

Quantum dynamics in random media and localization lengths in dimension 3

Thomas Chen
Courant Institute, NYU
chenthom@cims.nyu.edu

Abstract

We report on recent work, [1], concerning lower bounds on the localization length of eigenfunctions in the three-dimensional Anderson model at weak disorders, that uses an extension of methods developed by L. Erdős and H.-T. Yau. Our results are similar to those obtained by C. Shubin, W. Schlag and T. Wolff, [8], for dimensions one and two. Furthermore, we show that the macroscopic limit of the corresponding lattice random Schrödinger dynamics is governed by the linear Boltzmann equations.

1 Introduction

In d dimensions, the Anderson model is defined by the discrete random Schrödinger operator

$$(H_\omega\psi)(x) = -\frac{1}{2}(\Delta\psi)(x) + \lambda\omega(x)\psi(x) ,$$

acting on $\ell^2(\mathbb{Z}^d)$, where λ is a small coupling constant,

$$(\Delta\psi)(x) := 2d\psi(x) - \sum_{|x-y|=1} \psi(y)$$

is the nearest neighbor lattice Laplacian, and $\omega(x)$ are, for $x \in \mathbb{Z}^d$, bounded, i.i.d. random variables. We here report on [1], where we study the case $d = 3$, and prove that with probability one, most eigenfunctions of H_ω have localization lengths bounded from below by $O(\frac{\lambda^{-2}}{\log \frac{1}{\lambda}})$. In contrast to $d = 1, 2$, we note that there are no restrictions on the energy range for this result to hold. Furthermore, we derive the macroscopic limit of the quantum dynamics in this system, and prove that it is governed by the linear Boltzmann equations.

The paper [1] is closely related to work of L. Erdős and H.-T. Yau in [3], where the weak coupling and hydrodynamic limit is derived for a random Schrödinger equation in the continuum \mathbb{R}^d , $d = 2, 3$, for a Gaussian random potential. For macroscopic time and space variables (T, X) , microscopic variables (t, x) , and the scaling $(X, T) = \lambda^2(x, t)$, where λ is the coupling constant in the continuum analogue of H_ω , they established in the limit $\lambda \rightarrow 0$ that the macroscopic dynamics is governed by the *linear Boltzmann equations*, and thus ballistic, for all $T > 0$. We note that the corresponding result for sufficiently small values of T was first proved by H. Spohn [9]. For larger time scales, it has very recently been established that the macroscopic dynamics in $d = 3$ is determined by a diffusion equation, [4].

[1] is also closely related to a recent work of C. Shubin, W. Schlag and T. Wolff, [8], who established, by techniques of harmonic analysis, for the Anderson model at small disorders in $d = 1, 2$, that with probability one, most eigenstates are in frequency space concentrated on shells of thickness $\leq \lambda^2$ in $d = 1$, and $\leq \lambda^{2-\delta}$ in $d = 2$. The eigenenergies are required to be bounded away from the edges of the spectrum of $-\frac{1}{2}\Delta_{\mathbb{Z}^d}$, and in $d = 2$, also away from its center. By the uncertainty principle, this implies lower bounds of order $O(\lambda^{-2})$ in $d = 1$, and $O(\lambda^{-2+\delta})$ in $d = 2$, on the localization lengths in position space. Closely related to their work are the papers [5, 6] by J. Magnen, G. Poirot, V. Rivasseau, and [7] by G. Poirot, which address properties of the Greens functions associated to H_ω .

The proof of our main results uses an extension of the time-dependent techniques of L. Erdős and H.-T. Yau in [3] to the lattice, and to non-Gaussian random potentials. Higher correlations are now abundant, but are shown to have an insignificant effect, hence the character of our results does not differ from that obtained in the Gaussian case.

2 Localization Lengths

We shall first address the lower bounds on the localization lengths. For the random potential, it is assumed in [1] that $\mathbb{E}[\omega_x^{2m+1}] = 0 \ \forall x \in \mathbb{Z}^3, \ \forall m \geq 0$. This helps to reduce some of the notation, but for the methods to apply, only $\mathbb{E}[\omega_x] = 0$ is necessary. In addition, the uniform moment bounds

$$\mathbb{E}[\omega_x^{2m}] =: \tilde{c}_{2m} \leq c_\omega \ , \ \tilde{c}_2 = 1 \ , \ \forall x \in \mathbb{Z}^3 \ , \ \forall m \geq 1 \ , \quad (1)$$

are assumed, where the constant $c_\omega < \infty$ is independent of m . H_ω is a selfadjoint linear operator on $\ell^2(\mathbb{Z}^3)$ for every realization of V_ω .

