Feynman graphs and renormalization in quantum diffusion *

László Erdős

Mathematisches Institut, Universität München, Theresienstr. 39, D-80333 München lerdos@mathematik.uni-muenchen.de

Manfred Salmhofer

Institut für Theoretische Physik, Universität Leipzig, Postfach 100920, 04009 Leipzig and Max–Planck–Institut für Mathematik, Inselstr. 22, D-04103 Leipzig salmhofer@itp.uni-leipzig.de

Horng-Tzer Yau

Mathematics Department, Harvard University, Cambridge, MA 02138, USA htyau@math.harvard.edu

June 28, 2008

Abstract

We review our proof that in a scaling limit, the time evolution of a quantum particle in a static random environment leads to a diffusion equation. In particular, we discuss the role of Feynman graph expansions and of renormalization.

1 Introduction

The emergence of irreversibility from reversible dynamics in large systems has been one of the fundamental questions in science since the days of Maxwell and Boltzmann. The famous debate about the statistical character of the second law of thermodynamics and the related controversy about Boltzmann's *Stoßzahlansatz* in the derivation of his transport equation has been very fruitful for physics and

^{*}Talk given by M. Salmhofer at the conference in honour of Wolfhart Zimmermann's 80th birthday, Ringberg Castle, February 3–6, 2008

mathematics. After Lanford's rigorous justification of the Boltzmann equation for a classical many-particle system at short kinetic time scales[1], the mathematical justification of the Boltzmann equation at longer timescales has remained a challenge up to the present time. The analogous statement for quantum systems remains open even at the short kinetic timescale.

A related important question is to understand how Brownian motion emerges as an effective law from time-reversal-invariant microscopic physical laws, as given by a Hamiltonian system or the Schrödinger equation. Kesten-Papanicolaou[2] proved that the velocity distribution of a classical particle moving in an environment consisting of random scatterers (i.e., Lorenz gas with random scatterers) converges to a Brownian motion in a weak coupling limit in dimensions $d \ge 3$. In this model the bath of light particles whose fluctuations lead to the Brownian motion of the observed particle is replaced with random static impurities. A similar result was obtained in d = 2 dimensions[4]. Recently[3], the same evolution was controlled on a longer time scale and the position process was proven to converge to Brownian motion as well. Bunimovich and Sinai[5] proved the convergence of the periodic Lorenz gas with a hard core interaction to a Brownian motion. In this model the only source of randomness is the distribution of the initial condition. Finally, Dürr, Goldstein and Lebowitz[6] proved that the velocity process of a heavy particle in a light ideal gas, which is a model with a dynamical environment, converges to the Ornstein-Uhlenbeck process.

Although Brownian motion was discovered and first studied theoretically in the context of classical dynamics, it also describes the motion of a quantum particle in a random environment, on a timescale that is long compared to the standard kinetic timescale[7, 8, 9]. In the following we describe this result and the strategy of the proof in a bit more detail. Besides the motivation discussed above, the random Schrödinger operator that we study is also the standard model for transport of electrons in metals with impurities, which plays a central role in the theory of the metal-insulator transition[10, 11]. The outstanding open mathematical question in this area is the proof of the extended states conjecture, stating that in dimensions $d \ge 3$, at weak disorder, the spectrum of such Hamiltonians is absolutely continuous. Despite much effort, this conjecture has up to now only been proven[12, 13, 14] on the Bethe lattice, which can be interpreted as the case $d = \infty$. In a system with a magnetic field, the existence of dynamical delocalization at certain energies near the Landau levels has been proven recently[15].

2 The problem and the main result

We consider random Schrödinger operators, both on a lattice and in the continuum, in $d \ge 3$ dimensions. In this presentation, we focus on the case d = 3. The time evolution of the *Anderson Model* (AM) is generated by

$$i\frac{\partial}{\partial t}\psi(t) = H\psi(t), \ \psi(0) = \psi_0 \text{ with } H = -\frac{1}{2}\Delta + \lambda V_\omega \text{ on } \ell^2(\mathbb{Z}^d)$$
(1)

where $-\Delta$ is the standard discrete Laplacian and the potential is given by $V(x) = \sum_{a \in \mathbb{Z}^d} V_a(x)$, with $V_a(x) = v_a \delta_{x,a}$, and v_a independent identically distributed (i.i.d.) random variables. We assume that $m_k = \mathbb{E}(v_a^k)$ satisfies

$$\forall i \le 2d : m_i < \infty, \qquad m_1 = m_3 = m_5 = 0, \quad m_2 = 1.$$
 (2)

