Internal Lifshitz tails for random Schrödinger operators

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Abstract. We present new results on Lifshitz tails at internal band edges for the density of states of random Schrödinger operators on $\mathbb{R}^2$. In particular, we show the existence and compute the value of the Lifshitz exponent in the case when the band edge is simple.

0. Introduction

In the early 60's (see [**16, 18**]), I.M. Lifshitz produced a heuristic showing that, at the fluctuational band edges of the spectrum of a random Schrödinger operator, the density of states decays exponentially fast. This differs dramatically from the behavior of the density of states of a periodic Schrödinger operator : in this case, the band edge decay is polynomial. One of the major consequences of this difference is that the band edge spectral behaviors for these two classes of operators are radically different: in the random case, the spectrum is localized and, in the periodic case, the spectrum is extended.

To be more specific, let us turn to the random model we will study. As our results will only be valid in dimension 2, we will restrict everything to this case. Moreover to simplify the exposition, we will not give optimal assumptions (see [**13**] for details).

1. The continuous Anderson model

Let W be a $\mathbb{Z}^2$-periodic potential in $L^2_{\text{loc}}(\mathbb{R}^2)$ and consider the periodic Schrödinger operator $H=-\Delta+W$ acting on $L^2(\mathbb{R}^2)$. It is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^2)$; let Σ_p be its spectrum.

The *continuous Anderson model* is defined to be the random Schrödinger operator

$$H_\omega = H + V_\omega = H + \sum_{\gamma\in\mathbb{Z}^2} \omega_\gamma V_\gamma, \tag{1.1}$$

where $V_\gamma(\cdot)=V(\cdot-\gamma)$, $V:\ \mathbb{R}^2\to\mathbb{R}$ is a potential and $(\omega_\gamma)_{\gamma\in\mathbb{Z}^2}$ are independent identically distributed random variables. We assume that
(H.1)

1. $0\not\equiv V$ is continuous and compactly supported.
2. V is non-negative.
3. The i.i.d. random variables $(\omega_\gamma)_{\gamma\in\mathbb{Z}^2}$ are bounded and their support is the interval $[\omega^-,\omega^+]$.

Let us recall a few well known facts from the theory of random Schrödinger operators (see e.g. [**24, 5**] or [**2**]). For all ω, H_ω is essentially self-adjoint on $\mathcal{C}_0^\infty(\mathbb{R}^2)$, and we denote by H_ω its self-adjoint extension. There exists Σ, a closed subset of $\mathbb{R}$ such that, for almost all ω, the spectrum of H_ω coincides with Σ. This set is called the *(almost sure) spectrum* of H_ω. Our assumptions on V_ω and H imply that Σ is lower semi-bounded.

It follows from the Bethe-Sommerfeld conjecture (see e.g. [**28, 4**]) and the standard characterization of Σ using admissible periodic operators (see e.g.[**6, 24**]) that Σ is a finite union of intervals (see figure 1).

The connected components of $\mathbb{R}\setminus\Sigma$ will be the gaps of Σ. The edges on the gaps are the points in $\Sigma\cap\overline{\mathbb{R}\setminus\Sigma}$.

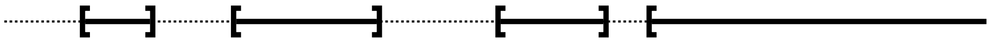

FIGURE 1. A typical Σ

One defines the integrated density of states of H_ω in the following way. Let $H_\omega^{l,D}$ to be the Dirichlet restriction of H_ω to the cube C_l centered in 0 of side length l. The operator $H_\omega^{l,D}$ has only discrete spectrum. For $E\in\mathbb{R}$, we define

$$N_\omega^l(E)=\frac{1}{\mathrm{Vol}(C_l)}\sharp\{\text{eigenvalues of } H_\omega^{l,D}\leq E\} \tag{1.2}$$

where $\sharp\mathcal{E}$ denotes the number of points of the set $\mathcal{E}$ and $\mathrm{Vol}(C_l)$, the volume of C_l.

