INTERNAL LIFSHITZ TAILS FOR DISCRETE SCHRÖDINGER OPERATORS

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We consider random Schrödinger operators H_ω acting on $l^2(\mathbb{Z}^d)$. We adapt the technique of the periodic approximations used in (2003) for the present model to prove that the integrated density of states of H_ω has a Lifshitz behavior at the edges of internal spectral gaps if and only if the integrated density of states of a well-chosen periodic operator is nondegenerate at the same edges. A possible application of the result to get Anderson localization is given.

1. Introduction

We consider the following random operator acting on $l^2(\mathbb{Z}^d)$:

$$(H_\omega \psi)(n) = 2d\psi(n) - \sum_{|m-n|=1} \psi(m) + W_{\text{per}}(n)\psi(n) + V_\omega(n)\psi(n). \qquad (1.1)$$

Here, for $n = (n_1, \ldots, n_d) \in \mathbb{Z}^d$, $|n| = \sum_{i=1}^d |n_i|$. It is a second-order finite difference analogous to the Schrödinger equation. These operators have been of interest for a long time in mathematics, and also in physics where they appear in the tight binding approximation of the condensed matter system. The discrete version has the advantage of being less technical and more transparent than the continuous one.

Let us start by defining the main object of our study: the integrated density of states. For this, for $L \in \mathbb{N}$ let H_ω^L be the $(2L+1)^d \times (2L+1)^d$ matrix obtained by restricting H_ω to sites $n = (n_1, \ldots, n_d)$ with $|n_i| \le L$. Let, for $E \in \mathbb{R}$, $\sharp(H_\omega^L \le E)$ denote the number of eigenvalues of H_ω^L smaller than or equal to E. We consider

$$N(E) = \lim_{L \to \infty} \frac{1}{(L+1)^d} \sharp(H_\omega^L \le E). \qquad (1.2)$$

It is shown that the limit in (1.2) exists almost surely for all E and ω is independent. It is called the *integrated density of states* of H_ω (IDS) (see [15]). In 1964, Lifshitz [10] argued using physical interpretations that for the continuous case N should decrease exponentially fast at the bottom of the spectrum. This behavior of the IDS is known as *Lifshitz tails* (for more details see [15, part IV.9.A]). This behavior is a characteristic of random operators; it has been proved mathematically in several papers. See [9, 11–13, 17, 18].

The works already existing in the discrete case are based on the Temple inequality. See [11] for the internal case in one dimension, [18] for the multidimensional one, and [17] in the external edges of the spectrum.

For the discrete model, the IDS was also the subject of [8], where the band edge behavior of the IDS of random Jacobi matrices in dimension 1 was proved.

Hamiltonians with a potential energy, which is the sum of periodic potential and a random one, give other examples of models with gaps in the spectrum and for which the investigation of the internal Lifshitz tails is a natural problem. They occur, for example, in the study of an electron in crystal with impurities. If the support of the one site distribution of the purely random part of the potential is contained in a compact set with a diameter smaller than the size of the gaps of the periodic potential, then the spectrum of the full operator will still have gaps. For such an operator, the IDS exists and its topological support is equal to the almost sure spectrum. Hence it is constant on these gaps and one could try to determine as before the behavior of the IDS near these gap edges, this is the subject of the present work. The mathematics are more technical and more difficult because of the presence of the periodic potential and the only known results on this context concerns external edges or internal edges, with gaps due to gaps on the probability density as the case in [17, 18].

In the present work we adapt the technique of [9, 12] to the discrete case. It is based on the uncertainty principle and the periodic approximation which allows us to relax some technical assumptions.

1.1. The model.   We consider H_ω as in (1.1), with

(i) $W_{\text{per}}(\cdot)$ is a bounded periodic function such that there exists a vector $q_0 = (q_1,\ldots,q_d) \in \mathbb{Z}^d$ with positive components such that

$$\forall x \in \mathbb{Z}^d, \quad W_{\text{per}}(x + q') = W_{\text{per}} \quad \forall q' \in q_0 \cdot \mathbb{Z}; \tag{1.3}$$

(ii) $(V_\omega(n))_{n \in \mathbb{Z}^d}$ is a family of nonconstant and positive independent identically distributed random variables whose common probability measure is noted by $\mathbb{P}_{\omega_0}$. We note the probability space by $(\Omega, \mathscr{F}, \mathbb{P})$. We assume that $\mathbb{P}_{\omega_0}$ is compactly supported.