Let $L \in \mathbb{N}$ with $L \gg \lambda^{-2}$, and $\Lambda_L = \{-L, -L+1, \dots, -1, 0, 1, \dots, L-1, L\}^3 \subset \mathbb{Z}^3$, and let $\{\psi_\alpha^{(L)}\}$ denote an orthonormal basis in $\ell^2(\Lambda_L)$ of eigenfunctions of H_ω restricted to Λ_L . That is,

$$(H_\omega - e_\alpha^{(L)})\psi_\alpha^{(L)} = 0 \text{ on } \Lambda_L \text{ and } \psi_\alpha^{(L)} = 0 \text{ on } \partial\Lambda_L := \Lambda_{L+1} \setminus \Lambda_L \ , \quad (2)$$

for $\alpha \in \mathcal{A}_L := \{1, \dots, |\Lambda_L|\}$, and $e_\alpha^{(L)} \in \mathbb{R}$. Let $\text{Box}_\ell(x)$ denote the translate of the cube $\mathbb{Z}^3/(\ell\mathbb{Z})^3$ that is centered at x , for $1 \ll \ell \ll L$, and let $R_{x,\delta,\ell}$ denote a suitable approximate characteristic function for the shell $\text{Box}_\ell(x) \setminus \text{Box}_{\delta\ell}(x)$. Then, we define

$$\mathcal{A}_{L,\varepsilon,\delta,\ell} := \left\{ \alpha \in \mathcal{A} \left| \sum_x |\psi_\alpha^{(L)}(x)| \left\| R_{x,\delta,\ell} \psi_\alpha^{(L)} \right\|_{\ell^2(\Lambda_L)} < \varepsilon \right. \right\},$$

for $\varepsilon > 0$. For ε small, $\{\psi_\alpha^{(L)} | \alpha \in \mathcal{A}_{L,\varepsilon,\delta,\ell}\}$ contains the class of exponentially localized states concentrated in balls of radius $\sim \frac{\delta\ell}{\log \ell}$ or smaller, where δ is independent of ℓ . This observation and Lemma 2.1 below are joint results of the author with L. Erdős and H.-T. Yau.

The following main theorem states that most eigenstates are expected to have localization lengths larger than $O(\frac{\lambda^{-2}}{|\log \lambda|})$.

Theorem 2.1 *Assume for $L \gg \lambda^{-2}$, that $\{\psi_\alpha^{(L)}\}$ is an orthonormal H_ω -eigenbasis in $\ell^2(\Lambda_L)$, satisfying (2) with $\alpha \in \mathcal{A}_L$, and $e_\alpha \in \mathbb{R}$. Then, for $\lambda^{\frac{14}{15}} < \delta < 1$, $\varepsilon_\delta := \delta^{\frac{3}{7}}$,*

$$\mathbb{E} \left[\frac{|\mathcal{A}_L \setminus \mathcal{A}_{L,\varepsilon_\delta,\delta,\lambda^{-2}}|}{|\mathcal{A}_L|} \right] \geq 1 - c\delta^{\frac{3}{14}} - \frac{c(\ell)}{L},$$

for a constant $c < \infty$ independent of L, δ, λ . Furthermore,

$$\mathbb{P} \left[\liminf_{L \rightarrow \infty} \frac{|\mathcal{A}_L \setminus \mathcal{A}_{L,\varepsilon_\delta,\delta,\lambda^{-2}}|}{|\mathcal{A}_L|} \geq 1 - c\delta^{\frac{3}{14}} \right] = 1$$

for $\lambda > 0$ sufficiently small, and a constant $c < \infty$ that is uniform in λ and δ .

This theorem is a corollary of Lemmata 2.1, 2.2, and 2.3 below. Lemma 2.1 links the dynamics generated by H_ω to lower bounds on the localization lengths.

