Spectral Theory of Sparse Potentials

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Dedicated to Sergio Albeverio on the occasion of his 60$^{\text{th}}$ birthday.

Abstract

We give a number of results concerning different possible spectral types for Schrödinger operators with sparse potentials. These potentials are in between stationary (e.g., random) potentials and the short range potentials familiar from scattering theory. They decay at infinity in some averaged sense, however in such a way that there is enough "space" for surprising spectral properties.

For a broad class of sparse potentials we establish existence of absolutely continuous spectrum above zero with scattering theory ideas. At the same time these potentials generically also possess negative essential spectrum. We classify this negative spectrum to some extend. It turns out to be pure point in many cases. In some cases the negative essential spectrum is countable, in fact it may be finite, but still does not belong to the discrete part of the spectrum. In other cases we find dense point spectrum.

Finally, we treat "surface potentials" and prove analogous results for these "generalized sparse potentials".

Contents

1 Introduction

In this paper we consider the spectral theory of Schrödinger operators with sparse or slowly decaying potentials. By sparse potentials we mean such functions $V(x)$ which do not decay to zero as $|x| \to \infty$ but which become small near infinity in an averaged sense.

A typical example is a potential of the form

$$V(x) = \sum f(x - x_n), \tag{1.1}$$

where f is an attractive short-range potential on $\mathbb{R}^d$, for instance with compact support, and x_n an infinite sequence of points in $\mathbb{R}^d$, such that $\mathrm{dist}(x_n, \{x_m\}_{m \neq n}) \to \infty$ as $n \to \infty$. Such types of potentials are intermediate between potentials decaying at infinity and stationary potentials (such as periodic, almost periodic or stationary random ones).

The spectral theory for short-range potentials V is well-understood. Roughly speaking these are potentials decaying at infinity faster than $|x|^{-(1+\epsilon)}$. For such potentials V the essential spectrum of $H := H_0 + V$ is purely absolutely continuous and the corresponding states are scattering states (in chapter 2 we will give a precise definition of these notions). There may be additional spectrum below zero. This spectrum is discrete, that is, it consists of isolated eigenvalues of finite multiplicity [35, 6], and the corresponding states are bound states. Zero may be an accumulation point of these negative eigenvalues depending on the fall-off of V at infinity.

If the potential V is relatively compact, roughly speaking if it has *some* decay at infinity, we still know that the essential spectrum of the Schrödinger operator $H = H_0+V$ is $[0, \infty)$, which is the spectrum of the "free" Schrödinger operator $H_0 = -\Delta$.

Potentials with "stationary" behavior at infinity are much less understood. The best investigated cases are periodic potentials. The corresponding Schrödinger operators have purely absolutely continuous spectrum which consists of a countable union of "bands", that is,

$$\sigma(H) = \bigcup_{n=0}^{\infty} [a_n, b_n]$$

with $a_n < b_n \leq a_{n+1}$. If $b_n < a_{n+1}$, we call the interval (b_n, a_{n+1}) a gap of the spectrum of the operator.

By stationary random potentials we mean a stochastic process on $\mathbb{R}^d$ which is stationary in the sense that the shifted processes $V_\omega(\cdot + i)$ for $i \in \mathbb{Z}^d$ have the same finite dimensional distributions regardless of the shift i. A typical example of such a potential, in fact the one which we will have in mind for the whole journey, is

$$V_\omega(x) = \sum_{i \in \mathbb{Z}^d} q_i(\omega) f(x - i), \tag{1.2}$$

where f is a non-positive function of compact support, say (for simplicity), $(q_i)_i$ a family of independent identically distributed random variables. It is known that $H_\omega = H_0 + V_\omega$ has dense pure point spectrum in dimension one (the most complicated case of Bernoulli distributions is treated in [4, 36] for the discrete Anderson model, for the continuous case see [8]).

Moreover, in $d \geq 2$, H_ω has dense pure point spectrum for energies near the bottom of its spectrum, near other band edges or for large disorder. (A way to talk about "large disorder" rigorously is to take λV_ω as the potential and to look at large $|\lambda|$.) We refer to [2, 5, 18, 24, 25, 39, 40, 41] for these results and to [1, 4, 9, 11, 12, 38] for the discrete analog.

We would like to emphasize that for all these results in $d \geq 2$ one has to assume that the distribution $\mathbb{P}_0$ of q_0 (which is the distribution of the other q_i, by stationarity) has a density with respect to the Lebesgue measure. So, in particular, the case of a Bernoulli distribution with $P(q_0 = \lambda_0) = p$, $P(q_0 = \lambda_1) = 1 - p$ *cannot* be handled up to now. However, physicists (and mathematicians) believe that there is pure point spectrum in this case as well.

The phenomenon of pure point spectrum for random quantum systems is known as Anderson localization. Physicists expect that for low disorder and away from the band edges, random Schrödinger operators should have absolutely continuous spectrum in dimension three and higher, while for dimension $d = 2$ they predict pure point spectrum for all energies no matter how small the disorder is, like it is rigorously known in $d = 1$. Both phenomena have not been proven rigorously, despite strong efforts over the past two decades.

The potentials we are going to consider in this article are somewhat in between the two extreme cases: Short-range potentials on the one hand and stationary on the other hand. While their study is interesting in its own right, at least from a mathematical point of view, our main goal is to produce examples of Schrödinger operators which have the spectral properties one expects for the stationary random case, that is, coexistence of absolutely continuous spectrum in the one energy regime and (dense) pure point spectrum for other energies. Moreover, these potentials can be looked upon as a "low concentration" limit of the stationary case (as was pointed out to one of us by S. Molchanov).

The theory of sparse potentials goes back at least to Pearson [32] who used potentials with sparse bumps to construct examples of Schrödinger operators with singular continuous spectrum. The paper by Klaus [26] has results about sparse potentials as well. We are going to use the results by Klaus in chapter 3. Finally, we mention the paper by Molchanov [30], which is closely related to our article.

From a different point of view Krishna Maddaly (see [27, 28]) considered "sparse" random potentials, in fact he investigated random potentials with decaying randomness similar to our Model III below. It was his idea to prove the existence of wave operators for such models. In chapter 2 we will rely on this method.

In this paper we will consider both random and deterministic sparse potentials. Let us start with a typical random example. Suppose $f \leq 0$ is a bounded function of compact support, for example $f = -\chi_{C_0}$, χ_{C_0} being the characteristic function of the unit cube C_0 in $\mathbb{R}^d$. Let $\{\xi_i\}_{i\in\mathbb{Z}^d}$ be independent random variables with values in $\{0, 1\}$. Then we consider

$$\textbf{Model I}: \qquad V_\omega(x) = \sum_{i\in\mathbb{Z}^d} \xi_i(\omega) f(x-i). \tag{1.3}$$

If the ξ_i are identically distributed then V_ω is a stationary random potential as discussed above. In fact, it is a Bernoulli-type potential since ξ_i takes only two values. So we know nothing about the measure theoretic nature of the spectrum for dimensions $d \geq 2$. To make (1.3) a sparse random potential we will chose the ξ_i not identically distributed. Setting $p_i := \mathbb{P}(\xi_i = 1)$ (so $\mathbb{P}(\xi_i = 0) = 1 - p_i$) we require that $p_i \to 0$ as $|i| \to \infty$. Of course, (1.3) becomes a short-range potential unless $\xi_i = 1$ infinitely often.

Introducing random couplings q_i in Model I we obtain

$$\textbf{Model II}: \qquad V_\omega(x) = \sum_{i\in\mathbb{Z}^d} q_i(\omega)\xi_i(\omega) f(x-i). \tag{1.4}$$

Here the q_i are independent identically distributed random variables (unless stated otherwise we assume $q_i \geq 0$ for simplicity).

For these two models we will prove that $[0, \infty)$ belongs to the absolutely continuous spectrum as long as $p_i = \mathbb{P}(\xi_i = 1)$ decays fast enough. Moreover, it turns out that there is additional essential spectrum below zero if $\sum p_i = \infty$. This essential spectrum is actually finite or countably infinite for Model I and consequently pure point. For Model II we prove that the spectrum below zero is pure point in many cases, especially it is dense pure point spectrum if the distribution of the q_i has a bounded density.

There is a third type of stochastic potentials which we will consider, namely a model with decaying but random coupling strength, that is,

$$\textbf{Model III}: \qquad V_\omega(x) = \sum_{i\in\mathbb{Z}^d} a_i q_i(\omega) f(x-i), \tag{1.5}$$

where the q_i's are again independent identically distributed random variables — as above— and $\{a_i\}_{i\in\mathbb{Z}^d}$ is a deterministic sequence decaying (fast enough) at infinity. See [20] for a discrete analog of this model. If the distribution $\mathbb{P}_0$ of the random variables q_i has a bounded support, every realization of model (1.5) is decaying at infinity, so not very interesting for our purpose.

In fact, V_ω is a standard short range potential then. However, if $\mathbb{P}_0$ has non-compact support the potential $V_\omega(x)$ may admit a sequence $x_n \to \infty$, such that $V_\omega(x_n) \to -\infty$, thus leaving space for essential, in fact, dense pure point spectrum below zero.

In chapter 2 we prove for a huge class of potentials with decaying randomness that the positive half axis belongs to their absolutely continuous spectrum. The class we consider contains all the above example (with certain conditions on the parameters). We obtain this result by methods from scattering theory. In fact, we prove that the corresponding wave operators exist. Since we try to construct examples with additional essential spectrum below zero we have to deal with potentials which are *not* relatively compact, that is, they are outside the scope of traditional scattering theory. Our main result is probabilistic in nature, that is, it claims the existence of the wave operators for a set of potentials of full measure. We complete our considerations by a deterministic result which contains and extends the probabilistic one.

In chapter 3 we prove that many of our models admit essential spectrum below zero. Although the spectrum itself is a (truly) random set the essential spectrum is not. Moreover, in various situations we prove that this part of the spectrum is pure point. Under certain conditions we actually show that the *essential* spectrum below zero is a *countable* or even *finite* set. In other situation we obtain dense point spectrum. The absence of absolutely continuous spectrum below zero can also be shown by the methods of [29]. This paper has a multidimensional version of the paper [37] (see also [23]).

Any potential above may be considered as a deterministic one, of course, by choosing the sequences ξ_i and q_i in a deterministic way. Then "almost sure" theorems will not give us anything for that particular potential. However, we will show a number of deterministic results which apply for a given choice of these sequences. For example, if we choose ξ_i in Model I in a deterministic way, we arrive at a potential of the form

$$V(x) = \sum_{n\in\mathbb{N}} f(x - x_n), \tag{1.6}$$

where $\{x_n\}$ is an enumeration of those points $i \in \mathbb{Z}^d$ which have $\xi_i = 1$. For this model there is, of course, no need for a restriction like $x_n \in \mathbb{Z}^d$ as we have for Model I.