The continuum analogue of this model is the *Quantum Lorentz Model* (QLM), where $H = -\frac{1}{2}\Delta + \lambda V_{\omega}$ on $L^2(\mathbb{R}^d)$, with Δ the standard Laplacian, $V_{\omega}(x) = \int_{\mathbb{R}^d} B(x-y) d\mu_{\omega}(y)$, where B is a fixed spherically symmetric Schwarz function with $0 \in \text{supp } \hat{B}$, μ_{ω} is a Poisson point process on \mathbb{R}^d with homogeneous unit density and i.i.d. random masses:

$$\mu_{\omega} = \sum_{\gamma=1}^{\infty} v_{\gamma}(\omega) \delta_{y_{\gamma}(\omega)}.$$
(3)

 $\{y_{\gamma}(\omega)\}\$ is Poisson, independent of the weights $\{v_{\gamma}(\omega)\}\$. Again, $m_k := \mathbb{E}_v v_{\gamma}^k$ is assumed to satisfy (2).

Suppose the initial state is localized, i.e. $\hat{\psi}_0$ is smooth. How does the solution $\psi(t) = e^{-itH}\psi_0$ behave for large t? If $\lambda = 0$, the time evolution is easily calculated in Fourier space: $\hat{\psi}(t,k) = e^{-ite(k)}\hat{\psi}_0(k)$, with $e(k) = k^2/2$ (QLM) or $e(k) = \sum_{i=1}^d (1 - \cos k_i)$ (AM). It is equally easy to see that the motion is ballistic, i.e.

$$\langle X^2 \rangle_t = \langle \psi(t), X^2 \psi(t) \rangle \sim t^2.$$
 (4)

If $\lambda \neq 0$, one expects either localization, $\langle X^2 \rangle_t = O(1)$ for all t, or diffusive behaviour (extended states), $\langle X^2 \rangle_t = O(t)$, depending on λ and $\hat{\psi}_0$. The localized behaviour corresponds to dense pure point spectrum at almost every energy; this was proven for large disorder[16, 17] and away from the spectrum of the Laplacian. Extended states correspond to absolutely continuous spectrum. As mentioned, the latter has been proven[12, 13, 14] on the Cayley tree for small $\lambda > 0$. At this time there is no proof of existence of extended states in d = 3. For a simpler case, namely that of randomness with a decaying envelopping function, i.e. $V_{\omega}(x) =$ $\omega_x h(x)$, ω_x i.i.d., h fixed, there is a proof[18, 19] that for $\eta > \frac{1}{2}$ and $h(x) \sim |x|^{-\eta}$ as $|x| \to \infty$, $H = -\Delta + V_{\omega}$ has absolutely continuous spectrum.

Our result is formulated in terms of the Wigner function

$$W_{\psi}(x,v) = \int \mathrm{d}y \,\mathrm{e}^{\mathrm{i}vy} \overline{\psi(x+\frac{y}{2})} \,\psi(x-\frac{y}{2}) \tag{5}$$

which can be thought of as an analogue of a phase space density (but can become negative). Its marginals are $\int W_{\psi}(x, v) dx = |\hat{\psi}(v)|^2$ and $\int W_{\psi}(x, v) dv = |\psi(x)|^2$. Moreover,

$$\hat{W}_{\psi}(\xi, v) = \int dx \ e^{-ix\xi} W_{\psi}(x, v) = \overline{\hat{\psi}(v - \xi/2)} \ \hat{\psi}(v + \xi/2).$$
(6)

On the lattice, one has to modify the definition of the Wigner transform slightly[9].

The kinetic scaling is given by

$$\eta = \lambda^2, \qquad \mathcal{T} = \eta t, \qquad \mathcal{X} = \eta x,$$
(7)

i.e. the microscopic time and space variables both become of order λ^{-2} , so that velocities remain unscaled.