Then, ω-almost surely, $N_\omega^l(E)$ has a limit when $l\to+\infty$. This limit is independent of the realization of ω. It is the *integrated density of states* or *IDS* of H_ω. We will denote it by $N(E)$. Physically, it represents the number of states per unit of volume below energy E for a system governed by H_ω. The function N is non random, non decreasing and right continuous. Its set of increasing points is Σ.

The integrated density of states is the main object of our study. Consider a gap in Σ, say (E_+,E_-) (see figure 1). Typically, if the random perturbation V_ω is not too large, this gap will be obtained by shrinking slightly a gap of Σ_p, say (e_+,e_-).

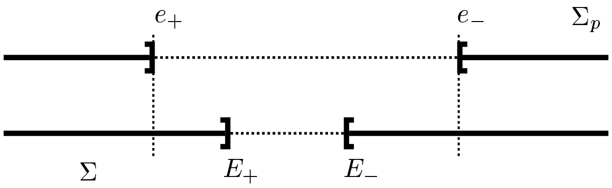

FIGURE 2. The band edges for Σ and Σ_p

Our main question then is:

(Q) how does $N(E)$ behave near $E_\pm$?

Before we state our result, let us review some of the known results on this question. Doing so, we will assume that we are working in dimension d; all the definitions and results we gave above can be generalized to this case.

2. Known results

Whether answers to (Q) are known or not depends crucially on the band edge one considers. One can distinguish essentially two cases : the bottom of the spectrum and internal band edges.

2.1. The bottom of the spectrum. This is the case that has been studied the most. Let us assume that $E_-=\inf(\Sigma)$. Translating the periodic potential by a constant, we may also assume that $E_-=0$.

In [**16, 17**], Lifshitz showed his heuristics not for the continuous Anderson model but for the Poisson model (the random potential is obtained by placing a nonnegative single site potential at every point of a Poisson process). He obtained the *Lifshitz tails*, namely

$$\log(N(E)-N(0))=\log N(E)\underset{E\to0^+}{\sim}-CE^{-d/2}. \tag{2.1}$$

Mathematical work on Lifshitz tails only appeared much later; the results were not obtained following the original Lifshitz heuristic but using Wiener integrals and the Donsker-Varadhan technique to estimate the Laplace transform of N (see [**22, 23**]). This point of view is directly related to the study of Brownian motion among Poissonian obstacles (see [**30**]).

Proofs of Lifshitz tails at the bottom of the spectrum for the continuous Anderson model following the original heuristic of Lifshitz were developed in the 80's (see [**7, 8, 19, 29**]). One does not obtain an asymptotic as precise as (2.1) but only the weaker version

$$\log|\log N(E)| \underset{E\to 0^+}{\sim} -\frac{d}{2}\log E. \tag{2.2}$$

2.2. Internal band edges. In this case, much fewer results are known. We will only describe results for the continuous Anderson model (the Poisson model does not have any internal gaps).

In dimension 1, in [**20**], (2.2) is proved at all band edges. In dimension larger than 1, much less is known. To fix ideas, let us assume that we work at the upper edge of a gap i.e. at the edge E_-. A lower edge can dealt with in the same way. Without restriction of generality, we will also assume $E_- = 0$. In [**14**], it is proved that (2.2) occurs if and only if $N_p(E)$, the density of states of a well chosen underlying periodic Schrödinger operator (see section 3.2.1) satisfies

$$\log N_p(E) \underset{E\to 0^+}{\sim} \frac{d}{2}\log E. \tag{2.3}$$

This result also holds at the bottom of the spectrum; it recovers all the cases previously described as it is known that the density of states of any periodic Schrödinger operator satisfies (2.3) at the bottom of the spectrum in any dimension and at all edges in dimension 1.

3. The results

We will start with the less precise but more general result.