Our Models I – III have straight forward analogs in the discrete case, that is, on the Hilbert space $l^2(\mathbb{Z}^d)$ instead of $L^2(\mathbb{R}^d)$. In this case the Laplacian is replaced with a finite difference operator which we also denote by H_0 (see, e.g., [6] for details and references). The theorems and proofs in this paper will easily transfer to the discrete case. In fact, the discrete case has one major advantage. While we stated above the existence of absolutely continuous spectrum and claimed $\sigma_{\mathrm{ac}}(H_\omega) = [0, \infty)$ almost surely, we carefully avoided claiming that there is no other spectrum there. In fact, we cannot rule out the possibility of some singular spectrum (pure point spectrum for example) inside the a.c. spectrum. For the discrete case, there is a remarkable paper by Jakšić and Last [14], which for many of our models immediately guarantees *purely* absolutely continuous spectrum in an interval I once we have established *some* absolutely continuous spectrum there. Unfortunately, the corresponding results for the continuous case, that is, for $L^2(\mathbb{R}^d)$, are not known.

There is a final class of "sparse" potentials which we are going to consider in this paper. They are various versions of potentials concentrated on a (hyper-) surface in $\mathbb{R}^d$ (or $\mathbb{Z}^d$). A typical example is a potential of the form

$$V_\omega(x) = \sum_{i \in \mathbb{Z}^{d-1} \times \{0\}} q_i(\omega) f(x - i), \tag{1.7}$$

for $x \in \mathbb{R}^d$. While this potential does not decay in the directions $x_1, \dots, x_{d-1}$ it has compact support in the x_d direction. Surface potentials have been well studied in the recent years, see e.g. [15, 16, 17] and the references therein. We will have a couple of things to say about this kind of potentials as well as on the case where the q_i occupy a half space.

2 The absolutely continuous spectrum

To prove existence of absolutely continuous spectrum for our various models, we will employ a few basic ideas from scattering theory. We refer to the books [34] and [6] as well as the review article by Enß [10] for a development of this theory. We would like to remark that Krishna [27, 28] was the first to observe that scattering theory can be applied to random potentials with decaying randomness.

2.1 A few basics of scattering theory

The basic idea of scattering theory is to compare the time evolution e^{-itH} of a quantum system described by a Hamiltonian H to the time evolution under the free evolution operator e^{-itH_0}. The central idea is that any "scattering state" ϕ should behave under the true "perturbed" evolution for large times $t \to \pm\infty$ like a state $\phi_\pm$ would behave under the "free" evolution e^{-itH_0}, that is, $\mathrm{e}^{-itH}\phi \sim \mathrm{e}^{-itH_0}\phi_\pm$ as $t \to \pm\infty$. These scattering states are thus the functions in the range of the *wave operators* (also known as Møller operators)

$$\Omega_\pm := \lim_{t\to\mp\infty} \mathrm{e}^{itH}\mathrm{e}^{-itH_0}. \tag{2.1}$$

(The strange convention about $\pm$ is for historical reasons.) The above limit is meant in the strong sense, that is, as convergence in the Hilbert space if the operators are applied to L^2-functions. Of course, the first step is to prove that the limit in (2.1) exists at all and that is what we are concerned with below.

The reason for us to care about the existence of the limit is the following well-known fact:

Theorem 2.1. *Suppose that for $H_0 = -\Delta$ and $H = H_0+V$ the limit $\Omega_-\phi = \lim_{t\to\infty} \mathrm{e}^{itH}\mathrm{e}^{-itH_0}\phi$ exists for all $\phi \in L^2(\mathbb{R}^d)$. Then the set $[0,\infty) = \sigma(H_0) = \sigma_{\mathrm{ac}}(H_0)$ is contained in $\sigma_{\mathrm{ac}}(H)$.*

The proof is easy and can be found in virtually any textbook on scattering theory. So, if we can establish the existence of (one of) the wave operators for a potential V we automatically have that $[0,\infty)$ is contained in the absolutely continuous spectrum of H_0+V. The main tool to prove existence of the wave operators for one-particle scattering is the well-known Cook's method.

Theorem 2.2. *Suppose $H = H_0 + V$. If for a dense (or total) set $\mathcal{D}_0$ in $L^2(\mathbb{R}^d)$ and some $T_0 > 0$*

$$\int_{T_0}^{\infty} \left\|V\mathrm{e}^{-itH_0}\phi\right\|_2 \, dt < \infty, \tag{2.2}$$

then the wave operator Ω_- exist.

This follows from differentiating $e^{itH}\mathrm{e}^{-itH_0}\phi$ with respect to t and integrating it again, confer the literature on scattering theory for a detailed proof.

The prototypical example for existence of wave operators is:

Theorem 2.3. *If V is a bounded function with $|V(x)| \leq C(1+|x|)^{-(1+\varepsilon)}$ for some $\varepsilon > 0$, then the integral in (2.2) is finite. Hence the wave operators $\Omega_{\pm}$ exist.*

Again, this result is well-known in scattering theory. We will actually prove this result in Section 2.3 as a by-product of a more general result which does not assume a pointwise decay. Note that we assumed boudedness of V in the above theorem merely for simplicity. Local singularities can be incorporated in scattering theory rather easily. It is the fall-off at infinity that limits the validity of scattering results.

2.2 The almost surely free lunch theorem

The results from scattering theory discussed in the previous chapter are not yet applicable for our purposes. From our discussion of scattering theory we know that $[0, \infty) \subset \sigma_{\mathrm{ac}}(H)$ if the potential V decays faster than a Coulomb potential. More precisely, if

$$V(x) \leq C(1 + |x|)^{-(1+\varepsilon)}. \tag{2.3}$$

It is clear that this is the case for Model I (or Model II) *only* if there are merely finitely many points $\xi_i = 1$. But then V_ω is a classical short-range potential. More generally, if (2.3) is true then the potential turns out to be relatively compact with respect to H_0. Consequently, by Weyl's theorem, the essential spectrum of H equals $[0, \infty)$. In other words, there is no chance to construct examples with dense point spectrum or even *any* essential spectrum below zero. Hence we have to go beyond the classical result of Section 2.1.

Common wisdom has it that there is not something like a free lunch. In scattering theory this might have led to the general belief that one can not go beyond the case (2.3) without hard work (if at all). However, in our situation there is a free lunch (almost surely) as we will explain below. Let $V_\omega(x)$ be a rather general random potential. We define $W(x) := \mathbb{E}(V_\omega(x)^2)^{1/2}$. As usual we denote by $\mathbb{E}$ the expectation with respect to the underlying probability measure $\mathbb{P}$.

Theorem 2.4 (Almost surely free lunch Theorem). *If the function W defined above satisfies Cook's criterion, then V_ω satisfies Cook's criterion almost surely.*

Proof.

$$\mathbb{E}\Big(\int_{T_0}^{\infty}\left\|V_\omega \mathrm{e}^{-itH_0}\phi\right\|_2\,dt\Big) = \int_{T_0}^{\infty}\mathbb{E}\Big(\big[\int V_\omega(x)^2|\mathrm{e}^{-itH_0}\phi(x)|^2\,dx\,\big]^{1/2}\Big)\,dt$$
$$\leq \int_{T_0}^{\infty}\Big(\int \mathbb{E}(V_\omega(x)^2)|\mathrm{e}^{-itH_0}\phi(x)|^2\,dx\,\big]^{1/2}\Big)\,dt = \int_{T_0}^{\infty}\left\|W\mathrm{e}^{-itH_0}\phi\right\|_2\,dt$$

by Jensen's inequality. Thus, if W satisfies Cook's criterion then the expectation of $\int_{T_0}^{\infty}\left\|V_\omega \mathrm{e}^{-itH_0}\phi\right\|_2\,dt$ is finite which implies that this quantity itself is finite almost surely. ∎

To show that we really gained something, let us apply this result to Model I. By a Borel-Cantelli argument we already saw that $V_\omega = \sum \xi_i(\omega) f(\cdot - i)$ is not a short-range potential if $\sum_{i\in\mathbb{Z}^d} p_i = \sum_{i\in\mathbb{Z}^d}\mathbb{P}(\xi_i = 1) = \infty$ which is the case if, for example, $p_i \sim |i|^{-\alpha}$ for some $\alpha < d$. Then we can obviously find a sequence $x_n \to \infty$ such that $V_\omega(y) \leq c < 0$ for $|y - x_n| \leq r_0$. This immediately implies that $\sigma_{\mathrm{ess}}(H_\omega) \cap (-\infty, 0) \neq \emptyset$ $\mathbb{P}$-almost surely if f is negative enough by construction of an appropriate Weyl sequence. Consequently, V_ω is *not* relatively compact (with probability one). (Chapter 3 contains more details about the construction of Weyl sequences. There it turns out that the condition on f to ensure essential spectrum for V_ω is that the operator $H_0 + f$ has a negative eigenvalue.)

Let us try to apply Theorem 2.4 to this potential. To simplify notation we will assume that the support of f is contained in the unit cell C_0 so that $f(\cdot - i)$ and $f(\cdot - j)$ do not overlap for $i \neq j$, $i, j \in \mathbb{Z}^d$. We simply compute: For $x \in C_0 + n$, $n \in \mathbb{Z}^d$

$$\mathbb{E}(V_\omega(x)^2)^{1/2} = \mathbb{E}(\xi_n^2)^{1/2} f(x - n) \leq C\mathbb{E}(\xi_n^2)^{1/2} = Cp_n^{1/2}$$

($p_n := \mathbb{P}(\xi_n = 1)$). So, we obtain $[0, \infty) \subset \sigma_{\mathrm{ac}}(H)$ almost surely as long as $\sqrt{p_n} \lesssim (1 + |n|)^{-(1+\varepsilon')}$, say, that is, if $p_n \leq C|n|^{-(2+\varepsilon)}$ for large n.

Thus we get both essential spectrum below zero and absolutely continuous spectrum above zero, if

$$p_n \sim |n|^{-\alpha} \qquad \text{for large } n$$

with $2 < \alpha < d$. We remark that this can be arranged for any dimension $d \geq 3$ but not for $d = 2$ (or $d = 1$).

This is consistent with the physical expectations for the stationary random case as we explained in the introduction. Depending on our mood, we either consider this as a hint or a mere coincidence.

The above discussion can be literally transformed to Model II. Thus we show

Theorem 2.5. *Set $V_\omega(x) = \sum q_i(\omega)\xi_i(\omega) f(x-i)$ with q_i i.i.d. random variables with a finite second moment and $\mathbb{P}(q_i > 0) > 0$, ξ_i independent $\{0,1\}$-valued random variables also independent from the q_i's, and f a non-positive function with compact support, $f(x) \le c < 0$ on some non-empty open set. Then for the operator $H_\omega = H_0 + V_\omega$ we have $\mathbb{P}$-almost surely:*
i) $[0,\infty) \subset \sigma_{\mathrm{ac}}(H_\omega)$ *if $p_i \lesssim |i|^{-\alpha}$ for an $\alpha > 2$,*
ii) $\sigma_{\mathrm{ess}}(H_\omega) \cap (-\infty, 0) \ne \emptyset$ *if $\sum p_i = \infty$ and f is negative enough.*

Remark 2.6. i) Of course, for $[0,\infty) \subset \sigma_{\mathrm{ac}}(H_\omega)$ we do not need the assumption $\mathbb{P}(q_i > 0) > 0$.
ii) We will later prove that the spectrum below zero is actually pure point in many cases.