As defined, H_ω is a bounded selfadjoint operator on $l^2(\mathbb{Z}^d)$.

Indeed, if τ_γ refers to the translation by γ, then $(\tau_\gamma)_{\gamma \in q\mathbb{Z}^d}$ is a group of unitary operators on $l^2(\mathbb{Z}^d)$, and for $\gamma \in q_0 \mathbb{Z}^d$ we have

$$\tau_\gamma H_\omega \tau_{-\gamma} = H_{\tau_\gamma \omega}. \tag{1.4}$$

Thus, according to [7, 15], we know that there exist Σ, Σ_{pp}, Σ_{ac} and Σ_{sc} closed and non-random sets of $\mathbb{R}$ such that Σ is the spectrum of H_ω with probability one and such that if σ_{pp} (resp., σ_{ac} and σ_{sc}) designs the pure point spectrum (resp., the absolutely continuous and singular continuous spectrum) of H_ω, then $\Sigma_{pp} = \sigma_{pp}$, $\Sigma_{ac} = \sigma_{ac}$, and $\Sigma_{sc} = \sigma_{sc}$ with probability one.

It is convenient to study H_ω as a perturbation of some background operator. For this, we set

$$(H_0\psi)(n) = 2d\psi(n) - \sum_{|m-n|=1} \psi(m) + W_{per}(n)\psi(n). \tag{1.5}$$

As $W_{per}(\cdot)$ is periodic, H_0 is a selfadjoint local periodic operator on $l^2(\mathbb{Z}^d)$.

Schrödinger operators with periodic potentials on $\mathbb{R}^d$ are the subject of the well-known Floquet-Bloch theory [16]. Modifications needed to extend the theory to our situation are brought in [4, Section 2]. We refer the reader to [3, 4] for more details on the theory of discrete periodic operators. We recall the following result concerning the band gap structure of the spectrum σ_0 of H_0.

THEOREM 1.1 [4]. *The spectrum σ_0 of H_0 consists of a finite number n_0 of intervals (bands), namely,*

$$\sigma_0 = \bigcup_{1 \le i \le n_0 - 1} [E_{2i}, E_{2i+1}], \quad E_{2i} \le E_{2i+1}, \quad 1 \le i \le n_0 - 1. \tag{1.6}$$

Remark 1.2. (i) There are many discrete models constructed with open spectral gaps [3, 4]. For instance, let $W_{per} = aw$, with a is a positive constant and w is the operator of the multiplication by a real, periodic nonconstant function $w(x)$. As the discrete Laplacian is a bounded operator, it is clear that H_0 has gaps in the spectrum when the constant a is large enough.

(ii) Even if one supposes that $W_{per} = 0$, it is still possible that H_ω exhibits spectral gaps, this is when there are gaps in the support of μ [18].

The periodic operator H_0 has an IDS which will be denoted by n. The behavior of n at a band edge 0 is said to be nondegenerate if

$$\lim_{\varepsilon \to 0^+} \frac{\log |n(\varepsilon) - n(0)|}{\log \varepsilon} = \frac{d}{2}. \tag{1.7}$$

Remark 1.3. It is proven in [9] that (1.7) is equivalent to saying that the Floquet eigenvalues reaching the band edge 0 have only nondegenerate quadratic extrima at that edge. That is, if θ^0 is such that $E_n(\theta^0) = 0$, then θ^0 is a nondegenerate quadratic extremum of E_n. Here E_n is a Floquet eigenvalue of H_0.

As we study the behavior of the IDS at the internal band edges we will just assume the existence of gaps in the spectrum of H_0 and H_ω.

As the operator is bounded, without loss of generality we can assume that 0 is an internal band edge of H_0; the thing that we do in the following.

More precisely

(A.1) There exists $\delta > 0$ such that $\sigma_0 \cap [0, \delta) = [0, \delta)$, and for any $t \in [0, 1]$, $\sigma(H_0 + t) \cap (-\delta, 0] = \varnothing$.