3.1. The density of states decays exponentially at band edges. We prove

THEOREM 3.1. *Assume (H.1). For any edge of a gap of Σ, say E_0, one has*

$$\limsup_{\substack{E\to E_0\\ E\in\Sigma}} \frac{\log|\log|N(E)-N(E_0)||}{\log|E-E_0|} < 0. \tag{3.1}$$

Theorem 3.1 says that the integrated density of states decays at least exponentially fast at any band edge of Σ. This is one of the ingredients necessary to prove band-edge localization for H_ω (see section 6).

3.2. The Lifshitz exponent. Under more restrictive assumptions on the random operator, we are able to compute the rate of exponential decay of the integrated density of states.
Therefore, we consider a random Schrödinger operator of the form (1.1) satisfying
(H.1')

1. $0 \not\equiv V$ is a continuous function with compact support.
2. V is non-negative.
3. $(\omega_\gamma)_{\gamma\in\mathbb{Z}^2}$ is a collection of independent identically distributed random variables; the support of these random variables is the interval $[\omega^-, \omega^+]$.
4. The common distribution of the $(\omega_\gamma)_{\gamma\in\mathbb{Z}^2}$ satisfies

$$\lim_{\varepsilon\to 0} \frac{\log|\log \mathbb{P}\{|\omega_0-\omega^\pm| \le \varepsilon\}|}{-\log\varepsilon} = 0$$

We need one more assumption. To state it, we will need to introduce some notations.

3.2.1. *The background operator.* The Lifshitz exponent is computed using a well chosen background periodic operator that can but need not be H. This background operator depends on the spectral edge E_0 one is considering. More precisely it depends on whether E_0 is the upper (resp. lower) edge (i.e. maximum (resp. minimum)) of a gap. Recall that the essential infimum (resp. supremum) of the random variables $(\omega_\gamma)_\gamma$ is ω_+ (resp. ω_-). Let H^+ (resp. H^-) be the periodic Schrödinger operator defined by $H^- = H + \omega_-\sum_{\gamma\in\mathbb{Z}^2} V_\gamma$ (resp. $H^+ = H + \omega_+\sum_{\gamma\in\mathbb{Z}^2} V_\gamma$). Then, one writes $H_\omega = H^- + V_\omega^-$ (resp. $H_\omega = H^+ + V_\omega^+$) where $V_\omega^- = \sum_{\gamma\in\mathbb{Z}^2}\omega_\gamma^+ V_\gamma$ and $\omega_\gamma^+ = \omega_\gamma - \omega_-$ (resp. $V_\omega^+ = \sum_{\gamma\in\mathbb{Z}^2}\omega_\gamma^- V_\gamma$ and $\omega_\gamma^- = \omega_\gamma - \omega_+$). The random variables $(\omega_\gamma^+)_\gamma$ (resp. $(\omega_\gamma^-)_\gamma$) are i.i.d. and non-negative (resp. non-positive). The results of [**6**] imply

- E_0 is the upper edge of a gap of Σ if and only if E_0 is the upper edge of a gap of the spectrum of H^-.
- E_0 is the lower edge of a gap of Σ if and only if E_0 is the lower edge of a gap of the spectrum of H^+.

For the sake of definiteness, let us assume that E_0 is the upper edge of a gap of Σ. Then, the correct background operator will be H^-.

3.2.2. *Floquet theory.* We recall some facts on the Floquet spectrum of H^- (see e.g. [**26, 15, 27**]). The Floquet spectrum of H^- is the spectrum of the differential operator H^- acting on $L^2_{\mathrm{loc}}(\mathbb{R}^2)$ with quasi-periodic boundary conditions. For $\theta \in \mathbb{T}^* = \mathbb{R}^2/(\mathbb{Z}^2)^*$ (here $(\mathbb{Z}^2)^* = 2\pi\mathbb{Z}^2$ is the dual lattice of $\mathbb{Z}^2$ i.e. for $\gamma \in \mathbb{Z}^2$ and $\gamma^* \in (\mathbb{Z}^2)^*$, one has $\gamma\gamma^* \in 2\pi\mathbb{Z}$), consider the following eigenvalue problem on $L^2_{\mathrm{loc}}(\mathbb{R}^2)$

$$\begin{cases} H^-\varphi = E\varphi \\ \varphi(x+\gamma) = e^{i\gamma\theta}\varphi(x), \ \forall x \in \mathbb{R}^2, \ \forall \gamma \in \mathbb{Z}^2. \end{cases} \tag{3.2}$$