Theorem 2.1

$$\mathbb{E}W^{\eta}_{\psi(\mathcal{T}\eta^{-1})}(\mathcal{X},\mathcal{V}) \xrightarrow[\eta \to 0]{} F(\mathcal{X},\mathcal{V},\mathcal{T}),$$
(8)

F the solution of the linear Boltzmann equation

$$\frac{\partial}{\partial \mathcal{T}} F(\mathcal{X}, \mathcal{V}, \mathcal{T}) + (\nabla e)(\mathcal{V}) \cdot \nabla_{\mathcal{X}} F(\mathcal{X}, \mathcal{V}, \mathcal{T})$$

= $2\pi \int d\mathcal{U} \, \delta(e(\mathcal{U}) - e(\mathcal{V})) \left| \hat{B}(\mathcal{U} - \mathcal{V}) \right|^2 \left[F(\mathcal{X}, \mathcal{U}, \mathcal{T}) - F(\mathcal{X}, \mathcal{V}, \mathcal{T}) \right] (9)$

This theorem was first proven for the continuum for small time \mathcal{T} [20], then for arbitrary time[21], and later extended to the lattice case[22].

The *diffusive scaling* is defined by

$$\varepsilon = \lambda^{2+\kappa/2}, \qquad X = \varepsilon x, \qquad T = \varepsilon \lambda^{\kappa/2} t = \lambda^{\kappa+2} t.$$
 (10)

This is long compared to the kinetic timescale: the kinetic variables \mathcal{X} and \mathcal{T} diverge as $\lambda \to 0$ when X and T are kept fixed,

$$\mathcal{X} = \lambda^{-\kappa/2} X, \qquad \mathcal{T} = \lambda^{-\kappa} T.$$
 (11)

A first hint at diffusion is that under this scaling $\mathcal{X}^2/\mathcal{T} = X^2/T$ is independent of λ . The result for the Anderson model is

Theorem 2.2 Let d = 3, $\psi_0 \in \ell^2(\mathbb{Z}^3)$ and $\psi(t)$ be the solution to the random Schrödinger equation with initial condition ψ_0 . If $\kappa > 0$ is small enough and $\varepsilon = \lambda^{2+\kappa/2}$, then in the limit $\lambda \to 0$, $\mathbb{E}W^{\varepsilon}_{\psi(\lambda^{-2-\kappa}T)}$ converges weakly to the solution f of a heat equation.

More precisely: denote $\langle F \rangle_E = \Phi(E)^{-1} \int dv \ F(v) \delta(E-e(v))$, where $\Phi(E) = \int dv \ \delta(E-e(v))$. Let $E \in (0,3)$ and $D_{ij}(E) = \frac{1}{2\pi\Phi(E)} \langle \nabla_i e \ \nabla_j e \rangle_E$, and let f be the solution of the heat equation

$$\frac{\partial}{\partial T}f(T,X,E) = \nabla_X \cdot D(E)\nabla_X f(T,X,E)$$
(12)

$$f(0, X, E) = \delta(X) \langle |\psi_0|^2 \rangle_E.$$
(13)

Let $\mathcal{O}(x, v)$ be a Schwartz function on $\mathbb{R}^d \times \mathbb{R}^d / 2\pi \mathbb{Z}^d$. Then

$$\lim_{\varepsilon \to 0} \sum_{X \in (\varepsilon \mathbb{Z}/2)^d} \int \mathrm{d}v \ \mathcal{O}(X, v) \ \mathbb{E} W^{\varepsilon}_{\psi(\lambda^{-\kappa-2}T)}(X, v)$$
$$= \int_{\mathbb{R}^d} \mathrm{d}X \int \mathrm{d}v \ \mathcal{O}(X, v) \ f(T, X, e(v)). \tag{14}$$

The limit is uniform on $[0, T_0]$ for any $T_0 > 0$.

We discuss some of the ideas in the proof of this theorem in Section 3.

If $\hat{\psi}_0 \in C^1$ and λ is small enough, we have the more detailed error estimate

$$\int dv \int d\xi \,\hat{\mathcal{O}}(\xi, v) \,\mathbb{E}\hat{W}^{\varepsilon}_{\psi(\lambda^{-2-\kappa}T)}(\xi, v)$$

$$= \int d\xi \int \Phi(E) dE \,e^{-\frac{T}{2}\langle \xi, \, D(E)\xi \rangle_E} \langle \hat{\mathcal{O}}(\xi, \cdot) \rangle_E \,\langle \hat{W}_{\psi_0}(\varepsilon\xi, \cdot) \rangle_E + o(1).$$
(15)

The Boltzmann equation also gives the same diffusion equation in the long time limit, but it was itself derived from the quantum mechanical time evolution only for shorter timescales. The main difficulty in the proof is to deal with contributions that vanish for $\lambda \rightarrow 0$ under kinetic scaling, but that become important under the above-defined diffusive scaling. More technically speaking, in the Feynman expansion done to analyze the time evolution, most of these terms would even diverge under diffusive scaling if we did not renormalize the propagator.