   We note that if the support of $\mathbb{P}_{\omega_0}$ is connected, the assumption (A.1) can be replaced by the following.

(A.1.bis) There exists $\delta' > 0$ such that $\Sigma \cap [-\delta', 0) = \varnothing$.

   By adding a disorder parameter λ in the equation which defines H_ω, that is,

$$(H_\omega \psi)(n) = 2d\psi(n) - \sum_{|m-n|=1} \psi(m) + W_{\mathrm{per}}(n)\psi(n) + \lambda V_\omega(n)\psi(n), \qquad (1.8)$$

we can choose λ small enough so that the spectral gap in $\sigma(H_0)$ will not be closed after the perturbation [4].

(A.2)

$$\limsup_{\varepsilon \to 0^+} \frac{\log |\log \mathbb{P}_{\omega_0}([0, \varepsilon])|}{|\log \varepsilon|} = 0. \qquad (1.9)$$

Remark 1.4. Here we allowed the probability distribution to decrease rapidly but at least not more than exponentially fast at 0. In [11, 17, 18], it is asked that the distribution does not decrease more than polynomially fast. Precisely it is required that $\mathbb{P}_{\omega_0}([0, \varepsilon]) \geq C\varepsilon^l$; for some C and l.

2. Results and discussion

The main result of this note is stated below.

THEOREM 2.1. *Assume assumptions (A.1) and (A.2) hold, then*

$$\begin{aligned}
&(i) \quad \liminf_{\varepsilon \to 0^+} \frac{\log |\log (N(\varepsilon) - N(0))|}{\log \varepsilon} \geq -\frac{d}{2}, \\
&(ii) \quad \lim_{\varepsilon \to 0^+} \frac{\log |\log (N(\varepsilon) - N(0))|}{\log \varepsilon} = -\frac{d}{2} \iff \lim_{\varepsilon \to 0^+} \frac{\log (n(\varepsilon) - n(0))}{\log \varepsilon} = \frac{d}{2}.
\end{aligned} \qquad (2.1)$$

Remark 2.2. (i) The result of Theorem 2.1 is stated for lower band edges. Under adequate assumptions the corresponding result can be proved for upper band edges.

   (ii) We notice that the Lifshitz component is $-d/2$ only if the IDS of the periodic operator is nondegenerate. This is the case for the free Schrödinger operators ($W_{\mathrm{per}} = 0$) and thus we get already known results in this particular case [11, 17, 18].

2.1. Application. Now we give a possible application of Theorem 2.1. We can use the result of Theorem 2.1 to get initial estimates to show Anderson localization [4, 21] under assumptions on the distribution of the random variables weaker than those required in these references. Indeed if we assume that the probability measure $\mathbb{P}_{\omega_0}$ has density, then H_ω satisfies a Wegner estimate [4, 21], that is, for some $\alpha > 0$ and $n > 0$ for $E \in \mathbb{R}$ for $k \geq 1$ and $0 < \varepsilon < 1$, there exists $C(E) > 0$ such that one has

(P2):

$$\mathbb{P}\big(\big\{\mathrm{dist}\,(\sigma(H_{\omega,\Lambda_k}),\,E)\leq\varepsilon\big\}\big)\leq C(E)\cdot|\Lambda_k|^{\alpha}\cdot\varepsilon^n. \tag{2.2}$$

Here H_{ω,Λ_k} is H_ω restricted to the box of size k, Λ_k.

THEOREM 2.3. *Let H_ω defined by (1.1). Assume that (A.1), (A.2), and (P2) hold. There exist $\varepsilon_0 > 0$ such that*
  (i) $\Sigma\cap[0,\varepsilon_0]=\Sigma_{\mathrm{pp}}\cap[0,\varepsilon_0]$,
  (ii) *an eigenfunction corresponding to an eigenvalue in $[0,\varepsilon_0]$ decays exponentially.*