As H^- is elliptic, one knows that the eigenvalues of (3.2) are discrete; when repeated according to multiplicity, we denote them by $E_0(\theta) \leq E_1(\theta) \leq \cdots \leq E_n(\theta) \leq \ldots$. They are called the *Floquet eigenvalues* of H^-. These functions are Lipschitz continuous in the variable θ; when simple, they are even analytic in θ. Moreover, Weyl's law tells us that

$$E_n(\theta) \to +\infty \text{ as } n \to +\infty \text{ (uniformly in } \theta). \tag{3.3}$$

The spectrum of H^- is given by $\sigma(H^-) = \cup_{n\geq 0} E_n(\mathbb{T}^*)$. Let E be in the spectrum of H^-. E will be *simple* if the set $\{p \in \mathbb{N};\ \exists \theta \in \mathbb{T}^*,\ E_p(\theta) = E\}$ is reduced to a single integer. Note that, by (3.3), this set of integers is always finite. An edge of a gap of Σ will be called simple if it is simple for H^- (resp. H^+) and it is the upper edge (resp. the lower edge) of a gap of Σ. By [**12**], we know that for a generic periodic potential, edges of gaps are simple.

3.2.3. *The result.* We prove

THEOREM 3.2. *Let E_0 be an edge of a gap of Σ that is simple. Then, there exists $0 < \alpha \leq +\infty$ such that*

$$\lim_{\substack{E \to E_0 \\ E \in \Sigma}} \frac{\log|\log|N(E) - N(E_0)||}{\log|E - E_0|} = -\alpha. \tag{3.4}$$

The exponential decay on the integrated density of states at the edges of the spectrum Σ is known as "Lifshitz tails" for the IDS. The exponent α is called the *Lifshitz exponent.* The computation of α is not obvious; section 4 is devoted to its description.

4. How to compute the Lifshitz exponent

We now assume that (H.1') is satisfied. For the sake of definiteness, let us assume that E_0 is the upper edge of a gap of Σ. Assume E_0 is simple. Let $E_{n_0}(\cdot)$ be the unique Floquet eigenvalue taking the value E_0. Define the set $\mathcal{S} = \{\theta \in \mathbb{T}^*;\ E_{n_0}(\theta) = E_0\}$. Then, there exists $\eta > 0$ such that

- For $n < n_0$, for all $\theta \in \mathbb{T}^*$, $E_n(\theta) < E_0 - \eta$.
- For $n > n_0$, for all $\theta \in \mathbb{T}^*$, $E_n(\theta) > E_0 + \eta$.

This implies that, for θ in some neighborhood of $\mathcal{S}$, the Floquet eigenvalue $E_{n_0}(\theta)$ is simple, hence, the function $\theta \mapsto E_{n_0}(\theta)$ is real analytic in some neighborhood of $\mathcal{S}$. The Lifshitz exponent will depend on the way E_{n_0} vanishes at $\mathcal{S}$ and on the curvature of $\mathcal{S}$.

To describe it precisely, we need to introduce some objects from analytic geometry. If $\mathcal{E}$ is a set contained in the closed first quadrant in $\mathbb{R}^2$ then its *exterior convex hull* is the convex hull of the union of the rectangles $R_{xy} = [x, \infty) \times [y, \infty)$, where the union is taken over all $(x, y) \in \mathcal{E}$.

Pick $\theta_0 \in \mathcal{S}$ and consider the Newton diagram of E_{n_0} at θ_0, i.e.,

1. Express E_{n_0} as a Taylor series at θ_0, $E_{n_0}(\theta^1, \theta^2) = \sum_{ij} a_{ij}(\theta^1 - \theta_0^1)^i(\theta^2 - \theta_0^2)^j$, $\theta = (\theta^1, \theta^2)$.