The allowed values of κ are in an interval $[0, \kappa_0)$, where κ_0 is a universal constant. For technical reasons, κ_0 has to be chosen very small in the proof. Heuristically, i.e. ignoring many of the technical complications and assuming optimal bounds, one would expect the remainder of the renormalized Feynman graph expansion to vanish up to $\kappa_0 = 2$, and to diverge for $\kappa_0 > 2$.

The diffusive scaling leads to a diffusion on the energy shells. A diffusion mixing energy shells is expected to start at $t = \lambda^{-4}$.

An intuitive way of interpreting the expansion described below is as an expansion in the number N of collisions of the particle with the randomly (but statically) arranged obstacles represented by the potential. As compared to the previous results[21, 22], the main new feature here is that under diffusive scaling, the effective number of collisions of the particle diverges. That is, not only is it necessary to expand to an order N that diverges as $\lambda \to 0$, but also the main contribution does not come from terms with a finite number of collisions.

3 Collision histories, Feynman graphs, and ladders

We discuss some of the ideas of the proof for the example of the Anderson model, i.e. the lattice situation. For the detailed bounds of Feynman graphs, the lattice leads to a number of complications[9], but for the presentation it is easier.

3.1 Collision histories

Let us start with a formal time–ordered expansion, setting $H_0 = -\frac{1}{2}\Delta$ and expanding in λV . Then $\psi(t) = e^{-itH}\psi_0 = \sum_{n\geq 0} \psi^{(n)}(t)$ with

$$\psi^{(n)}(t) = (-i\lambda)^n \int d\mu_{n+1}(s) e^{-is_n H_0} V e^{-is_n H_0} \dots V e^{-is_0 H_0} \psi_0 \quad (16)$$

where $s = (s_0, ..., s_n)$ and

$$d\mu_{n+1}(s) = \int_{[0,\infty)^{n+1}} ds_0 \dots ds_n \,\delta\left(t - \sum_{j=0}^n s_j\right).$$
 (17)

Because $V = \sum_{a \in \mathbb{Z}^d} V_a$, it is natural to split each $\psi^{(n)}$ further, $\psi^{(n)}(t) = \sum_{\mathbf{a}_n} \psi^{(n)}_{\mathbf{a}_n}(t)$. Every sequence of obstacle labels $\mathbf{a}_n = (a_1, \ldots, a_n) \in (\mathbb{Z}^d)^n$ represents a *collision history*, and for $k \in \{1, \ldots, n-1\}$, the time variables s_k in (17) are the time differences between two subsequent collisions. The delta function in (17) enforces the constraint that these time differences, together with the propagation times s_0 before the first collision and s_n after the last one, add up to the total time t. We shall discuss convergence questions about this expansion later.

Our detailed analysis takes place in momentum space, where each V acts as a convolution operator, so that

$$\hat{\psi}_n(t,p_n) = (-\mathbf{i})^n \int \mathrm{d}\mu_{n+1}(s) \int \prod_{j=0}^{n-1} \frac{\mathrm{d}^d p_j}{(2\pi)^d} \,\mathrm{e}^{-\mathbf{i}s_j e(p_j)} \prod_{j=1}^n \hat{V}(p_j \cdot p_{j-1}) \hat{\psi}_0(p_0).$$
(18)

Very schematically, one can represent this as follows, where each of the dashed lines represents a factor λV and each of the full lines gets a phase factor $e^{-is_j e(p_j)}$.

T	T	T	T	T	T	T
1	1	1	1	1	1	1
1		1			1	

As the convolution formula shows, one can define a momentum flow in this graph, where the momentum change $p_j - p_{j+1}$ flows away through the dashed line. Before the disorder average, there is no translation invariance in the system, so every scattering at an obstacle changes the momentum of the particle.