Lemma 2.1 *Let $\{\psi_\alpha^{(L)}\}$ denote an orthonormal basis in $\ell^2(\Lambda_L)$, consisting of eigenvectors of H_ω satisfying (2), and assume that $1 \ll \ell \ll L$. Let*

$$\mathcal{A}_{L,\varepsilon,\delta,\ell}^c := \mathcal{A}_L \setminus \mathcal{A}_{L,\varepsilon,\delta,\ell},$$

and suppose that for all $x \in \mathbb{Z}^3$,

$$\mathbb{E} \left[\left\| R_{x,\delta,\ell} e^{-itH_\omega} \delta_x \right\|_{\ell^2(\mathbb{Z}^3)}^2 \right] \geq 1 - \varepsilon \tag{3}$$

is satisfied for some $\varepsilon = \varepsilon(\delta, \ell, t) > 0$. Then,

$$\mathbb{E} \left[\frac{|\mathcal{A}_{L,\varepsilon,\delta,\ell}^c|}{|\mathcal{A}_L|} \right] \geq 1 - 2\varepsilon^{1/2} - \frac{c(\ell)}{L},$$

where $c(\ell)$ is a constant that only depends on ℓ .

Proof. To prove this result, we represent δ_x on the left hand side of (3) in the basis $\{\psi_\alpha^{(L)}\}$, and separate the contributions stemming from $\mathcal{A}_{L,\varepsilon,\delta,\ell}$ and its complement by a Schwarz inequality. Averaging over Λ_L (where $|\Lambda_L| = |\mathcal{A}_L|$), we find

$$\frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \|R_{x,\delta,\ell} e^{-itH_\omega} \delta_x\|_{\ell^2(\Lambda_L)}^2 \leq (1 + \varepsilon^{1/2}) \frac{|\mathcal{A}_{L,\varepsilon,\delta,\ell}^c|}{|\mathcal{A}_L|} + 1.1\varepsilon^{1/2}. \quad (4)$$

The left hand side and

$$\frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \|R_{x,\delta,\ell} e^{-itH_\omega} \delta_x\|_{\ell^2(\mathbb{Z}^3)}^2 \quad (5)$$

differ only by boundary terms of order $O(\frac{1}{L})$. Taking expectations, the assertion of the lemma follows.

Lemma 2.2 *Under the same assumptions as in Lemma 2.1,*

$$\mathbb{P} \left[\liminf_{L \rightarrow \infty} \frac{|\mathcal{A}_{L,\varepsilon,\delta,\ell}^c|}{|\mathcal{A}_L|} \geq 1 - 2\varepsilon^{1/2} \right] = 1.$$

Proof. We note that by unitarity of the translation operator on $\ell^2(\mathbb{Z}^3)$,

$$(5) = \frac{1}{|\Lambda_L|} \sum_{x \in \Lambda_L} \|R_{0,\delta,\ell} e^{-itH_{\tau_{-x}\omega}} \delta_0\|_{\ell^2(\mathbb{Z}^3)}^2, \quad (6)$$

where $\tau_x : \omega_y \mapsto \omega_{x+y}$, for $x \in \mathbb{Z}^3$, is the family of shift transformations, which acts ergodically on the probability space on which the random potential is realized. The assertion of the lemma follows from (4), and from applying the Birkhoff-Khinchin ergodic theorem to (6).

Lemma 2.3 provides the condition (3).

Lemma 2.3 *Let $t = \delta^{\frac{6}{7}} \lambda^{-2}$, and $H_0 := -\frac{1}{2}\Delta$. Then, for λ sufficiently small, $0 < \delta < 1$, and all $x \in \mathbb{Z}^3$, the free evolution term satisfies*

$$\|R_{x,\delta,\frac{1}{\lambda^2}} e^{-itH_0} \delta_x\|_2 \geq 1 - c\delta^{\frac{3}{7}}, \quad (7)$$

while the sum over collision histories yields

$$\mathbb{E} \left[\left\| R_{x,\delta,\frac{1}{\lambda^2}} (e^{-itH} - e^{-itH_0}) \delta_x \right\|_2^2 \right] \leq c'\delta^{\frac{6}{7}} + t^{-\frac{1}{3}}, \quad (8)$$

for positive constants $c, c' < \infty$ that are independent of x, λ and δ .

