqq C\int_{-\infty}^{+\infty} \tilde{g}(s) \int_0^\infty te^{-\beta t}e^{-\alpha j\arctan\frac{t}{|s|}}ds\,dt. \qquad (4.1)\end{aligned}$$

Using that

$$\int_0^\infty te^{-\beta t}e^{-\alpha j\arctan\frac{t}{|s|}}dt \leqq \frac{K(1+s^2)}{1+j^2}, \qquad (4.2)$$

we conclude that

$$(4.1) \leqq \frac{\tilde{C}}{1+j^2}\int |\tilde{g}(s)|(1+s^2)ds \leqq \frac{\bar{C}}{1+j^2}$$

for a g-dependent constant $\bar{C}$.

Note that the regularity assumption on g is used to get $\int|\tilde{g}(s)|(1+s^2)ds$ finite, as well as to justify the Fourier inversion formula. (Recall what if $g, g' \in L^2$ then $\tilde{g} \in L^1$.)

5. Extensions and Modifications

Let us consider once more the alloy type model with

$$V_\omega^\pm(x) = \sum q_i^\pm(\omega) f^\pm(x-i).$$

In the case the "mixed system" V_ω consisting of the system "$-$" in the left half space and of the system "$+$" in the right half space might be modelled by setting

$$\tilde{V}_\omega(x) = \sum_{i_1<0} q_i^-(\omega)f^-(x-i) + \sum_{i_1 \geqq 0} q_i^+(\omega)f^+(x-i),$$

which, of course, differs significantly from the V_ω discussed above.

Our results in the previous section still can be proven in this case by modifications of the proofs. To get the existence of the density of surface states, however, our proof seems to require f to decay exponentially fast. While we feel this assumption is much stronger than necessary, we don't see how to avoid it. Similar considerations apply also for potentials with Poisson distributed sources.

It is not difficult to extend our theorem to cover discrete Schrödinger operators. In place of the path integral used in the continuum case, one can use a simple perturbation expansion in H_0.

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