3.2 Disorder average and graphs

Recalling (6), we have

$$\mathbb{E}\left[\hat{W}_{\psi(t)}(\xi,v)\right] = \sum_{n,n'} \sum_{\mathbf{a}_{n},\mathbf{a}'_{n'}} \mathbb{E}\left[\overline{\hat{\psi}_{\mathbf{a}_{n}}^{(n)}(t,v-\xi/2)}\hat{\psi}_{\mathbf{a}'_{n'}}^{(n')}(t,v+\xi/2)\right].$$
 (19)

Note that there are now two, a priori independent, collision histories, one for ψ and one for $\overline{\psi}$. It will be part of the proof to show that, in the scaling limit we consider, the only contributions after self-energy renormalization come from the so-called ladder graphs, where the two collision histories are identical: n = n' and $\mathbf{a}_n = \mathbf{a}'_n$.

Because the disorder is i.i.d., translation invariance holds for the average, which means that momentum conservation also holds for the dashed lines, which for the Anderson model simply correspond to a factor λ^2 , since the second moment of the disorder was normalized to 1 in (2).

The result can be represented as a graph built of two particle lines, particle– disorder vertices, which are joined by disorder lines, and, if the randomness is non-Gaussian, disorder-disorder vertices, which correspond to the higher moments of the disorder distribution. An example is



Particle lines get propagators $e^{-is_j e(p_j)}$, interaction lines give factors λ^2 , and the disorder-disorder vertex of degree four corresponds to a factor $m_4\lambda^4$.

It is clear that in the way the expansion was introduced above, one really needs the assumption that arbitrary moments, not just the first 2d ones, exist. The expansion employed in the true proof contains a stopping rule which avoids high

moments, but we shall not discuss this here in more detail. In fact, we shall in the following assume for simplicity that the disorder is Gaussian, so that there are no vertices of higher degree for the dashed lines, and the average just corresponds to a pairing of interaction lines.

An example of a pairing is as follows



Note that here, there is a crossing of the two pairing lines in the graphical representation, but there are no vertices in which more than one interaction line enters.

A special class of pairings are the *up-down pairings*, where n = n' and the pairing corresponds to a permutation $\sigma \in S_n$:



The most important term turns out to be the *ladder graph*, corresponding to $\sigma = id$:



3.3 Graph bounds

In the following, we give a brief discussion of bounds of the contributions of individual graphs, restricting to up-down pairings. If one takes a bound in the representation (18), each phase factor is replaced by 1. This leads to a bound of order $(\lambda t)^n/n!$ (where the n! comes from the time ordering implied by the delta function in (17)), which does not even allow to consider the kinetic scaling where $\lambda^2 t$ is fixed. For this reason, the following *propagator representation* is useful. Let $\eta > 0$. Then, inserting the Fourier representation of the delta function,

$$\int_{[0,\infty)^{n+1}} \mathrm{d}^{n+1}s \,\delta\left(t - \sum_{j=1}^{n+1} s_j\right) \prod_{j=1}^{n+1} \mathrm{e}^{-\mathrm{i}s_j e(p_j)}$$

$$= e^{t\eta} \int_{[0,\infty)^{n+1}} d^{n+1}s \,\delta\left(t - \sum_{j=1}^{n+1} s_j\right) \prod_{j=1}^{n+1} e^{-is_j(e(p_j) - i\eta)}$$

$$= e^{t\eta} \int \frac{d\alpha}{2\pi} e^{-it\alpha} \int_{[0,\infty)^{n+1}} d^{n+1}s \prod_{j=1}^{n+1} e^{-is_j(\alpha - e(p_j) + i\eta)}$$

$$= i^{-n} e^{t\eta} \int \frac{d\alpha}{2\pi} e^{-i\alpha t} \prod_{j=1}^{n+1} \frac{1}{\alpha - e(p_j) + i\eta}.$$
(20)

It is convenient to choose $\eta = t^{-1}$.

The contribution of a permutation $\sigma \in S_n$, corresponding to an up–down pairing graph Γ_{σ} , to $\langle \hat{\mathcal{O}}, \hat{W}_{\psi}^{\varepsilon} \rangle$ is

$$Val(\Gamma_{\sigma}) = \lambda^{2n} e^{2t\eta} \int \frac{d\alpha d\beta}{(2\pi)^2} e^{i(\beta-\alpha)t}$$
$$\int d\xi \int \prod_{j=0}^{n} \frac{d^d p_j}{(2\pi)^d} \int \prod_{k=0}^{n} \frac{d^d q_k}{(2\pi)^d} \quad \hat{\mathcal{O}}(\xi, p_n) \hat{W}_{\psi_0}^{\varepsilon}(\xi, p_0)$$
$$\prod_{j=0}^{n} \frac{1}{\beta - \omega(q_j - \frac{\varepsilon\xi}{2}) - i\eta} \frac{1}{\alpha - \omega(p_j - \frac{\varepsilon\xi}{2}) - i\eta}$$
$$\prod_{j=1}^{n} \delta \left(p_j - p_{j-1} - (q_{\sigma(j)} - q_{\sigma(j)-1}) \right).$$
(21)

At the moment, $\omega(p) = e(p) \in \mathbb{R}$; later, ω will change under renormalization and become complex.