Proof. The bound (7) follows from a simple stationary phase argument. The proof of (8) in [1] is based on an extension of methods in [3] to the lattice system and non-Gaussian distributed random potentials, and comprises the following four key steps.

1. The small parameters are λ and $t^{-1} = O(\lambda^2)$.

We expand $\phi_t = e^{-itH_\omega} \delta_x$ into a truncated Duhamel series with remainder term $\phi_t = \sum_{n=0}^N \phi_{n,t} + R_{N,t}$, where

$$\phi_{n,t} = (-i\lambda)^n \int ds_0 \cdots ds_n \delta\left(\sum_{j=0}^n s_j - t\right) e^{-is_0 H_0} V_\omega e^{-is_1 H_\omega} \cdots V_\omega e^{-is_n H_0} \delta_x ,$$

and

$$R_{N,t} = -i \int_0^t ds e^{-i(t-s)H_\omega} V_\omega \phi_{N,s} .$$

The number N remains to be determined. Evidently, the left hand side of (8) is bounded by $2 \sum_{n=1}^N \mathbb{E}[\|\phi_{n,t}\|_{\ell^2}^2] + 2\mathbb{E}[\|R_{N,t}\|_{\ell^2}^2]$.

2. For every fixed n with $1 \leq n \leq N$, we determine the expectation $\mathbb{E}[\|\phi_{n,t}\|_{\ell^2(\mathbb{Z}^3)}^2]$ explicitly by taking all possible contractions among random potentials. This produces $O(n!)$ terms containing only pairing contractions, and $\leq O(2n^{2n})$ terms containing higher order contractions.

To estimate the individual integrals, we classify them according to their contraction structure, which we represent as Feynman graphs.

To this end, we draw two parallel, horizontal solid "particle lines" accounting for $\phi_{n,t}$ and $\phi_{n,y}^*$, respectively. On each particle line, away from its endpoints, we insert n vertices, corresponding to n copies of V_ω . The $n + 1$ edges on each particle line thus obtained correspond to free particle propagators. The particle lines are joined together at, say, both left ends, to account for the ℓ^2 -inner product. Furthermore, we draw dotted "interaction lines" interconnecting those vertices which are mutually contracted. Letting $\Gamma_{n,n}$ denote the set of all such graphs on $n + n$ vertices, we have

$$\mathbb{E}[\|\phi_{n,t}\|_{\ell^2(\mathbb{Z}^3)}^2] \leq \sum_{\gamma \in \Gamma_{n,n}} |Amp(\gamma)| ,$$

where $Amp(\gamma)$ is the integral (Feynman amplitude) corresponding to the graph γ .

Let $\Gamma_{n,n}^{(pair)}$ denote the subset of graphs in $\Gamma_{n,n}$ that comprise only *pairing* contractions among the random potentials. The a priori bound

$$|Amp(\gamma)| \leq P(n, t) \tag{9}$$

holds for all $\gamma \in \Gamma_{n,n}^{(pair)}$, with $P(n, t) := (\log t)^3 (ct\lambda^2 \log t)^n$. Due to the factorially large number of pairings, this bound is insufficient ($n!P(n, t)$ is not summable), and it is thus necessary to perform a finer classification of graphs.

The set $\Gamma_{n,n}^{(pair)}$ is subdivided into:

- (i) The *ladder* graph $\{l_n\}$, where the j -th vertex on the upper particle line is contracted with the j -th vertex on the lower particle line, for $j = 1, \dots, n$ (enumerated along the same direction on both lines).
- (ii) *Simple pairings*, which correspond to decorated ladders. On each particle line, between the rungs of the ladder, there are possibly progressions of *immediate recollisions*, that is, pairings between neighboring copies of V_ω . By definition, simple pairings include $\{l_n\}$.
- (iii) *Crossing* and *nested* graphs, accounting for all non-simple pairing graphs.