We will not give the details of the proof of Theorem 2.3 but we notice that the proof of localization can be based on the use of the method of the multiscale analysis [19]. This method was used for the first time by Fröhlich and Spencer, at the early eighties [5], and it knew many extensions and simplifications. This analysis makes it possible to obtain information on the operator in the whole space, starting from information on the operator restricted to cubes of finished size [21]. The proof of Theorem 2.3 is then reduced on a simple verification of the so-called initials estimates (P2) and
  (P1):

$$\mathbb{P}\left(\left\{\mathrm{dist}\,(\sigma(A_{\omega,\Lambda_{k^\alpha}}),\,E_+)\leq\frac{1}{k}\right\}\right)\leq\frac{1}{k^p}. \tag{2.3}$$

To check (P1) one uses the fact that N, the IDS of H_ω, decreases exponentially fast at 0 which is the result of Theorem 2.1. This is given in [14, 20]. Indeed, from (P1) we get that the Green function decreases exponentially fast to define regular boxes.

Remark 2.4. Anderson localization was the subject of many studies. For discrete operators we mention that the method for proving localization in the multidimensional case is the fractional moment introduced by Aizenman and Molchanov [1, 6].

3. The proof of Theorem 2.1

To prove Theorem 2.1, we prove lower and upper bounds on $N(E)-N(0)$. The lower and the upper bounds are proven separately. For the first one is now classic and we just need the right lower for the probability that $H_{\omega,\Lambda}$ has an eigenvalue in $[-\varepsilon,\varepsilon]$. As for the second it is more technical.

3.1. The lower bound. The lower bound is proved by constructing a large enough number of orthogonal approximate eigenfunctions of H_{ω,Λ_k} associated with approximate eigenvalues in $[-\varepsilon,\varepsilon]$ for $\varepsilon < \delta$ (see assumption (A.1)). This will enable us to lower bound the number of the eigenvalues of $H_{\omega,\Lambda}$ in the interval $[0,\varepsilon]$. By assumption (A.1), there is a spectral gap below 0 of length at least $\delta > 0$. Thus, for $\varepsilon < \delta'$ we have

$$N(\varepsilon)-N(0)=N(\varepsilon)-N(-\varepsilon). \tag{3.1}$$

Then, we will lower bound $N(\varepsilon)-N(-\varepsilon)$. Indeed, for k large, we can show that H_{ω,Λ_k} (H_{ω,Λ_k} is H_ω restricted to Λ_k with Dirichlet boundary conditions) has a large number

of eigenvalues in $[-\varepsilon,\varepsilon]$ with a large probability. For this we construct a family of approximate eigenvectors associated to approximate eigenvalues of A_{ω,Λ_N} in $[-\varepsilon,\varepsilon]$. These functions will be constructed from a Floquet eigenvector of H_0 associated with 0. Locating this eigenvector in θ and imposing to $V_\omega(n)$ to be small for n in some well-chosen box Λ_{k_ε}, for k_ε fixed below, one obtains an approximate eigenfunction of H_{ω,Λ_N}. Locating the eigenfunction in x in several disjointed places, we get several eigenfunctions two by two orthogonal. If we denote by $N(\varepsilon)$ the number of disjoint boxes Λ_{k_ε} contained in Λ_k, then we get

$$
\begin{aligned}
N_{\Lambda_N}(\varepsilon) - N_{\Lambda_N}(-\varepsilon) &= \frac{1}{(2k+1)^d}\mathbb{E} \quad (\#\{\text{eigenvalues of } H_{\omega,\Lambda_k} \text{ in } [-\varepsilon,\varepsilon]\}) \\
&\geq \frac{N(\varepsilon)}{(2k+1)^d}\mathbb{P} \quad \{\text{for any } n \in \Lambda_{k_\varepsilon} \cap \mathbb{Z}^d,\ V_\omega(n) \in (0,\varepsilon)\} \qquad (3.2) \\
&= \frac{N(\varepsilon)}{(2k+1)^d}\mathbb{P} \quad \{V_\omega(0) \in (0,\varepsilon)\}^{\#(\Lambda_{k_\varepsilon} \cap \mathbb{Z}^d)}.
\end{aligned}
$$

Here $k_\varepsilon = \varepsilon^{-(1/2)s+\alpha}$ with $1/2 > \alpha > 0$ small and $s < 1$ (resp. $= 1$) if n is degenerate (resp., nondegenerate) at 0. Notice as α small one gets that there exists $C > 0$ such that

$$
N(\varepsilon) \geq \frac{(k\varepsilon^s)^d}{C}. \qquad (3.3)
$$

Taking into account (3.2), (3.3), and assumption (A.2) computing the limit for k to infinity, we get

$$
\liminf_{\varepsilon \to 0^+} \frac{\log |\log (N(\varepsilon) - N(0))|}{\log \varepsilon} \geq -s\frac{d}{2}. \qquad (3.4)
$$

This ends the proof of the lower bound.