We will have more detailed results of this genre and a precise condition on f in the next chapter.

We turn to Model III:

$$V_\omega(x) = \sum a_n q_n(\omega) f(x-n).$$

In this case it is easy to show that the almost free lunch Theorem applies if $\mathbb{E}(q_n^2) < \infty$ and $|a_n| \le C(1+|n|)^{-(1+\varepsilon)}$. Moreover, it can be shown that $\sigma_{\mathrm{ess}}(H_\omega) \cap (-\infty, 0) \ne \emptyset$ almost surely as long as the distribution of the q_n has "heavy tails" in the sense that $\mathbb{P}(q_0 \le -a) \sim \int_{-\infty}^{a} |\lambda|^{-\beta} \, d\lambda$ for β large enough. The distribution measure $|\lambda|^{-\beta} \, d\lambda$ is finite if $\beta > 1$ and has a finite second moment if $\beta > 3$.

Analogously to [20], one proves that as long as $a_n \sim |n|^{-\alpha}$ then there is essential spectrum below zero if $\beta < 1 + d/\alpha$. Again, coexistence of pure point and absolutely continuous spectrum can be arranged iff $d \ge 3$.

2.3 A deterministic free lunch

Here we want to generalize the preceding discussion to show the existence of wave operators for deterministic sparse potentials .

Theorem 2.7. *Let V be locally square integrable and $\mu(r) := \int_{|x|\le r} V(x)^2 \, dx$. If μ is bounded by $\mu(r) \le C(1+r)^\alpha$ with some $\alpha < d-2$, then the wave operators exist.*

Remark 2.8. i) If the potential is random, a sufficient condition for the existence of the wave operators is $\mathbb{E}\mu(r) \le C(1+r)^\alpha$ with some $\alpha < d-2$.
ii) This result is optimal in the sense that for spherically symmetric monotone potentials it allows for a decay like $|x|^{-(1+\varepsilon)}$ at infinity, which is known to be the borderline case.

The proof of Theorem 2.7 uses an ancient method for establishing existence of the wave operators: Cook's method with Gaussians (see [34], p. 56). Let ϕ_γ be $\phi_\gamma(x) := \gamma^{d/4}\exp(-\gamma x^2/2)$. These wavefunctions together with their translates form a total set in $L^2(\mathbb{R}^d)$. The strategy to prove Theorem 2.7 is basically to do the calculation as explicit as possible, avoiding any estimates. The main technical observation is

Lemma 2.9. *With μ as defined in Theorem 2.7, we have*

$$\int_T^\infty \left\|V\mathrm{e}^{-itH_0}\phi_\gamma\right\|_2 \, dt = C_\gamma \int_{2\gamma T}^\infty dt(1+t^2)^{-d/4} \left[\int_0^\infty \mu(r\sqrt{1+t^2}/\sqrt{\gamma})\, r\mathrm{e}^{-r^2}\, dr\right]^{1/2}$$

Proof. The free time evolution of ϕ_γ is easily computed,

$$(\mathrm{e}^{-itH_0}\phi_\gamma)(x) = \gamma_t^{d/4}\exp(-\gamma_t x^2/2 + i\beta_t),$$

where $\gamma_t := \gamma(1+4\gamma^2t^2)^{-1}$ and β_t is real valued (see [34], p. 56).Thus

$$\begin{aligned} \left\|V\mathrm{e}^{-itH_0}\phi_\gamma\right\|_2^2 &= \gamma_t^{d/2}\int_{\mathbb{R}^d} V(x)^2\mathrm{e}^{-\gamma_t x^2}\, dx = \gamma_t^{d/2}\int_0^\infty \left(\frac{d}{dr}\mu(r)\right)\mathrm{e}^{-\gamma_t r^2}\, dr \\ &= \gamma_t^{d/2} 2\gamma_t \int_0^\infty \mu(r) r\mathrm{e}^{-\gamma_t r^2}\, dr = 2\gamma_t^{d/2}\int_0^\infty \mu(r/\sqrt{\gamma_t}) r\mathrm{e}^{-r^2}\, dr \end{aligned}$$

by the definition of μ, partial integration, and a change of variables. Calculating $\int dt \left\|V\mathrm{e}^{-itH_0}\phi_\gamma\right\|_2$ by a change of variables gives the result. ∎

Remark 2.10. If the potential is random we can take the expectation in Lemma 2.9. This yields the condition $\mathbb{E}\mu(r) \le C(1+r)^\alpha$ with some $\alpha < d-2$ for existence of the wave operators in the random case.

Proof of Theorem 2.7. If $\mu(r) = \int_{|x|\le r} V(x)^2 dx \lesssim (1+r)^\alpha$ then, by Lemma 2.9 we have

$$\int_T^\infty \left\|V\mathrm{e}^{-itH_0}\phi_\gamma\right\|_2 \, dt \le C_\gamma \int_{2\gamma T}^\infty dt(1+t^2)^{-d/4}(1+t^2)^{\alpha/4} < \infty$$

as long as $\alpha < d-2$. The same estimate holds for shifted Gaussians, and hence for a total set of vectors. Cook's criterion, Theorem 2.2, applies. ∎

Let us apply Theorem 2.7 to a deterministic potential of the form $V(x) = \sum_{n\in\mathbb{N}} f(x - x_n)$ with the single-site potential f having compact support. Then

$$\int_{|x|\leq R} V(x)^2\, dx \leq C\#\{x_n \mid |x_n| \leq R\}.$$

Assume that the centers x_n are such that the minimal distance $d_n = \inf_{m\neq n} |x_n - x_m| \to \infty$. Without loss we may assume that $x_0 = 0$. Moreover, by reordering the centers if necessary we may also assume that the sequence d_n is nondecreasing. If the ball $B_R(0)$ of radius R around the origin contains the center x_n then the ball $B_{d_n}(x_n)$ of radius d_n around x_n must be contained in the ball $B_{2R}(0)$. Note that $d_n \leq R$ since $x_0 = 0$. Consequently, if $B_R(0)$ contains n centers then

$$\sum_{j=1}^{n} d_j^d \leq 2^d R^d$$

If, for example, $d_n \geq Cn^\gamma$ with $\gamma \geq 0$ then it follows that

$$\#\{x_n \mid |x_n| \leq R\} \leq C_1 R^{\frac{d}{\gamma d+1}}$$

Hence the lemma applies if $\gamma \geq \frac{2}{d(d-2)}$ (for $d \geq 3$).

This shows

Theorem 2.11. *Let $V(x) = \sum_{n\in\mathbb{N}} f(x-x_n)$ with a square integrable single-site potential f of compact support. If the centers x_n satisfy*

$$d_n := \inf_{m\neq n} |x_m - x_n| \gtrsim n^\gamma$$

for some $\gamma > \frac{2}{d(d-2)}$ then the operator $H_0 + V$ has absolutely continuous spectrum containing $[0, \infty)$.

Note that for non-positive f these operators can have essential spectrum below zero. The existence of negative essential spectrum for these types of operators is easy to see, Theorem 3.1 below.

Let us reconsider Model II: The random potential is of the form $V_\omega(x) = \sum q_i(\omega)\xi_i(\omega) f(x-i)$. Under the same assumptions as in Theorem 2.5 we get

$$\mathbb{E}\mu(r) = \int_{|x|\leq r} \mathbb{E}[V_\omega(x)^2] dx \leq C \sum_{|n|\leq r} p_n \quad \text{with } p_n := \mathbb{P}(\xi_n = 1).$$

If the p_n decay polynomial we recover the result in Theorem 2.5, since for $p_n \lesssim (1+|n|)^{-\beta}$

$$\sum_{|n|\leq R} p_n \lesssim \int_{|x|\leq R} (1+|x|)^{\beta}\, dx \sim \int_0^R \frac{r^{d-1}}{(1+r)^{\beta}}\, dx \sim R^{d-\beta}.$$

So we have to have $d-\beta < d-2 \Leftrightarrow \beta > 2$. Nevertheless, the probabilistic version of Theorem 2.7 also applies if the p_n's do not decay polynomially:

Theorem 2.12. *Set $V_\omega(x) = \sum q_i(\omega)\xi_i(\omega) f(x-i)$ with q_i independent identically distributed random variables with a finite second moment and $\mathbb{P}(q_i < 0) > 0$, ξ_i independent $\{0,1\}$-valued random variables also independent from the q_i's, and f a non-positive function with compact support, $f(x) \leq c < 0$ on some non-empty open set. Then for the operator $H_\omega = H_0 + V_\omega$ we have $\mathbb{P}$-almost surely:*
i) $[0,\infty) \subset \sigma_{\mathrm{ac}}(H_\omega)$ if $\sum_{|i|\leq R} p_i \lesssim 1 + R^\alpha$ for some $\alpha < d-2$,
ii) $\sigma_{\mathrm{ess}}(H_\omega) \cap (-\infty, 0) \neq \emptyset$ if $\sum p_i = \infty$.
That is, we have a non-trivial model if $\sum p_i = \infty$ which has some absolutely continuous spectrum as long as $\sum_{|i|\leq R} p_i$ does not grow too fast.

3 The essential spectrum below zero

3.1 Existence of negative essential spectrum

In this chapter we investigate the spectrum of Schrödinger operators with sparse potentials at negative energies. We start with a criterion for the existence of negative essential spectrum.

Theorem 3.1. *Let f be a bounded function of compact support. Suppose $E < 0$ is an eigenvalue of $H_f = H_0 + f$. Let x_{n_j} be points in $\mathbb{R}^d$, such that as $n \to \infty$. Consider the operator $H = H_0 + V$, $V(x) = \sum_n f_n(x - x_n)$. If $f = f_{n_j}$ for infinitely many j, then $E \in \sigma_{\mathrm{ess}}(H)$.*

Proof. Let ψ be an eigenfunction of H_f for the eigenvalue E, $H_f\psi = E\psi$, $\|\psi\| = 1$. Let x_{n_j} be a subsequence of x_n such that $\mathrm{dist}(x_{n_j}, \{x_m\}_{m\neq n_j}) \to \infty$ and $f_{n_j} = f$ and set $\psi_j(x) = \psi(x - x_{n_j})$. Then $(\psi_j)_j$ is a Weyl sequence for the operator H and the energy E, that is,

$$(H-E)\psi_j \to 0, \quad \|\psi_j\| = 1$$

and $\psi_j \to 0$ weakly as $j \to \infty$. ∎

Remark 3.2. The proof of the above theorem also gives the following consequence: If we drop the sparseness condition $\text{dist}(x_n, \{x_m\}_{m\neq n}) \to \infty$ but assume $f \leq 0$ then we still get $\sigma_{\text{ess}}(H) \cap (-\infty, 0] \neq \emptyset$

Example: In Model I suppose that $H_f = -\Delta + f$ has a negative eigenvalue E. If $\sum p_n = \infty$, the Borel-Cantelli lemma implies that $\xi_n = 1$ for infinitely many $n \in \mathbb{N}$. By the above remark we learn that there is some essential spectrum in $(-\infty, E]$.