2. Form the exterior convex hull of the points (i,j) with $a_{ij} \neq 0$. This is a convex polygon, called the *Newton polygon*.
3. The boundary of the polygon is the *Newton diagram*.

The Newton decay exponent is then defined as follows. The Newton diagram consists of certain line segments. Extend each to a complete line and intersect it with the diagonal line $\theta^1 = \theta^2$. This gives a collection of points (a_k, a_k), one for each boundary segment. Take the reciprocal of the largest a_k and call this number $\tilde{\alpha}(E_{n_0}, \theta_0)$; it is the *Newton decay exponent.* Define $\alpha(E_{n_0}, \theta_0) = \min\{\tilde{\alpha}(E_{n_0} \circ T_0, \theta_0) : T_0(\cdot) = \theta_0 + T(\cdot - \theta_0),\ T \in SL(2,\mathbb{R})\}$.

Similarly, define $\alpha(E_{n_0}, \theta)$ if θ is any other point in $\mathcal{S}$, the zero set of E_{n_0}. Then, the *Lifshitz exponent* α is defined by

$$\alpha = \min_{\theta \in \mathcal{S}} \alpha(E_{n_0}, \theta). \tag{4.1}$$

The Lifshitz exponent α is positive as $\theta \mapsto \alpha(E_{n_0}, \theta)$ is a positive, lower semi-continuous function and $\mathcal{S}$ is compact.

To conclude this subsection, let us compare N to N_p, the density of states of the underlying periodic operator H. Up to a constant factor, $N_p(E_0 + \varepsilon) - N_p(E_0)$ is the volume of $\{\theta \in \mathbb{T}^*;\ E_{n_0}(\theta) \leq E_0 + \varepsilon\}$. From the equivalence between (2.2) and (2.3) (see section 2.2), one may have conjectured that, at band edges N behaves roughly like e^{-1/N_p} (if one takes the double logarithm of both terms). We see here that this will not be true in general if the set $\mathcal{S}$ has some curvature. For example, if we assume that $E_{n_0}(\theta) - E_0$ vanishes to constant order q on a curve, and if the maximum order of vanishing of the curvature of the curve is m (thus non-vanishing curvature means $m = 0$) then $\alpha = \frac{m+3}{q(m+2)}$ and the volume will have the exponent $\frac{1}{q}$.

5. The main ideas of the proof

To fix ideas let us assume that we work at the upper edge of a gap i.e. at the edge E_-. A lower edge can dealt with in the same way. Without restriction of generality, we will also assume $E_- = 0$

First, following the ideas developed in [**14**], we show that the study of the density of states of H_ω near E_- can be reduced to the study of the density of states of a discrete random operator. This discrete Hamiltonian is the sum of a kinetic energy part and a potential energy part. The kinetic energy part is made of the Floquet eigenvalues giving rise to the band starting at E_- for the background periodic operator H^-. The potential energy part is the random potential projected onto the space of states generating the band starting at E_-. This discrete Hamiltonian, that we will call the reduced operator, can be realized as an operator acting on the torus $\mathbb{T}^*$. To perform this reduction, one needs to know that the edge E_- of Σ corresponds to an edge of a single periodic realization (namely H^-). Therefore we first need the positivity assumption of V and, second, we need to know that, when switching on the random potential (remember that H^- is now the unperturbed Hamiltonian), none of the spectrum below E_- passes above E_-. In the present exposition, this is ensured by the fact that the gap below E_- is open in Σ and by the assumption that the random variables have connected support. Another natural setting where there cannot be any crossing is when one assume that H^- has a gap and that the random perturbation V_ω^- is smaller than the length of the gap.