3.2. The upper bound. The upper bound is based on the reduction procedure which consists in decomposing the operator H_ω according to various translation-invariants subspaces. The random operators thus obtained are reference operators. They will be used for the upper bound on the IDS. We prove that for an energy E close to 0, $N(E) - N(0)$ can be upper bounded by $N_{\mathscr{E}_0}(E)$, the IDS of the bounded random operator $H_\omega^0 = \Pi_0 H_\omega \Pi_0$. Here Π_0 is the spectral projection for H_0 on the band starting at 0. So to study the behavior of $N(E) - N(0)$, we investigate the behavior of $N_{\mathscr{E}_0}(E)$. Precisely, we use the following result.

THEOREM 3.1. *Let H_ω be defined by (1.1). Assume that (A.1) and (A.2) hold. There exists $E_0 > 0$ and $C > 1$ such that, for $0 \leq E \leq E_0$,*

$$
0 \leq N(E) - N(0) \leq N_{\mathscr{E}_0}(C \cdot E), \qquad (3.5)
$$

where $N_{\mathscr{E}_0}$ is the IDS of $H_\omega^0 = \Pi_0 H_\omega \Pi_0$.

The proof of **Theorem 3.1** is based on the use of the technique of periodic approximations which consists in approaching the density of states of H_ω by the density of states of well-chosen periodic operators.

The periodic approximations. For $k \in \mathbb{N}^*$. Let $H_{\omega,k}$ be the following periodic operator:

$$(H_{\omega,k}\psi)(n) = (H_0\psi)(n) + V_{\omega,k}(\tilde{n})\psi(n). \tag{3.6}$$

With $\tilde{n} \in \mathbb{Z}_k^d = \{q \in q_0\mathbb{Z}^d; \; |q| \le k\}$ and $\tilde{n} = n$ modulo $(2k+1)q_0\mathbb{Z}^d$.

As $H_{\omega,k}$ is periodic, the Floquet theory is still valid in this case. The IDS of $H_{\omega,k}$ is denoted by $N_{\omega,k}$. Let $dN_{\omega,k}$ be the derivative of $N_{\omega,k}$ in the distribution sense. As $N_{\omega,k}$ is increasing, $dN_{\omega,k}$ is a positive measure; it is the density of states of $H_{\omega,k}$. We denote by dN the density of states of H_ω. It is proven [9, 12] that $dN_{\omega,k}$ converge to dN in the distribution sense. First we prove an analogous result to **Theorem 3.1** for the Floquet operators. Then, by a simple integration, we get the same result in **Theorem 3.1** for the new periodic operators $H_{\omega,k}$.

We notice that for the upper bound we suppose that the IDS, n is nondegenerate. Now to prove the upper bound we use **Theorem 3.1**. Indeed to prove the upper bound, it is enough to prove the same upper bound on $N_{\mathscr{C}_0}$ (defined in **Theorem 3.1**). To do this, we show that when n has a nondegenerate behavior at energy E_+, then $N_{\mathscr{C}_0}$ (and so N) may be compared to the IDS of some well-chosen, discrete Andreson model (whose behavior of its IDS is already known). This represents several advantages: first, H_ω^0 is equivalent to a random Jacobi matrix acting on $L^2(\mathbb{T}^*) \otimes \mathbb{C}^n$ [12]. The second advantage is that while 0 is an interior edge of a gap for H_ω, it becomes the bottom of the spectrum for H_ω^0. We prove that when n, the IDS of the periodic operator H_0, is nondegenerate at 0, H_ω^0 is lower bounded by the usual discrete Schrödinger random operator whose behavior of the IDS at the edges of the spectral gaps is already known [2, 17, 18]. This lower bound on the operator immediately yields an upper bound on the density of states. Precisely if n is nondegenerate at 0, then we get

$$\limsup_{\varepsilon \to 0^+} \frac{\log |\log(N(\varepsilon) - N(0))|}{\log \varepsilon} \le -\frac{d}{2}. \tag{3.7}$$

We notice that there exists a constant $C > 0$ such that the operator $C \cdot H_\omega^0$ is lower bounded by the same discrete operator as those used in [9, 12].