Let us denote by Ξ the random set $\Xi = \{n \in \mathbb{Z}^d |\, \xi_n = 1\}$. We have shown that $\#\Xi = \infty$ almost surely, if $\sum p_n = \infty$. Moreover, we have:

Proposition 3.3. *If $p_n \to 0$ as $|n| \to \infty$, but $\sum p_n = \infty$ then with probability one, there exists an infinite sequence $n_j \in \Xi$, such that $\text{dist}(n_j, \Xi \backslash \{x_j\}) \to \infty$ as $|j| \to \infty$.*

With this proposition we can apply Theorem 3.1 to Model I.

Proof. We first fix an arbitrary integer $L \geq 1$. Since $\sum p_n = \infty$ there is a sequence $k_i \in \mathbb{Z}^d$, such that $|k_i - k_j| \geq L+1$ for $i \neq j$ and $\sum p_{k_i} = \infty$. For a given k_i we denote by A_i^L the event that in the cube $\Lambda_L(k_i) := \{n \in \mathbb{Z}^d |\, |n - k_i| \leq L/2\}$ $\xi_i = 1$, but $\xi_j = 0$ for all $j \in \Lambda_L(k_i) \backslash \{k_i\}$, that is,

$$A_i^L := \{\omega |\, \Xi \cap \Lambda_L(k_i) = \{k_i\}\}\,.$$

The event A_i^L occurs with probability

$$\mathbb{P}(A_i^{(L)}) = p_{k_i} \prod_{j \in \Lambda_L(k_i) \backslash \{k_i\}} (1 - p_j) \geq \frac{1}{2^{L^d}} p_{k_i}$$

if $|k_i|$ is large enough. Consequently, $\sum \mathbb{P}(A_i^{(L)}) = \infty$, so by the Borel–Cantelli lemma we conclude that $A_\infty^{(L)} = \{\omega |\, \omega \in A_i^{(L)} \text{ for infinitely many } i\}$ has probability one. Thus, $B := \bigcap_{L=1}^{\infty} A_\infty^{(L)}$ has full probability as well. For $\omega \in B$ there is a sequence $n_j \in \Xi$ with $\xi_{n_j} = 1$, and $\xi_m = 0$ for all $|m - n_j| \leq L/2$ and $m \neq n_j$. With the diagonal sequence trick we can find a subsequence which is separated from the rest by an arbitrary distance near infinity. ∎

Remark 3.4. An inspection of the proof of Proposition 3.3 shows that the assertion is also valid in the stationary case, that is, for $p_n \equiv p$. In fact what is needed is merely $0 < c_0 \leq p_n \leq c_1 < 1$.

We will investigate the essential spectrum of operators in the Model I class in more details in the next section.

The spectrum of operators with Model II potentials, that is, with potentials of the form

$$V_\omega(x) = \sum_{n\in\mathbb{Z}^d} q_n(\omega)\xi_n(\omega)f(x - x_n)$$

with q_n independent identically distributed (and independent of the ξ_n) can be treated in a similar way as the model considered above. We assume $f \le 0$ and $\sum p_n = \sum \mathbb{P}(\xi_n = 1) = \infty$.

Let us denote by $\mathbb{P}_0$ the probability distribution of q_0 (and hence of a general q_n). To avoid notational inconvenience we assume $\operatorname{supp}\mathbb{P}_0 \subset [0,\infty)$. For any $\lambda \ge 0$ we denote by H_λ the operator $H_\lambda = H_0 + \lambda f$ and by $E_n(\lambda)$ its eigenvalues $E_0(\lambda) < E_1(\lambda) \le E_2(\lambda) \le \ldots < 0$.

Theorem 3.5. *For $\lambda \in \operatorname{supp}\mathbb{P}_0$ and any n, the energy $E_n(\lambda)$ belongs to the essential spectrum $\sigma_{\mathrm{ess}}(H_\omega)$ of H_ω almost surely.*

Proof. Since $\lambda \in \operatorname{supp}\mathbb{P}_0$ and $\sum p_l = \infty$ we find (with probability one) a sequence n_j, $|n_j| \to \infty$, such that

$$\xi_{n_j} = 1 \quad \text{and} \quad q_{n_j} \in (\lambda - 1/j, \lambda + 1/j)\,,$$

and in addition $\xi_m = 0$ for all $m \in \Lambda_j(n_j)$. With ψ the eigenfunction of H_λ corresponding to the energy $E_n(\lambda)$ and $\psi_j(x) := \psi(x - n_j)$, we have $\psi_j \overset{w}{\to} 0$ and $(H_\omega - E_n(\lambda))\psi_j \to 0$ by construction. ∎

We turn to Model III, that is, potentials of the form

$$V_\omega(x) = \sum a_n q_n(\omega) f(x - n)$$

with (deterministic) $a_n \to 0$ and q_n independent identically distributed with common distribution $\mathbb{P}_0$. If $\operatorname{supp}\mathbb{P}_0$ is compact, then $V_\omega(x) \to 0$ as $|x| \to \infty$, so V_ω is relatively compact and $\sigma_{\mathrm{ess}}(H_\omega) = [0,\infty)$. As above, denote by H_λ the operator $H_\lambda = H_0 + \lambda f$ and by $E_n(\lambda)$ its ordered eigenvalues (below zero). We can redo the above construction of Weyl sequences for $E_n(\lambda)$ if there is a sequence of points $n_j \in \mathbb{Z}^d$ such that $|a_{n_j} q_{n_j} - \lambda| < \varepsilon$ for arbitrary $\varepsilon > 0$ and $q_n \le$ const near n_j. By Borel-Cantelli this happens with probability one if $\sum_n \mathbb{P}\big(q_n \in (a_n^{-1}(\lambda - \varepsilon), a_n^{-1}(\lambda + \varepsilon))\big) = \infty$. Assume that a_n decays like $|n|^{-\alpha}$

(some $\alpha > 1$). Then, if $\mathbb{P}(q_n > a) \le C_1 \exp(-C_2 a)$, the above sum obviously converges. However, if $\mathbb{P}(q_n \in [a,b]) \sim \int_a^b s^{-\beta}\, ds$ (for a, b large), then

$$\mathbb{P}\left(q_n \in\ |n|^\alpha]\lambda - \varepsilon, \lambda - \varepsilon[\right) \sim \int_{|n|^\alpha(\lambda-\varepsilon)}^{|n|^\alpha(\lambda+\varepsilon)} s^{-\beta}\, ds \sim |n|^{-\alpha\beta+\alpha} \qquad \beta > 1$$

which is not summable if

$$\beta \le 1 + d/\alpha. \tag{3.1}$$

In case $\alpha > 1$ and $\beta > 3$ (to ensure $\mathbb{E}(q_i^2) < \infty$) we know from section 2.2 that $[0,\infty) \subset \sigma_{\mathrm{ac}}(H_\omega)$ in three and more dimensions. If α is close to 1 and the dimension is at least three, we can choose β such that (3.1) is satisfied *and* $\beta > 3$. Thus in these cases we know that there is absolutely continuous spectrum above zero and additional essential spectrum below. The corresponding discrete model (i.e., on $l^2(\mathbb{Z}^d)$) was considered in [20]. There it is proven that the spectrum below zero is pure point.

3.2 Klaus' theorem

In this section we prove a partial converse to Theorem 3.1. We consider *deterministic* sparse potentials of the form

$$V(x) = \sum f(x - x_n)$$

with $\operatorname{dist}(x_n, \{x_m\}_{m\neq n}) \to \infty$ as $n \to \infty$. As above f is a non-positive (say bounded) function of compact support. Later we will actually allow the "single-site potential" f to vary with the center x_n.

We already know from our discussion above that the Schrödinger operator $H = H_0 + V$ has absolutely continuous spectrum including $[0,\infty)$ if the centers x_n are "sparse enough" (see Theorems 2.7 and 2.11). Moreover, Theorem 3.1 tells us that the eigenvalues E_n ($n = 0, 1, \dots$) of the "model operator" $H_f = H_0 + f$ belong to the essential spectrum of H.

The following theorem guarantees that there is no other essential spectrum of H below zero.

Theorem 3.6 (Klaus). *If the potential is sparse, that is,* $\operatorname{dist}(x_n, \{x_m\}_{m\neq n}) \to \infty$ *as* $n \to \infty$ *then*

$$\sigma_{\mathrm{ess}}(H) = \{E_n |\, n \in \mathbb{N}\} \cup [0,\infty).$$

Remark 3.7. This theorem is due to Martin Klaus [26] who stated it for the one-dimensional case only. Klaus proved this result by Birman-Schwinger techniques. An alternative proof can be found in [6]. We give a third proof below. Klaus' paper deals with the more general situation of potentials $V(x) = \sum f_n(x - x_n)$ which we shall also discuss below.

The physical idea behind Klaus' theorem is simple: An approximate eigenfunction (Weyl sequence) corresponding to essential spectrum will mainly live close to infinity. Since the distance between the centers x_n grows near infinity, these "eigenfunctions" must behave like an eigenfunction of the operator with just one center.

Our proof uses the IMS-localization formula [6, Section 3.1] to separate the single bumps. Let j_n be a partition of unity, that is a sequence of $\mathcal{C}^\infty$-functions, $0 \le j_n(x) \le 1$ with $\sum j_n(x)^2 = 1$, and $\sup \sum |\nabla j_n(x)|^2 < \infty$.