A simple Schwarz inequality separating the dependence on the p_i and that on the q_i implies that for all σ

$$|Val(\Gamma_{\sigma})| \le Val(\Gamma_{id}). \tag{22}$$

The ladder is easy to calculate at $\xi = 0$, and a ladder of length n is of order $\frac{1}{n!}(\lambda^2 t)^n = \frac{1}{n!}T^n$.

A crucial observation is that the values of graphs with *crossings* get inverse powers of t, as compared to the ladder. This follows from the bound

$$\int \mathrm{d}p \, \frac{1}{|\alpha - \omega(p) + \mathrm{i}\eta|} \, \frac{1}{|\beta - \overline{\omega(\pm p + q)} - \mathrm{i}\eta|} \le C |\log \eta|^3 \frac{\eta^{-b}}{||q|| + \eta} \tag{23}$$

 $(b = 0 \text{ for the continuum; } 1/2 \le b \le 3/4 \text{ on the lattice}). |||p||| = |p| \text{ in the continuum, } |||p||| = \min\{|p - v| : v_i \in \{0, \pm \pi\}\} \text{ on the lattice. Again, here }$

 $\omega(p) = e(p)$. This motivates why the ladder graph gives the dominant contribution under kinetic scaling. However, the number of graphs goes like n!, which cancels the 1/n!, hence expanding to infinite order one gets majorants by geometric series, which converge only on very short kinetic timescales \mathcal{T} . This is the reason for the restriction to small kinetic timescales in the first proof[20] of the Boltzmann equation for the QLM.

3.4 Expansions to finite order and remainder terms

Major progress[21] came from the realization that one can do an expansion to finite order with an efficient remainder estimate. A natural way to generate a finite–order expansion is the *Duhamel formula*

$$\psi(t) = e^{-itH}\psi_0 = e^{-itH_0}\psi_0 + \int_0^t ds \ e^{-i(t-s)H}\lambda V e^{-isH_0}\psi_0.$$
(24)

Iteration gives

$$\psi(t) = \sum_{n=0}^{N-1} \psi^{(n)}(t) + \Psi_N(t), \qquad (25)$$

where

$$\Psi_N(t) = (-\mathrm{i}) \int_0^t \mathrm{d}s \; \mathrm{e}^{-\mathrm{i}(t-s)H} \lambda V \psi^{(N-1)}(s) \tag{26}$$

and

$$\psi^{(n)}(t) = (-i\lambda)^n \int d\mu_{n+1}(s) e^{-is_n H_0} V \dots V e^{-is_0 H_0} \psi_0.$$
 (27)

An alternative way of looking at this is via its relation to the resolvent formula

$$R_z = R_z^{(0)} + R_z \lambda V R_z^{(0)}$$
(28)

where $R_z = (z - H)^{-1}$ and $R_z^{(0)} = (z - H_0)^{-1}$. Iteration of the resolvent equation and using the Fourier transform gives the above propagator representation directly. The Duhamel formula is obtained via

$$e^{-itH} = -e^{t\eta} \int \frac{d\alpha}{2\pi i} e^{-i\alpha t} R_{\alpha+i\eta}.$$
 (29)

The second crucial ingredient is that one can use the unitarity of the full time evolution to reduce all terms to ones where no H appears in the time evolution any more:

$$\|\Psi_N(t)\| \leq \int_0^t \mathrm{d}s \, \left\| \mathrm{e}^{-\mathrm{i}(t-s)H} \lambda V \psi^{(N-1)}(s) \right\| \leq \int_0^t \mathrm{d}s \, \left\| \lambda V \psi^{(N-1)}(s) \right\| (30)$$

Thus

$$\|\Psi_N(t)\|^2 \le t \ |\lambda|^2 \int_0^t \mathrm{d}s \ \left\|V\psi^{(N-1)}(s)\right\|^2.$$
(31)

The remaining integral over *s* effectively gives a factor *t*, which is the price to pay for this unitarity bound. To control this factor, one needs exhibit more factors t^{-1} in graphs with several independent crossings, and treat graphs with only one crossing explicitly (in the resolvent iteration, the unitarity bound would be replaced by $||R_{\alpha+i\eta}|| \leq \eta^{-1}$).