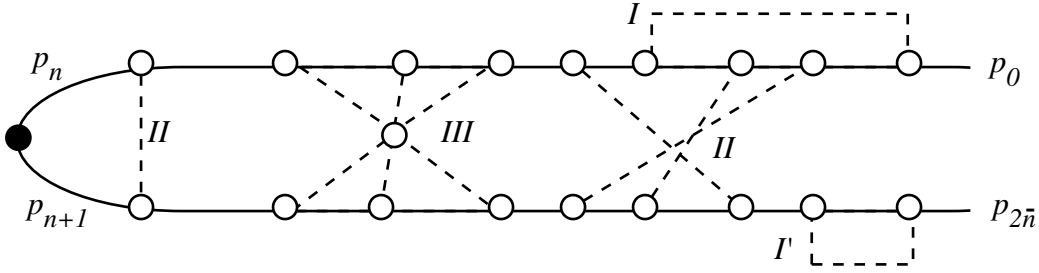


Figure 1. A graph containing pairing (types I, I', II) and non-pairing (type III) contractions.

A key ingredient of the proof are the bounds

$$|Amp(\{l_n\})| \leq \frac{ct\lambda^2}{(n!)^{\frac{1}{2}}} \quad (10)$$

$$|Amp(\gamma \in \Gamma_{n,n}^{(pair)} \setminus \{l_n\})| \leq t^{-\frac{1}{2}} P(n, t), \quad (11)$$

obtained from the corresponding singular momentum space integrals. In this part of the analysis, there are significant differences between the lattice situation of [1], and the continuum case studied in [3]. The bound (10) on the ladder graph $\{l_n\}$ is summable in n , and by (11), all other pairings yield integrals that are, due to strong phase cancellations, at least $O(t^{-\frac{1}{2}})$ smaller than the a priori bound (9) on pairing contractions. Furthermore, it is shown that

$$\sum_{\gamma \in \Gamma_{n,n} \setminus \Gamma_{n,n}^{(pair)}} |Amp(\gamma)| \leq Q(n, t) := C(t^{-\frac{1}{2}}(n!) + t^{-2}(2n)^{4n})P(n, t)$$

holds for the sum of all non-pairing graphs (which are absent in [3]). Thus,

$$\sum_{n=1}^N \sum_{\gamma \in \Gamma_{n,n}} |Amp(\gamma)| \leq ct\lambda^2 + CNQ(N, t)$$

follows.

3. We estimate $\mathbb{E}[\|R_{N,t}\|_{\ell^2(\mathbb{Z}^3)}^2]$ by splitting the time integration into κ intervals of equal size, and by exploiting the rarity of the event that a large number of quantum collisions take place in a small time interval. The result is

$$\mathbb{E}[\|R_{N,t}\|_{\ell^2(\mathbb{Z}^3)}^2] \leq \left(N^2 \kappa^2 + \frac{t^2}{\kappa^N} \right) CNQ(4N, t)$$

4. For a choice

$$\begin{aligned} N(t) &\sim \frac{\beta_1 \log t}{\log \log t} \\ \kappa(t) &\sim (\log t)^{\beta_2}, \end{aligned}$$

and some positive constants β_1, β_2 that are independent of t , we have $1 \ll N(t), \kappa(t) \ll t$, and the asserted estimate (8) follows. In other words, we prove that the sum of all graphs containing crossing, nested, and non-pairing contractions, only contributes to a small error of order at most $O(t^{-\frac{1}{3}})$. The sum of contributions from ladder diagrams for $n \geq 1$ is bounded by $t\lambda^2$, up to a multiplicative constant that is independent of λ and t .

3 Linear Boltzmann Equations

In this section, we discuss the derivation of the macroscopic limit for the quantum dynamics for the system at hand. Let $\phi_t \in \ell^2(\mathbb{Z}^3)$ solve the random Schrödinger equation

$$\begin{cases} i\partial_t \phi_t = H_\omega \phi_t, \\ \phi_0 \in \ell^2(\mathbb{Z}^3) \end{cases} \quad (12)$$

for a fixed realization of the random potential. Then, $W_{\phi_t} : \mathbb{Z}^3 \times \mathbb{T}^3 \rightarrow \mathbb{C}$,

$$W_{\phi_t}(x, v) = \sum_{y \in \mathbb{Z}^3} \overline{\phi_t(x+y)} \phi_t(x-y) e^{2\pi i y v}, \quad (13)$$

defines its Wigner transform.