The IMS-formula reads

$$H = \sum_n j_n H j_n - \sum_n |\nabla j_n|^2.$$

In our proof of Klaus' theorem we will use a different version of this type of formula, since we have to compute $\|(H - E)\varphi\|$:

$$\begin{aligned}
\|(H-E)\varphi\|^2 &= \sum_n \langle j_n(H-E)\varphi, j_n(H-E)\varphi\rangle \\
&= \sum_n \langle j_n(H-E)\varphi, (H-E)j_n\varphi\rangle + \sum_n \langle j_n(H-E)\varphi, [j_n, H_0]\varphi\rangle \\
&= \sum_n \langle (H-E)j_n\varphi, (H-E)j_n\varphi\rangle + \sum_n \langle [j_n, H_0]\varphi, j_n(H-E)\varphi\rangle \\
&\quad + \sum_n \langle j_n(H-E)\varphi, [j_n, H_0]\varphi\rangle - \sum_n \langle [j_n, H_0]\varphi, [j_n, H_0]\varphi\rangle \\
&= \sum_n \langle (H-E)j_n\varphi, (H-E)j_n\varphi\rangle + L_E(\varphi).
\end{aligned}$$

Using the explicit expression $[j_n, H_0] = (\Delta j_n) + 2(\nabla j_n)\nabla$ for the commutator and the fact that V is infinitesimally small w.r.t. H_0, an easy but tedious calculation shows that the localization error can be bounded by

$$\begin{aligned}
|L_E(\varphi)| &\le \sum_n \left(\|j_n(H-E)\varphi\| \, \|[j_n, H_0]\varphi\| + \|[j_n, H_0]\varphi\|^2 \right) \\
&\le C \sum_n \sup_{\operatorname{supp}\varphi} \left(|\Delta j_n(x)| + |\nabla j_n(x)| \right) \qquad (3.2)
\end{aligned}$$

where the constant depends on $\|\varphi\|$, $\|(H-E)\varphi\|$, and $\|\Delta\varphi\|$ and is therefore uniformly bounded for a Weyl sequence. We now turn to the

Proof of Theorem 3.6: It is obvious that $[0,\infty) \subset \sigma_{\text{ess}}(H)$. This is simply due to the fact that the potential is sparse. From the sparseness it also follows that there are *huge* regions where the potential is zero and we have a lot of space to construct Weyl sequences for non-negative energies. To control the negative essential spectrum we choose a partition of unity $\{j_n\}_{n=0,1,\dots}$ such that the function j_n is concentrated near the point x_n while j_0 takes care of the region where the potential is zero. More precisely, we choose the partition of unity such that:

i) $\operatorname{supp} j_n$ is compact for $n \neq 0$ and $j_n(x)j_m(x) = 0$ for $n \neq m$, and $n, m \neq 0$,

ii) $\exists N \in \mathbb{N}$ such that $j_n(x)V(x) = f(x - x_n)$ for $n \geq N$,

iii) $\exists R_0$ such that $V \equiv 0$ on $\operatorname{supp} j_0 \cap \{|x| \geq R_0\}$,

iv) $\sup_{|x|\geq R} \sum_n (|\nabla j_n(x)| + |\Delta j_n(x)|) \to 0$ as $R \to \infty$,

So, $j_n = 1$ on $\operatorname{supp} f(\cdot - x_n)$ for large enough n and decays to zero outside. Note that by i) condition iv) will follow as soon as $\|\nabla j_n\|_\infty \to 0$, $\|\Delta j_n\|_\infty \to 0$ as $n \to \infty$, and $\sup_{|x|\geq m} |\nabla j_0(x)|$, $\sup_{|x|\geq m} |\nabla j_0(x)| \to 0$ as $m \to \infty$. Since x_n is far away from the other centers for large n, j_n can indeed decay slowly ($\|\nabla j_n\|_\infty$ and $\|\Delta j_n\|_\infty$ small) without overlapping the other j_m's and still ensuring condition ii). The rest is gathered in j_0, whose support contains the major part of the region where the potential V vanishes.

Let φ_k be a Weyl sequence for H corresponding to an energy $E < 0$ in $\sigma_{\text{ess}}(H)$. We may assume that $\varphi_k \in \mathcal{C}_0^\infty$ and $\operatorname{supp} \varphi_k \cap B_k(0) = \emptyset$. By the definition of a Weyl sequence we have $\|\varphi_k\| = 1$ and $\|(H-E)\varphi_k\| \to 0$ as $k \to \infty$. Our goal is to construct from this a Weyl sequence for the model operator $H_f = H_0 + f$. The calculation above gives

$$\|(H-E)\varphi_k\|^2 = \sum_n \|(H-E)j_n\varphi_k\|^2 + L_E(\varphi_k). \tag{3.3}$$

By iv) above, the assumption on the support of the Weyl sequence, and the bound (3.2) on the localization error $L_E(\varphi_k)$, we see that $L_E(\varphi_k) \to 0$ as

$k \to \infty$. Consequently, we get

$$\sum_n \|(H-E)j_n\varphi_k\|^2 \to 0 \qquad \text{as } k \to \infty. \tag{3.4}$$

We remind the reader that the sum in (3.4) is actually finite since φ_k has compact support. Given $0 < \varepsilon < |E|$ we can take k large enough, such that

$$\sum_n \|(H-E)j_n\varphi_k\|^2 < \varepsilon^2/2. \tag{3.5}$$

It follows that for this k there exists at least one $n \in \{0, 1, 2, \dots\}$ with

$$\|(H-E)j_n\varphi_k\| < \varepsilon \|j_n\varphi_k\|.$$

For otherwise $\sum_n \|(H-E)j_n\varphi_k\|^2 \geq \varepsilon^2 \sum_n \|j_n\varphi_k\|^2 = \varepsilon^2$, since $\sum \|j_n\varphi_k\|^2 = \|\varphi_k\|^2 = 1$, which contradicts (3.5). Furthermore, since the potential vanishes on the support of $j_0\varphi_k$ for $k \geq R_0$, we have $\|(H-E)j_0\varphi_k\|^2 \geq |E|^2 \|j_0\varphi_k\|^2 > \varepsilon^2 \|j_0\varphi_k\|^2$. Thus there exists an $n_k \geq 1$ for which $\|j_{n_k}\varphi_k\| > 0$ and

$$\|(H-E)j_{n_k}\varphi_k\| < \varepsilon \|j_{n_k}\varphi_k\|.$$

Hence we get existence of a sequence $\{n_k\}_k$ such that

$$\frac{\|(H-E)j_{n_k}\varphi_k\|}{\|j_n\varphi_k\|} \to 0 \qquad \text{as } k \to \infty.$$

Next we define a Weyl sequence for H_f by setting

$$\psi_k(x) := j_{n_k}(x + x_{n_k})\varphi_k(x + x_{n_k}) / \|j_{n_k}\varphi_k\|.$$

In fact, $\|\psi_k\| = 1$ by construction and

$$\|(H_f - E)\psi_k\| = \frac{\|(H_f - E)j_{n_k}(. + x_{n_k})\varphi_k(. + x_{n_k})\|}{\|j_{n_k}\varphi_k\|} = \frac{\|(H-E)j_{n_k}\phi_k\|}{\|j_n\varphi_k\|} \to 0$$

as $k \to \infty$. ∎

The above proof actually works for the more general situation where

$$V(x) = \sum_n f_n(x - x_n). \tag{3.6}$$

If again $\operatorname{dist}(x_n, \{x_m\}_{m \neq n}) \to \infty$ and the f_n are, say, bounded functions of compact support with $\|f_n\|_\infty$ bounded, then the following theorem holds:

Theorem 3.8 (Klaus, general case). *Set* $H_m = H_{f_m}$. *Denote by* $\mathcal{E}$ *the set of energies*

$$\begin{aligned}\mathcal{E} \;=\; & \big\{E < 0 \mid \textit{there exists a sequence } n_j, \textit{ and energies} \\ & \qquad E_{n_j} \in \sigma(H_{n_j}) \text{ with } \mathrm{E_{n_j}} \to E\big\}.\end{aligned}$$

Then $\sigma_{\text{ess}}(H) = \mathcal{E} \cup [0, \infty)$.

Remark 3.9. For these results the boundedness of f (equivalently V) is not essential. It is enough to assume an L^p condition on f for some p large enough (depending on the dimension) which, since the centers x_n are sparse and f has compact support, leads to a uniform local L^p condition for V. This is enough to ensure that V is infinitesimally operator small with respect to $H_0 = -\Delta$.

3.3 Klaus' type spectrum for sparse random potentials

In this section we will apply Klaus' theorem to random potentials. We start with Model I, that is,

$$V_\omega(x) = \sum_n \xi_n(\omega) f(x-n)$$

with the assumptions and notations made throughout the text; in particular, f has compact support and $p_n = \mathbb{P}(\xi_n = 1)$, $\mathbb{P}(\xi_n = 0) = 1 - p_n$.

By Borel-Cantelli we know that there are infinitely many "bumps" $f(x-n)$, that is, the set $\Xi = \{n \,|\, \xi_n = 1\}$ is infinite (almost surely), if and only if $\sum_{n\in\mathbb{Z}^d} p_n = \infty$. As we have seen in Section 3.1, this condition implies that the negative eigenvalues E_n of $H_0 + f$ belong to the essential spectrum of H_ω. Klaus' theorem tells us that this is all of the negative essential spectrum of H_ω, *provided* that the set Ξ does not cluster at infinity. We prove that this is, indeed, true under an additional assumption on the p_n:

Theorem 3.10. *If* $\sum p_n = \infty$ *but* $\sum p_n^2 < \infty$ *then*

$$\sigma_{\text{ess}}(H_\omega) = \{E_n \,|\, n = 0, 1, \dots\} \cup [0, \infty) \quad \mathbb{P}\text{-}a.s.$$

Proof. Let Λ be an arbitrary cube in $\mathbb{R}^d$ with center in $\mathbb{Z}^d$. We define the event

$$A_2(\Lambda) := \{\omega \mid \text{ For at least two } n, m \in \Lambda, n \neq m, \xi_n = \xi_m = 1\}\,. \tag{3.7}$$

Then

$$\mathbb{P}(A_2(\Lambda)) \leq \sum_{i,j\in\Lambda} p_i p_j = (\sum_{i\in\Lambda} p_i)^2 \leq |\Lambda| \sum_{n\in\Lambda} p_n^2. \tag{3.8}$$

where we used Jensen's inequality.

For fixed L we set

$$A_2(L) = \left\{\omega \in A_2(\Lambda_L(n)) \text{ for infinitely many } n \in \mathbb{Z}^d\right\}.$$

Since

$$\sum_n \mathbb{P}(A_2(\Lambda_L(n))) \leq C_L \sum_{n\in\mathbb{Z}^d} p_n^2 < \infty$$

we conclude that $\mathbb{P}(A_2(L)) = 0$. Consequently,

$$A_2 := \bigcup_{L=1}^{\infty} A_2(L)$$

has zero probability as well. For ω in the complement of A_2 we have: If $n_j \in \Xi = \{n|\,\xi_n = 1\}$, $n_j \to \infty$, then $\mathrm{dist}(n_j, \Xi\backslash\{n_j\}) \to \infty$. So Klaus' theorem (Theorem 3.6) applies in this situation. ∎

The same reasoning gives a similar result for Model II, where

$$V_\omega(x) = \sum_{n\in\mathbb{Z}^d} q_n(\omega)\xi_n(\omega) f(x-n).$$

Here the q_n are independent random variables with common distribution $\mathbb{P}_0$. We denote by $\{E_n(\lambda)\}$ the eigenvalues of $H_\lambda = H_0 + \lambda f$.

Corollary 3.11. *If* $\sum p_n = \infty$ *and* $\sum p_n^2 < \infty$ *then*

$$\sigma_{\mathrm{ess}}(H_\omega) = \overline{\{E_n(\lambda)|\; \lambda \in \operatorname{supp}\mathbb{P}_0, n = 0, 1, \dots\}} \cup [0,\infty) \quad \mathbb{P}\text{-}a.s.$$

For Model III a similar consideration shows that the behavior of the probability measure $\mathbb{P}_0$, the distribution of the q_n determines the essential spectrum. More precisely, let $G(x) := \mathbb{P}_0([x,\infty))$ and assume $G(x) \sim x^{-\alpha}$ near infinity. Then, for any fixed $\gamma > 0$ we have

$$\mathbb{P}(a_n q_n \in [\gamma,\infty)) = G(a_n^{-1}\gamma) \sim a_n^{\alpha}.$$

So, if $\sum_{n\in\mathbb{Z}^d} a_n^\alpha = \infty$ we have infinitely many wells of depth at least γ. Moreover, if $\sum a_n^{2\alpha} < \infty$, we have only single wells near infinity.