By a Schwarz inequality, one can see that the Wigner transform is continuous in L^2 norm:

$$\left| \mathbb{E} \left(\langle \hat{\mathcal{O}}, \hat{W}_{\psi_1}^{\varepsilon} \rangle - \langle \hat{\mathcal{O}}, \hat{W}_{\psi_2}^{\varepsilon} \rangle \right) \right| \le C \int \mathrm{d}\xi \, \sup_{v} \left| \hat{\mathcal{O}}(\xi, v) \right| \sqrt{\mathbb{E} \|\psi_1\|^2 \, \mathbb{E} \|\psi_1 - \psi_2\|^2}.$$
(32)

Thus the unitarity bound can also be used for the Wigner transform. The proof of the Boltzmann equation[21] on an arbitrarily large kinetic timescale \mathcal{T} uses an expansion up to order $N \sim \log t$. The ladder terms give the gain term in the Boltzmann equation. The lowest order self-energy correction gives the loss term in the Boltzmann equation. It corresponds to the "gate" graph



3.5 Long time scale: renormalization

Because the ladder with n rungs is of order $(\lambda^2 t)^n/n!$, it diverges under diffusive scaling, and so do other graphs. To increase the time beyond λ^{-2} , we need to do a renormalization. Formally, one can think of this as a resummation of the gate diagrams, which are of self-energy type, but this geometric series converges only for small $\lambda^2 t$. A way to avoid such formal resummations is to change the way H is split into a "free" and an interaction part, i.e., expand around a different H_0 . For $\varepsilon > 0$ set

$$\Theta_{\varepsilon}(\alpha) = \int \mathrm{d}q \frac{1}{\alpha - e(q) + \mathrm{i}\varepsilon} \,. \tag{33}$$

This is the value of the gate diagram at energy α in the Anderson model (in the QLM, the integrand contains an additional factor from the interaction function). The limit $\Theta(\alpha) = \lim_{\varepsilon \to 0+} \Theta_{\varepsilon}(\alpha)$ exists and is Hölder continuous[7] in α of order 1/2. Let

$$\theta(p) = \Theta(e(p)). \tag{34}$$

The idea is now to put $\lambda^2 \theta(p)$ as a counterterm, which by construction subtracts every insertion of a gate diagram at the point $\alpha = e(p)$ where the particle propagator is singular. Because α and η appear only as auxiliary quantities in the expansion, it was necessary to take $\varepsilon \to 0$ above and define θ in an α -independent way.

The counterterm is added and subtracted so that the Hamiltonian does not change: let $\omega(p) = e(p) + \lambda^2 \theta(p)$ and decompose

$$H = \omega(P) + U, \qquad U = \lambda V - \lambda^2 \theta(P) \tag{35}$$

(where P denotes the momentum operator). The function ω can be thought of as a new dispersion relation of energy as a function of momentum. However, ω also has a negative imaginary part, roughly of order λ^2 . More precisely, for $d \ge 3$ there is c > 0 such that

$$\operatorname{Im} \omega(p) \le -c\lambda^2 ||p||^{d-2}.$$
(36)

Thus H_0 is no longer selfadjoint. However, the negative sign of Im ω implies that the resolvent $R_{\alpha+i\eta}$ is still well-defined, since the imaginary parts add up with the same sign. Correspondingly, the time evolution operator e^{-isH_0} is no longer unitary but it remains bounded for $s \ge 0$. Both the Duhamel and the resolvent iteration are thus well-defined. Besides the new propagator $(\alpha + i\eta - \omega(p))^{-1}$, the important change is that every factor U now also contains a counterterm insertion $-\lambda^2 \theta(p)$. The point about these iterations is that they can be stopped (or even modified) after every expansion step. It is thus clear that one can group the counterterms that appear in the expansion together with the gates that get created when taking the average over the disorder. The cancellation among these two terms provides a small factor that makes such terms vanish in the diffusive scaling limit. Moreover, it is clear that one can implement rules for stopping the expansion independently of the subsequent disorder average. In particular, because the randomness is i.i.d., one can avoid moments beyond the power 2d by stopping the expansion when a given site has appeared in the collision history d times. The terms to which no such repetition or renormalization cancellation applies are expanded up to order $n \sim \lambda^2 t \lambda^{-\delta} \sim \lambda^{-\kappa-\delta}$, where $\delta > 0$ depends on κ . The intuition behind this is that certain graphs with $n \sim \lambda^2 t \sim \lambda^{-\kappa}$ give the main contribution, and expanding up to an order that is $\lambda^{-\delta}$ higher leads again to small factors.