Acknowledgments

References

[1] M. Aizenman and S. Molchanov, *Localization at large disorder and at extreme energies: an elementary derivation*, Communications in Mathematical Physics **157** (1993), no. 2, 245–278.

[2] R. Carmona and J. Lacroix, *Spectral Theory of Random Schrödinger Operators*, Probability and Its Applications, Birkhäuser, Massachusetts, 1990.

[3] A. Figotin, *Existence of gaps in the spectrum of periodic dielectric structures on a lattice*, Journal of Statistical Physics **73** (1993), no. 3-4, 571–585.

[4] A. Figotin and A. Klein, *Localization phenomenon in gaps of the spectrum of random lattice operators*, Journal of Statistical Physics **75** (1994), no. 5-6, 997–1021.

[5] J. Fröhlich and T. Spencer, *Absence of diffusion in the Anderson tight binding model for large disorder or low energy*, Communications in Mathematical Physics **88** (1983), no. 2, 151–184.

[6] G. M. Graf, *Anderson localization and the space-time characteristic of continuum states*, Journal of Statistical Physics **75** (1994), no. 1-2, 337–346.

[7] W. Kirsch, *Random Schrödinger operators. A course*, Schrödinger Operators (Sønderborg, 1988), Lecture Notes in Phys., vol. 345, Springer, Berlin, 1989, pp. 264–370.

[8] F. Klopp, *Band edge behavior of the integrated density of states of random Jacobi matrices in dimension 1*, Journal of Statistical Physics **90** (1998), no. 3-4, 927–947.

[9] ———, *Internal Lifshitz tails for random perturbations of periodic Schrödinger operators*, Duke Mathematical Journal **98** (1999), no. 2, 335–396.

[10] I. Lifshitz, *Structure of the energy spectrum of impurity bands in disordered solid solutions*, Soviet Physics JETP **17** (1963), 1159–1170.

[11] G. A. Mezincescu, *Internal Lifschitz singularities for one-dimensional Schrödinger operators*, Communications in Mathematical Physics **158** (1993), no. 2, 315–325.

[12] H. Najar, *Lifshitz tails for random acoustic operators*, Journal of Mathematical Physics **44** (2003), no. 4, 1842–1867.

[13] ———, *Asymptotic behavior of the integrated density of states of acoustic operators with random long range perturbations*, Journal of Statistical Physics **115** (2004), no. 3-4, 977–996.

[14] ———, *2-dimensional localization of acoustic waves in random perturbation of periodic media*, Journal of Mathematical Analysis and Applications **322** (2006), no. 1, 1–17.

[15] L. Pastur and A. Figotin, *Spectra of Random and Almost-Periodic Operators*, Fundamental Principles of Mathematical Sciences, vol. 297, Springer, Berlin, 1992.

[16] M. Reed and B. Simon, *Methods of Modern Mathematical Physics. IV. Analysis of Operators*, Academic Press, New York, 1978.

[17] B. Simon, *Lifschitz tails for the Anderson model*, Journal of Statistical Physics **38** (1985), no. 1-2, 65–76.

[18] ———, *Internal Lifschitz tails*, Journal of Statistical Physics **46** (1987), no. 5-6, 911–918.

[19] P. Stollmann, *Caught by Disorder Bounded States in Random Media*, Birkhäuser, Massachusetts, 2001.

[20] I. Veselić, *Localization for random perturbation of periodic Schrödinger operators with regular Floquet eigenvalues*, Tech. Rep., University of Bochum, Bochum, 2005.

[21] H. von Dreifus and A. Klein, *A new proof of localization in the Anderson tight binding model*, Communications in Mathematical Physics **124** (1989), no. 2, 285–299.

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