In all these cases we obtain as a by-product that the essential spectrum of H_ω is (almost surely) *independent* of the ω. This *does not* follow from general nonsense (as in [21]) since our potentials are not stationary. In fact, the discrete spectrum *will* depend on ω. Below we will show the invariance of the essential spectrum in fair generality.

The method of Klaus' theorem can be used for cases when "impurities" cluster at infinity as well. Let us define this exactly for the case of Model I. For a finite subset F of $\mathbb{Z}^d$ we set

$$H_F = H_0 + \sum_{n\in F} f(\cdot - n). \tag{3.9}$$

Operators of this type will be called model operators of rank $|F|$. The eigenvalues of H_F will be denoted by $E_n(F)$. They are always negative, for fixed F there are only finitely many of them (f has compact support). We are going to show that the essential spectrum of H_ω is determined by a given subset of these eigenvalues.

We will call a finite subset F of $\mathbb{Z}^d$ essential (for H_ω) if

$$\mathbb{P}(F+n \subset \Xi \text{ for infinitely many } n) = 1$$

(recall $F+n = \{m+n |\ m\in F\}$), that is, if

$$\sum_{n\in\mathbb{Z}^d} \prod_{l\in F} p_{l+n} = \infty. \tag{3.10}$$

As long as $\sum p_n^k < \infty$ only sets F of rank at most $k-1$ can be essential. To see this, consider the obvious generalization $A_k(\Lambda)$ of the set $A_2(\Lambda)$ in (3.7)

$$A_k(\Lambda) = \{\omega |\ \exists \text{ at least } k \text{ distinct points } n_l \text{ in } \Lambda \text{ with } \xi_{n_l} = 1\}.$$

As for $A_2(\Lambda)$ we have the bound $\mathbb{P}(A_k(\Lambda)) \leq (\sum_{i\in\Lambda} p_i)^{\,k} \leq (|\Lambda|)^{\,k-1}\ \sum_{i\in\Lambda} p_n^k$. Thus by Borel-Cantelli $A_k(L) = \limsup A_k(\Lambda_L)$ and $A_k = \bigcup_{L=1}^\infty A_k(L)$ have zero probability as soon as $\sum p_n^k < \infty$. In other words, if $\sum p_n^k < \infty$ we have that near infinity, a maximum of $k-1$ distinct points can have $\xi_n = 1$ in arbitrary large boxes, that is, the essential sets have at most rank $k-1$.

Theorem 3.12. *Let $\mathcal{E} = \{E_n(F) \mid F \text{ is essential for } H_\omega\}$. If $\sum p_n^k < \infty$ for some k then*

$$\sigma_{\text{ess}}(H_\omega) = \mathcal{E} \cup [0,\infty) \quad \mathbb{P}\text{-}a.s.$$

Proof. We apply Klaus' theorem (general case) to the possible (finite) clusters F. We obtain that $\sigma_{\text{ess}}(H_\omega) = \overline{\mathcal{E}} \cup [0,\infty)$. It remains to show that $\mathcal{E}$ is a closed set. We write $\mathcal{E} = \bigcup_{j=1}^{k-1} \mathcal{E}_j$ with

$$\mathcal{E}_j = \{E_n(F) |\, |F| = j\}\,.$$

For each finite F the set of negative eigenvalues of H_F, $E(F) = \{E_n(F)\}$, is finite. By shifting F if necessary we may assume that the origin belongs to F and, moreover, $F \subset (\mathbb{Z}_+)^d$. The possible accumulation points in $\mathcal{E}_j$ come from sequences F_j such that F_j splits asymptotically into at least two clusters. The corresponding eigenvalues converge to an eigenvalue of one of those clusters, that is, belong to $\mathcal{E}_l$ with $l < j$. ■

Remark 3.13. If we drop the condition $\sum p_n^k < \infty$ and assume only $p_n \to 0$ as $n \to \infty$, percolation theory shows that still only finite sets occur as essential clusters near infinity. So, in this case we have $\sigma_{\text{ess}}(H_\omega) = \overline{\mathcal{E}} \cup [0,\infty)$ but we don't know whether (the still *non-random* set) $\mathcal{E}$ is closed. Of course, the possible cluster points of $\mathcal{E}$ come from eigenvalues of some of the H_F with F essential for H_ω, so these cluster points might be called thresholds. The above theorem then says that the negative essential spectrum of H_ω is given by the negative eigenvalues of some of the model operators H_F together with the thresholds.

The above method allows us to describe the essential spectra of the operators from Model II and III as well in a straightforward way. We only remark

Theorem 3.14. *The essential spectrum of Schrödinger operators with sparse random potentials* (*of type I–III*) *is independent of* ω $\mathbb{P}$*-almost surely.*

We pause for a short summary about sparse random potentials of type I:

In Section 2.2 we proved that $[0,\infty)$ belongs to the a.c. spectrum if $p_n \le C(1+|n|)^{-(2+\varepsilon)}$. There exists essential spectrum below zero if $\sum p_n = \infty$. If $p_n \le C|n|^{-\alpha}$ for large n ($\alpha > 0$ arbitrary), the essential spectrum below zero is countable, hence pure point spectrum. The essential spectrum below zero is finite if $\sum p_n^2 < \infty$. It consists of the negative eigenvalues of the operator $H_1 = H_0 + f$. If $\sum p_n^2 = \infty$ it may happen that the eigenvalues of the operator $H_{n,m} = H_0 + f(\cdot - x_n) + f(\cdot - x_m)$, $n \ne m$ belong to the essential spectrum, in fact they do if and only if $\sum_{r\in\mathbb{Z}^d} p_{n+r}p_{m+r} = \infty$. Those eigenvalues may accumulate only at the eigenfunctions of H_1! If

$\sum p_n^3 = \infty$ this "hierarchy" goes on, that is, the eigenvalues of the operators $H_{n,m,l} = H_0 + f(\cdot - x_n) + f(\cdot - x_m) + f(\cdot - x_l)$ belong to the essential spectrum of H_ω if and only if $\sum_{r\in\mathbb{Z}^d} p_{n+r}p_{m+r}p_{l+r} = \infty$, etc. The essential spectrum is always a non-random set, while the discrete spectrum will vary with ω. Although discrete essential spectrum is certainly somewhat unusual, the measure theoretic nature of the spectrum fits pretty well into the picture physicists have of stationary (ergodic) random potentials.

The occurrence of countable or even finite essential spectrum is perhaps somewhat surprising. There are two ways to produce such spectrum. The first is to have eigenvalues of infinite multiplicity. While we can not rule out them in general, there are certainly no such eigenvalues in dimension one. The other, more likely mechanism to pruduce isolated points in the essential spectrum is that eigenvalues from the discrete spectrum can accumulate. We believe this is what is happening in our case.

For low energies the spectrum is pure point; for high energies it has an absolutely continuous component if $d \geq 3$. Note that in our case as well we can establish coexistence of a.c. spectrum at high and p.p. spectrum at low energies only for space dimension 3 and higher!

3.4 Dense point spectrum

We turn to Model II:

$$V_\omega(x) = \sum q_n(\omega)\xi_n(\omega)f(x_n).$$

We saw that the essential spectrum of H_ω in this case depends on the support of the distribution $\mathbb{P}_0$ of q_n, in fact,

$$\sigma_{\text{ess}} = \bigcup_{k=1}^{\infty} \mathcal{E}_k \cup [0,\infty), \tag{3.11}$$

where

$$\mathcal{E}_k = \Big\{\sigma(H_0 + \sum_{i=1}^{k} \lambda_i f(x - n_i)) \mid \lambda_i \in \inf \operatorname{supp} \mathbb{P}_0 \text{ and } \sum_{r\in\mathbb{Z}^d} p_{n_1+r}\dots p_{n_k+r} = \infty\Big\}.$$

We assumed above (and will assume in the following) that $p_n \leq C|n|^{-\alpha}$ for large $|n|$ and some $\alpha > 0$. The union in (3.11) is finite in this case. So, if supp $\mathbb{P}_0$ is countable the essential spectrum below zero is countable as well, hence pure point. This includes the case of the Bernoulli distribution which turns out to be very hard in the stationary case.

If the support of $\mathbb{P}_0$ is uncountable we can in certain cases apply multi-scale analysis (see [11, 12, 9, 5, 18, 24]).

Let us suppose that $\mathbb{P}_0$ is absolutely continuous with a bounded density of compact support. Moreover, we assume that $\sum p_n = \infty$ and $p_n \leq C|n|^{-(2+\varepsilon)}$ to ensure the existence of essential spectrum below zero and absolutely continuous spectrum above zero.

The multi-scale analysis requires a number of modifications before it can be applied to our case of sparse potentials. We will not give complete details here but rather concentrate on the critical change required, which is the proof of a Wegner estimate for our case.

We follow the proof in [18] for the Wegner estimate. Moreover, to avoid technicalities, we give this proof for the discrete case only (i.e., for operators on $l^2(\mathbb{Z}^d)$). A complete proof will be given in a subsequent paper [19]. We keep the notation from [18]. The crucial step there is to show that

$$\sum_{k\in\Lambda} \frac{\partial E_n(q_i,\xi_i)}{\partial q_k} \geq C > 0. \tag{3.12}$$

Here $E_n(q_i,\xi_i)$ are the negative eigenvalues of the discrete Schrödinger operator $h_0 + \sum_{i\in\Lambda} q_i(\omega)\, \xi_i(\omega) |i\rangle\langle i|$ on $l^2(\Lambda)$, Λ a box in $\mathbb{Z}^d$ with Dirichlet boundary conditions.

By the Feynman-Hellman theorem it is clear that

$$\sum_{k\in\Lambda} \frac{\partial E_n(q_i,\xi_i)}{\partial q_k} = \sum_{k\in\Lambda\cap\Xi} |\psi_n(k)|^2,$$

where ψ_n is a normalized eigenfunction corresponding to $E_n(q_i,\xi_i)$. Thus (3.12) is proved if we show

$$\sum_{k\in\Lambda\cap\Xi} |\psi_n(k)|^2 \geq C \sum_{k\in\Lambda} |\psi_n(k)|^2 = C.$$

For this it is enough to have a bound of the form

$$\|\psi\|^2_{l^2(\complement(\Xi))} \leq c\, \|\psi\|^2_{l^2(\Xi)}\,. \tag{3.13}$$

Since ψ_n is an eigenfunction we have (writing E and ψ instead of E_n and ψ_n and suppressing the box Λ in the notation)

$$0 = (h_0 + v - E)\psi = (h_0 - E)|_{\complement(\Xi)}\, \psi + (h_0 + v - E)|_{\Xi}\, \psi + \Gamma\psi$$

with the "boundary operator" $\Gamma\psi(j) := \sum_{i\in\Xi, |i-j|=1} \psi(i)$. So

$$\psi|_{\complement(\Xi)} = \big((h_0 - E)|_{\complement(\Xi)}\big)^{-1} (\Gamma(\psi|_{\Xi})).$$

Hence (3.13) follows, with a constant depending *only* on the energy E (and not on Λ), since $h_0|_{\Xi^c}$ is a non-negative operator, and thus $((h_0 - E)|_{\Xi^c})^{-1}\,\Gamma$ is bounded with norm uniform in the region Ξ. The above calculation is the main step in the proof of

Theorem 3.15. *Suppose that q_n are independent random variables with a common distribution $\mathbb{P}_0$ which has a bounded density of compact support. Let ξ_n be random variables taking values in $\{0, 1\}$, ξ_n independent of each other and of the q_n. Then the negative spectrum of $h_0 + v_\omega$ with $v_\omega(n) = q_n(\omega)\xi_n(\omega)$ is pure point.*

The above theorem can be proved for the continuous case with virtually the same techniques. Moreover, this proof can be transfered to potentials of Model III as well.