We introduce macroscopic variables $T := \epsilon t$, $X := \epsilon x$, $V := v$, and consider the rescaled Wigner transform

$$W_{\phi_t}^\epsilon(X, V) := \epsilon^{-3} W_{\phi_t}(X/\epsilon, V) \quad (14)$$

with $X \in (\epsilon\mathbb{Z})^3$, and $V \in \mathbb{T}^3$.

Theorem 3.1 *Let $\epsilon = \lambda^2$, and let ϕ_t^ϵ be a solution of (12) with initial condition*

$$\phi_0^\epsilon(x) = \epsilon^{3/2} h(\epsilon x) e^{iS(\epsilon x)/\epsilon}, \quad (15)$$

where $h, S \in S(\mathbb{R}^3)$. Then, for any $T > 0$,

$$\mathbb{E}[W_{\phi_{T/\epsilon}^\epsilon}^\epsilon(X, V)] \rightarrow F_T(X, V),$$

for $X \in \mathbb{R}^3$, $V \in \mathbb{T}^3$, weakly as $\epsilon \rightarrow 0$, where $F_T(X, V)$ solves the linear Boltzmann equation

$$\begin{aligned} \partial_T F_T(X, V) + 2 \sum_{j=1}^3 \sin 2\pi V_j \cdot \nabla_{X_j} F_T(X, V) \\ = \int_{\mathbb{T}^3} dU \sigma(U, V) [F_T(X, U) - F_T(X, V)], \end{aligned} \quad (16)$$

with collision kernel

$$\sigma(U, V) = 4\pi \delta(e(U) - e(V)),$$

and initial condition F_0 given by

$$W_{\phi_0^\epsilon}^\epsilon \rightarrow |h(X)|^2 \delta(V - \nabla S(X)) =: F_0(X, V), \quad (17)$$

weakly as $\epsilon \rightarrow 0$.

This result is established by extracting the main terms from the expectation of the Wigner distribution, consisting exclusively of simple pairings, which converge weakly to a solution of the linear Boltzmann equations as $\epsilon \rightarrow 0$, in analogy to the case in [3]. To prove that the errors stemming from the remaining classes of graphs tend to zero as $\epsilon \rightarrow 0$, one essentially uses the ℓ^2 -estimates described above.

Acknowledgements

I am profoundly grateful to Prof. L. Erdős, and in particular Prof. H.-T. Yau, for their support and generosity. It is a great pleasure to thank Prof. K. R. Ito, Prof. I. Ojima, and Prof. Y. Takahashi for their great kindness and warm hospitality during our visit in Kyoto. The author is supported by a Courant Instructorship, and in part by a grant from the NYU Research Challenge Fund Program.

References

- [1] Chen, T. *Localization Lengths and Boltzmann Limit for the Anderson Model at Small Disorders in Dimension 3*, submitted (2003).
- [2] Erdős, L., *Linear Boltzmann equation as the scaling limit of the Schrödinger evolution coupled to a phonon bath*, J. Stat. Phys. 107(5), 1043-1127 (2002).
- [3] Erdős, L., Yau, H.-T., *Linear Boltzmann equation as the weak coupling limit of a random Schrödinger equation*, Comm. Pure Appl. Math., Vol. LIII, 667 - 753, (2000).
- [4] Erdős, L., Salmhofer, M., Yau, H.-T., *announced*.
- [5] Magnen, J., Poirot, G., Rivasseau, V., *Renormalization group methods and applications: First results for the weakly coupled Anderson model*, Phys. A 263, no. 1-4, 131-140 (1999).
- [6] Magnen, J., Poirot, G., Rivasseau, V., *Ward-type identities for the two-dimensional Anderson model at weak disorder*, J. Statist. Phys., 93, no. 1-2, 331-358 (1998).
- [7] Poirot, G., *Mean Green's function of the Anderson model at weak disorder with an infra-red cut-off*, Ann. Inst. H. Poincaré Phys. Théor. 70, no. 1, 101-146 (1999).
- [8] Shubin, C., Schlag, W., Wolff, T., *Frequency concentration and localization lengths for the Anderson model at small disorders*, to appear in Journal d'analyse math.
- [9] Spohn, H., *Derivation of the transport equation for electrons moving through random impurities*, J. Statist. Phys., 17, no. 6, 385-412 (1977).