The next step is to show that, with good enough precision, we can estimate the integrated density of states of the reduced operator between E_0 and $E_0 + \varepsilon$ by the probability that the reduced operator (restricted to some large cube) has an eigenvalue in the interval $[E_0, E_0 + \varepsilon]$. If the band edge is simple, we then have to estimate the probability that, for $\delta > 0$ small, there exists $u \in L^2(\mathbb{T})$ such that such that the Fourier coefficients of u are supported in $[-M, M] \times [-M, M] \subset \mathbb{Z}^2$ and such that

$$\langle E_{n_0} \cdot u, u \rangle_{L^2(\mathbb{T}^*)} + \langle v_\omega u, u \rangle_{L^2(\mathbb{T}^*)} \leq \delta \tag{5.1}$$

Here $E_{n_0} \cdot u$ denotes the multiplication by the Floquet eigenvalue E_{n_0} and v_ω denotes the reduced potential. Notice that both terms in (5.1) are non-negative. In the general case, the situation is somewhat complicated by the possible multiplicities.

At last, we estimate these probabilities. Carrying out this estimation is essentially a problem in random Fourier series; indeed, thanks to assumption (H.1'.4), for our purpose, we can replace the random variables $(\omega_\gamma)_\gamma$ by i.i.d. Bernoulli random variables.

Let f be a nonnegative real analytic function on $\mathbb{T}^*$, let $\delta > 0$ and $M < \infty$ be parameters, let S be a random subset of the square $[-M, M] \times [-M, M]$ (in $\mathbb{Z}^2$) with (say) density $\frac{1}{2}$ and let $P(M, \delta)$ be the probability that there is a function $u \in L^2(\mathbb{T})$ such that

$$\int_{T^2} f(\theta)|u(\theta)|^2 < \delta \|u\|_2^2 \quad \text{and} \quad \operatorname{supp}(\hat{u}) \subset S.$$

Thus the Fourier coefficients of u are to be supported on the random set, and u is to be mostly supported near the zero set of f. We will study the behavior of the probability $P(M(\delta), \delta)$ as $\delta \to 0$, letting $M = M(\delta)$ go to ∞ in an appropriate manner. It turns out that $P(M(\delta), \delta)$ behaves roughly like $e^{-\delta^{-\alpha}}$.

One can apply this bound taking f to be roughly the Floquet eigenvalue E_{n_0} to complete the proofs of Theorems 0.1 and 0.2, in a manner analogous to the one dimensional case treated in [**11**].

A Newton decay exponent similar to the one introduced above arises in problems concerning estimation of oscillatory integrals - see [**31**] and [**25**] - and we show here that it also controls the behavior of certain random Fourier series, in a way which to some extent is suggested by the results of [**31**] and [**25**].

Though in [**13**] we only study the case of random Schrödinger operators, the methods we develop can be applied too many other families of random operators: acoustic operators, random magnetic fields, etc (see e.g. [**21, 3**]).

6. Application to localization

Our results can be applied to study band edge localization for the continuous Anderson model. Therefore, in addition to assumption (H.1), we need to assume that the random operator satisfies a *Wegner estimate* i.e that for some $\beta > 0$ and $\nu > 0$, for $E \in \mathbb{R}$, for $l \geq 1$ and $0 < \varepsilon < 1$, there exists $C(E) > 0$ such that one has

$$\mathbb{P}\left(\operatorname{dist}(\sigma(H^\theta_{\omega,C_l}, E) \leq \varepsilon\right) \leq C(E)\operatorname{Vol}(C_l)^\beta \varepsilon^\nu \tag{6.1}$$

where the constant $C(E)$ is locally uniform in energy. Here l is an integer and H^θ_{ω,C_l} is the operator H_ω restricted to the cube C_l with boundary conditions: $\varphi(x+\gamma) = e^{i\theta\gamma}\varphi(x)$ for any $\gamma \in 2l\mathbb{Z}^2$.
We prove

THEOREM 6.1. *Let H_ω be a random operator described by* (1.1) *such that (H.1) and estimate* (6.1) *are satisfied. Then, for every band edge of Σ, the almost sure spectrum of H_ω, there exists a neighborhood of that band edge where the spectrum of H_ω is purely punctual. Moreover the eigenfunctions associated to energies in that neighborhood are exponentially localized.*

This result is a direct application of Theorem 3.1 and the multi-scale analysis developed in [**10**] (see also [**1, 9**]).

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