4 Surface potentials

In this chapter we will demonstrate how to use some of the ideas above for random potentials which are concentrated around a hypersurface. We note that there are several recent publications about this subject, for example, [13, 31, 16, 15] where mainly the discrete "half-space" case is studied. We will mainly concentrate on the continuous case, more precisely on potentials of the following type:

$$V_\omega(x) = \sum_{n\in\mathbb{Z}^{d-1}} q_n(\omega) f(x - (n, 0)). \tag{4.1}$$

Here $x \in \mathbb{R}^d$ $(n, 0) \in \mathbb{Z}^d \subset \mathbb{R}^d$ for $n \in \mathbb{Z}^{d-1}$, f as usual is a non-positive bounded function of compact support, and q_n are independent identically distributed random variables, indexed by $n \in \mathbb{Z}^{d-1}$, with $q_n(\omega) \geq 0$ almost surely. We will also consider discrete analogs of the surface potentials (4.1) as well as those living on a half-space $\mathbb{R}^{d-1} \times \mathbb{R}_+$ only.

4.1 Absolutely continuous spectrum

For potentials as in (4.1) it is physically clear that a particle at positive energy with velocity pointing away from the surface will travel away from the surface $\mathbb{R}^{d-1} \times \{0\}$ once it escapes from the support of the potential. We will make this picture more rigorous by using techniques from Enß' theory (see [6, 10, 33] for the necessary background).

Let φ be a function of with support in the "upper" half-space $\mathbb{R}^{d-1} \times [a, \infty)$ for some $a > 0$. Furthermore, let g be a smooth function $0 \leq g \leq 1$ with support in $[\alpha, \beta]$ $(\alpha, \beta > 0)$ and consider $g(p_d)\varphi$, where p_d is the momentum operator in direction $(0, \dots, 0, 1)$, that is, perpendicular to the surface $\mathbb{R}^{d-1} \times \{0\}$. Then $g(p_d)\varphi$ may be considered as a state starting in the upper half plane and moving away from the surface $\mathbb{R}^{d-1} \times \{0\}$. In particular, the surface $\mathbb{R}^{d-1} \times \{0\}$ or, more precisely, the support of the potential V is inside the classically forbidden region of the configuration space. The quantum mechanical particle under the free motion is described by $\mathrm{e}^{-itH_0} g(p_d)\varphi$.

While the probability of finding the quantum mechanical particle inside the classically forbidden region is never exactly zero, it is exponentially small in the following sense:

Proposition 4.1. *For any $N \in \mathbb{N}$ there exists a constant $C_N(\varphi)$ (depending on N and on φ) such that for all $t \geq 0$*

$$\left\| \chi_{\{x_d \leq a\}} \mathrm{e}^{-itH_0} g(p_d)\varphi \right\| \leq C_N(\varphi)(1 + |t|)^{-N}.$$

This proposition is very similar to [10, Lemma 6.1] and can be proven in the same way as this result.

Given the proposition, it is easy to prove the existence of the wave operators Ω for such functions. In fact, we have

Proposition 4.2. *Let V be a bounded function, such that $\operatorname{supp} V \subset \mathbb{R}^{d-1} \times [-a, a]$ for some finite a. Let φ be an L^2-function with compact support on $\mathbb{R}^d$ and $g \in \mathcal{C}_0^\infty(\mathbb{R})$ with $\operatorname{supp} g \subset [\alpha, \infty)$ for some $\alpha > 0$. Then*

$$\int_0^\infty \left\| V \mathrm{e}^{-itH_0} g(p_d)\varphi \right\| \, dt < \infty.$$

Proof.

$$\left\| V \mathrm{e}^{-itH_0} g(p_d)\varphi \right\| \leq C \left\| \chi_{x_d \leq a} \mathrm{e}^{-itH_0} g(p_d)\varphi \right\| \leq \tilde{C}_2(\varphi)(1 + |t|)^{-2}$$

by Proposition 4.1. ∎

We conclude that $\Omega_- = \text{s-lim}\, \mathrm{e}^{itH}\mathrm{e}^{-itH_0}\psi$ exist for $\psi = g(p_d)\varphi$. Then

$$\langle \Omega_-\psi, \mathrm{e}^{-itH}\Omega_-\psi\rangle = \langle \Omega_-\psi, \Omega_-\mathrm{e}^{-itH_0}\psi\rangle = \langle \psi, \mathrm{e}^{-itH_0}\psi\rangle,$$

where we used the intertwining property of Ω_- and the fact that Ω_- is an isometry. So we get that the Fourier transform of the spectral measure corresponding to $\Omega_-\psi$ equals the Fourier transform of the spectral measure of H_0 corresponding to ψ. Thus these measures coincide and Ω_- belongs to the absolutely continuous subspace of the operator H.

We have proven

Theorem 4.3. *Let V be a bounded function on $\mathbb{R}^d$ with support in $\mathbb{R}^{d-1} \times [-a, a]$. Then $[0, \infty) \subset \sigma_{\mathrm{ac}}(H_0 + V)$.*

It is clear that the above argument shows in fact the following: Suppose that the potential V satisfies a short-range condition in the sense of section 2 for all x in an open cone $K \subset \mathbb{R}^d$. Then $[0, \infty) \subset \sigma_{\mathrm{ac}}(H_0 + V)$.

This applies especially to the situation where $V(x)$ is a random potential for $x_d \leq 0$ and $V(x) \equiv 0$ for $x_d > 0$. In dimension one such a potential was investigated by Carmona [3]. He proved that in this case the spectrum above zero is purely absolutely continuous while the spectrum below zero is pure point.

Proposition 4.2 does not apply directly to the half-space model $H^+ = H_0^+ + V$, where $H_0^+ = H_{0,d-1} + H_{0,d}^+$ is the Laplacian on $\mathbb{R}^{d-1} \times \mathbb{R}_+$ with Dirichlet boundary conditions at the $\{x_d = 0\}$-hypersurface. This is simply due to the fact that there is no selfadjoint momentum operator on $L^2(\mathbb{R}_+)$. However, with the help of dilations, it is still possible to define outgoing states.

We follow the reasoning in [6] very closely. To be more precise, define the group of dilation operators on $L^2(\mathbb{R}_+)$ by $U^D(t)\psi(x_d) = \mathrm{e}^{t/2}\psi(\mathrm{e}^t x_d)$. Furthermore, set $U\psi(t) = (U^D(t)\psi)(1)$. We will not distinguish between U^D and U and their natural extensions to $L^2(\mathbb{R}^{d-1}) \otimes L^2(\mathbb{R}_+) = L^2(\mathbb{R}^{d-1} \times \mathbb{R}_+)$. Observe that U^D is a strongly continuous group of unitary transformations and that $U(U^D(t)\psi)(x_d) = U\psi(x_d + t)$. So U^D acts as translations in the range of U and can be diagonalized by a "Fourier" transform:

Lemma 4.4. *Setting $M\psi(\lambda) = \frac{1}{\sqrt{2\pi}} \int \mathrm{e}^{-is\lambda}(U\psi)(s)\, ds$ we have*

$$(MU^D(t)\psi)(\lambda) = \mathrm{e}^{-it\lambda}(M\psi)(\lambda).$$

Proof. Simply a calculation of $MU^D(t)\psi$ for ψ in a nice dense subset of $L^2(\mathbb{R}_+)$. ∎

Let $H_{0,d}^+$ be the Dirichlet Laplacian on $L^2(\mathbb{R}_+)$. We want to diagonalize $H_{0,d}^+$ on $L^2(\mathbb{R}_+)$ with the help of the Fourier transform. For this we identify $f \in L^2(\mathbb{R}_+)$ with $\tilde{f} \in L^2(\mathbb{R})$ by $\tilde{f}(x_d) := \frac{1}{\sqrt{2}} f(x_d)$ for $x_d > 0$, $\tilde{f}(x_d) := -\frac{1}{\sqrt{2}} f(-x_d)$ for $x_d < 0$. Then the map $f \to \tilde{f}$ is unitary and we have

$$\langle f, \mathrm{e}^{-itH_{0,d}^+} g\rangle_{L^2(\mathbb{R}_+,dx)} = \langle \mathcal{F}_d \tilde{f}, \mathrm{e}^{-it\zeta^2} \mathcal{F}_d \tilde{g}\rangle_{L^2(\mathbb{R},d\zeta)}$$

with $\mathcal{F}_d$ the usual Fourier transform on $L^2(\mathbb{R})$. To state Perry's estimate we need another technical result.

Lemma 4.5. *For all $t \in \mathbb{R}$: $\mathcal{F}_d U^D(t) = U^D(-t)\mathcal{F}_d$. In particular, with A the infinitesimal generator of U^D and $P_+ = \chi_{(0,\infty)}(A)$, $P_- = \chi_{(-\infty,0)}(A)$ we have*

$$\mathcal{F}_d P_\pm = P_\mp \mathcal{F}_d.$$

Proof. A calculation of $\mathcal{F}_d U^D(t)\psi$ for $\psi \in \mathcal{C}_0^\infty(\mathbb{R})$, say. ∎

Again, we did not distinguish between operators on $L^2(\mathbb{R}_+)$ and their extensions (via $f \to \tilde{f}$) to $L^2(\mathbb{R})$. We have

Theorem 4.6 (Perry's estimate for the half-space). *Let g be a $\mathcal{C}_0^\infty$ function with support in $[a^2, b^2]$, $a>0$. Then for $N\in\mathbb{N}$, $\varphi\in L^2(\mathbb{R}^{d-1}\times\mathbb{R}_+)$ we have*

$$\left\| \chi_{\{0\le x_d \le at\}} \mathrm{e}^{-itH_{0,d}^+} g(H_{0,d}^+) P_+ \varphi \right\| \le C_N(\varphi)(1+t)^{-N} \quad \textit{for all } t \ge 0. \tag{4.2}$$

Proof. For $(x, x_d) \in \mathbb{R}^{d-1} \times \mathbb{R}_+$ set

$$\psi_t(x, x_d) := (e^{-itH_{0,d}^+} g(H_{0,d}^+) P_+ \varphi)(x, x_d) = \langle K_{x_d,t}, \mathcal{F}_d P_+ \tilde{\varphi}(x,\cdot)\rangle_{L^2(\mathbb{R},d\zeta)}$$

with $K_{x_d,t}(\zeta) = \frac{1}{\sqrt{2\pi}} e^{-it\zeta^2} g(\zeta^2)$, $\zeta \in \mathbb{R}$. By the above lemma $\mathcal{F}_d P_\pm = P_\mp \mathcal{F}_d$. This implies

$$|\psi_t(x, x_d)| \le \|P_- K_{x_d,t}\|_{L^2(\mathbb{R},d\zeta)} \|\psi(x,\cdot)\|_{L^2(\mathbb{R},dx)}$$

since $\mathcal{F}_d$ and $\psi \to \tilde{\psi}$ are unitary. Thus, using $\mathrm{e}^{-itH_0^+} = \mathrm{e}^{-itH_{0,d-1}} \otimes \mathrm{e}^{-itH_{0,d}^+}$ and the fact that $\mathrm{e}^{-itH_{0,d-1}}$ commutes with $\chi_{\{0\le x_d\le at\}}$,

$$\begin{aligned}\left\| \chi_{\{0\le x_d\le at\}} \mathrm{e}^{-itH_{0,d}^+} g(H_{0,d}^+) P_+\varphi \right\|^2 &= \left\| \chi_{\{0\le x_d\le a\}} \psi_t \right\|^2_{L^2(\mathbb{R}^{d-1}\times\mathbb{R}_+)} \\ &\le at \sup_{0\le x_d\le \delta t} \|P_- K_{x_d,t}\|^2_{L^2(\mathbb{R},d\zeta)} \|\psi\|^2_{L^2(\mathbb{R}^{d-1}\times\mathbb{R}_+)} .\end{aligned}$$

Lemma 4.4 implies

$$\|P_- K_{x_d,t}\|^2 = \|M(P_- K_{x_d,t})\| = \int_{-\infty}^{0} |M(K_{x_d,t})(\lambda)|^2 \, d\lambda.$$

We have $M(K_{x_d,t})(\lambda) = \int \mathrm{e}^{i\varphi(s)} g(\mathrm{e}^{2s}) \, ds/(2\pi)$ with
$\varphi(s) := -\lambda s + t\mathrm{e}^{2s} - x_d \mathrm{e}^{s} + s/2$. Since $\mathrm{supp} g \subset [a^2, b^2]$ and $x_d \le at$ we get

$$\varphi'(s) = -\lambda + \mathrm{e}^{s}(2t\mathrm{e}^{s} - x_d) + 1/2 \ge -\lambda + a^2 t + 1/2$$

for $\lambda \le 0$ and $t \ge 0$. Using stationary phase methods as in [6, 33] we conclude the bound (4.2). ∎

With this estimate we can use the same reasoning as in Theorem 4.2 to establish the existence of the wave operators and use this again to prove existence of a.c. spectrum for H^+:

Theorem 4.7. *Let V be a bounded (for simplicity) function on $\mathbb{R}^{d-1} \times \mathbb{R}_+$ with support in $\mathbb{R}^{d-1} \times [0, a]$ (or, obeying a short-range condition in the x_d direction). Then $[0, \infty) \subset \sigma_{\mathrm{ac}}(H_0^+ + V)$.*

4.2 Pure point spectrum

The multi-scale analysis can be applied to the spectrum below zero. In particular, we can prove the Wegner estimate for those energies in the same way as in section 3.4. The initial length scale estimate can be done as in [24] either for low energies (Lifshitz tails) or for high disorder.

There occurs a special case if we consider — in addition to a surface potential as in (4.1) — an impenetrable wall at the $\{x_d = 0\}$-hypersurface. More precisely, we consider the operator $H_\omega^+ = H_0^+ + V_\omega$ with Dirichlet boundary conditions at $\mathbb{R}^{d-1} \times \{0\}$. Again, H_0^+ is the corresponding free operator. Crucial for localization with a surface potential will be the fact that, due to the Dirichlet boundary condition at the $\{x_d = 0\}$-hypersurface, such a potential *cannot* create negative spectrum if it is not strong enough.

Lemma 4.8. *If V_0 is a bounded non-positive surface potential with support in $\mathbb{R}^{d-1} \times [0, a)$ for some $a \ge 0$ then there exists $\lambda_0 > 0$ such that $H_0^+ + \lambda V_0 \ge 0$ for all $\lambda \le \lambda_0$.*

Proof. By monotonicity (min-max-principle) it suffices to prove the assertion for $V_0(x) = M\chi_{[0,a]}(x_n)$. Since this potential is independent of x_ν, $\nu = 1, 2, \ldots, d-1$ we can seperate variables and reduce the claim to the assertion that $H_0^+ = \lambda V_0(x) \geq 0$ for the case of dimension $d = 1$. For this case one can either do an explicit calculation or see it as an immediate consequence of the Hardy inequality [7]

$$\tfrac{1}{4}\langle \varphi, \tfrac{1}{|x|^2}\varphi\rangle_{L^2(\mathbb{R}_+)} \leq \langle \varphi', \varphi'\rangle_{L^2(\mathbb{R}_+)} \qquad \text{for all } \varphi \in D(H_0^+),$$

which holds due to the Dirichlet boundary condition at zero. ∎

Now we consider a random surface potential of the form

$$V_\omega(x) = \sum_{n\in\mathbb{Z}^{d-1}} q_n(\omega) f(x - (n, 0)). \tag{4.3}$$

As before, we assume that $f \leq 0$ is a bounded function of compact support ($f \neq 0$ to avoid triviality). The random variables q_n are independent and have a a common distribution $\mathbb{P}_0$ with $\operatorname{supp}\mathbb{P}_0 \subset [0, \infty)$. As usual, to prove localization we assume that $\mathbb{P}_0$ has a bounded density. By V_α we denote the potential (4.3) with all coupling constants q_n set equal to α and by H_ω^+ and H_α^+ we mean the Schrödinger operators on $L^2(\mathbb{R}^{d-1} \times \mathbb{R}_+)$ with Dirichlet boundary conditions and the potential V_ω, and V_α, respectively. Note that the potential V_α is periodic with respect to integer shifts parallel to the hypersurface $\mathbb{R}^{d-1} \times \{0\}$.

Lemma 4.9. $\inf\sigma(H_\omega^+) = \inf_{\alpha\in\operatorname{supp}\mathbb{P}_0}(\inf\sigma(H_\alpha^+))$ $\quad \mathbb{P}$-*a.s.*

Proof. By construction of a Weyl sequence. ∎

In particular, if $\mathbb{P}_0$ is unbounded from above H_ω^+ is unbounded from below (and we have to check essential self-adjointness of H_ω^+ on a suitable subspace of H_0^+ via the method of [22], say). On the other hand, if $\operatorname{supp}\mathbb{P}_0$ is compact then $\inf\sigma(H_\omega^+) = \sigma(H_{\alpha_{\max}}^+)$ with $\alpha_{\max} = \sup(\operatorname{supp}\mathbb{P}_0)$ by the lemma above. Lemma 4.8 gives the existence of a critical $\alpha_0 > 0$ such that if $\alpha_{\max} \leq \alpha_0$ then $\inf\sigma(H_\omega^+) = 0$ while $\inf\sigma(H_\omega^+) < 0$ if $\alpha_{\max} \geq \alpha_0$. This peculiar phenomenon is due to the Dirichlet barrier at the surface which forces the wavefunctions to vanish for $x_d = 0$. The magnitude of $\alpha_{\max}$ is determined by the width (and depth) of the potential f.

Now, we consider the family of operators

$$H_\omega^+(\lambda) = H_0^+ + \lambda V_\omega \qquad \text{for } \lambda \geq 0.$$

By the above discussion we have a critical constant $\lambda_0 = \alpha_0/\alpha_{\max}$ such that $\inf \sigma(H_\omega^+(\lambda)) = 0$ for $\lambda \leq \lambda_0$ and $\inf \sigma(H_\omega^+(\lambda)) < 0$ for $\lambda > \lambda_0$. The threshold, λ_0 is zero if $\operatorname{supp} \mathbb{P}_0$ is unbounded, but $\lambda_0 > 0$ otherwise..

To formulate the initial length scale estimate needed for to prove localization by the multi-scale analysis, we consider the operator H_ω^+ restricted to a box $\Lambda_{L_0}^+$ of side length L_0,

$$\begin{aligned} \Lambda_{L_0}^+ = \big\{ x \in \mathbb{R}^d \mid -L_0/2 \leq x_\nu \leq L_0/2 \text{ for } \nu = 1, \ldots, d-1, \\ \text{and } 0 \leq x_d \leq L_0/2 \big\}, \end{aligned}$$

with Dirichlet boundary conditions on $\partial \Lambda_{L_0}$. The multi-scale analysis requires an estimate of the form

$$\mathbb{P}\left(|G_E^{L_0}(x,y)| \leq \mathrm{e}^{-\gamma|x-y|} \right) \geq 1 - 1/L_0^q, \tag{4.4}$$

where $G_E^{L_0}$ is the Green's function of $H_\omega^+|_{\Lambda_{L_0}^+}$ at energy E and L_0 and q are large enough.

We are going to show this estimate for some $\lambda > \lambda_0$, say $\lambda = \lambda_0 + \varepsilon$, $\varepsilon > 0$ small. To do so it suffices to show that

$$\mathbb{P}\left(H_\omega^+|_{\Lambda_{L_0}^+} \geq 0 \right) \to 1 \qquad \text{as } \lambda \searrow \lambda_0$$

because then $\operatorname{dist}(E, \sigma(H_\omega^+|_{\Lambda_{L_0}^+})) > 0$ for negative energies $E < 0$ and λ close to λ_0. Thus a standard Combes-Thomas argument gives the exponential decay as required in (4.4). Moreover, by taking λ even closer to λ_0 we can make this probability arbitrarily close to 1. It remains to show

Proposition 4.10.

$$\lim_{\lambda \searrow \lambda_0} \mathbb{P}\left(H_\omega^+|_{\Lambda_{L_0}^+} \geq 0 \right) = 1$$

Proof. Since $H_\omega^+|_{\Lambda_{L_0}^+} \geq 0$ if all the (random) couplings in $\Lambda_{L_0}^+$ are below the critical α_0, we have

$$\begin{aligned} \mathbb{P}\left(\inf \sigma(H_\omega^+|_{\Lambda_{L_0}^+}) < 0 \right) &\leq \mathbb{P}\left(\exists n \in \Lambda_{L_0}^+ : \ \lambda q_n > \alpha_0 \right) \\ &\leq \ |\Lambda_{L_0}^+| \ \mathbb{P}_0\left((\frac{\alpha_0}{\lambda}, \alpha_{\max}) \right) \to 0 \quad \text{as } \lambda \searrow \lambda_0 \end{aligned} \tag{4.5}$$

since $\alpha_{\max} = \sup(\operatorname{supp} \mathbb{P}_0)$ is not an atom for $\mathbb{P}_0$. ∎

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