The imaginary part of ω gives effectively a regularization $O(\lambda^2)$ instead of $O(\eta)$ for the denominators, which changes the values of all diagrams significantly. In particular, the integral for one rung of the ladder becomes

$$\int \frac{\lambda^2 \, \mathrm{d}p}{(\alpha - \overline{\omega}(p+r) - i\eta) \, (\beta - \omega(p-r) + i\eta)} = 1 + C_0 \lambda^{1 - O(\kappa)} \,. \tag{37}$$

where C_0 is a constant. Thus with this renormalization, the ladders become of order 1, so that one can go beyond kinetic scaling. Indeed, in the language of Feynman graphs, the main result can be stated informally as

After renormalization, the sum of the ladder graphs for the Wigner transform converges to a solution of the heat equation in the diffusive scaling limit.

The precise statements are Theorems 5.1, 5.2, and 5.3 in Ref.[7]. They involve in particular proving that the terms which do not correspond to pure up–down pairings vanish in the limit, and dealing with a number of technical complications which arise from the fact that one has to do an expansion to a finite order.

3.6 The key estimate for controlling combinatorics

We have had to leave out almost all technical details to avoid overloading the presentation, but we should like to at least mention the heart of the proof here at the end, to clarify the main ideas about the Feynman graph expansion.

Focusing on up-down pairings, we have to deal with a combinatorial problem of bounding the sum over the n! permutations $\sigma \in S_n$. As mentioned, with an expansion to infinite order, one cannot get beyond the kinetic scaling because of this factor n!. The control of the remainders is done here by choosing an appropriate stopping n for the expansion and by "beating down the combinatorics by power counting". That is, we prove exponential suppression of the values of Feynman graphs in the number of crossings they have, that is, loosely speaking, in their complexity.

The precise notion capturing the complexity of a permutation $\sigma \in S_n$ is its degree $d(\sigma)$, defined as the number of non-ladder and non-antiladder indices. Essentially, the ladder indices are those for which $\sigma(i + 1) = \sigma(i) + 1$, and the antiladder indices are those for which $\sigma(i + 1) = \sigma(i) - 1$.

Theorem 3.1 Let Γ_{σ} be the Feynman graph corresponding to σ . There is $\gamma > 0$ such that for all σ

$$|Val(\Gamma_{\sigma})| \le C\lambda^{\gamma d(\sigma)}.$$
(38)

This theorem is proven using a special integration algorithm for bounding the values of large Feynman graphs[7].

The number of permutations with degree D is

$$\mathcal{N}_{n,D} = |\{\sigma \in \mathcal{S}_n : d(\sigma) = D\}| \le 2(2n)^D.$$
(39)

Expanding up to $n = O(\lambda^{-\kappa-\delta}), \delta > 0$, we have by (38), if $\gamma - \kappa - \delta > 0$,

$$\sum_{\substack{\sigma \in S_n \\ d(\sigma) \ge D}} \lambda^{\gamma d(\sigma)} = \sum_{d=D}^k \lambda^{\gamma d} \mathcal{N}_{n,d} \le 2 \sum_{d=D}^k (2\lambda)^{d(\gamma-\kappa-\delta)} \le O(\lambda^{D(\gamma-\kappa-\delta)}).$$
(40)

Thus the contribution from the sum of all terms with degree $D \ge 2$ is small if $\gamma - \kappa - \delta > 0$, hence the essential restriction for the value of κ is that of γ . As mentioned, one would hope to get close to $\gamma = 2$ in (38), but γ has to be chosen smaller for technical reasons.

4 Conclusion

We have shown that, for random Schrödinger operators with a weak static disorder the quantum mechanical time evolution can be controlled on large space and time scales where a diffusion equation governs the behavior. The Schrödinger evolution is time–reversible – yet irreversibility on large scales emerges. This apparent controversy is resolved by noting that along the scaling limit microscopic degrees of freedom have been effectively integrated out.

Although the expansion methods we use bear some resemblance to those of constructive quantum field theory, there are also a few noteworthy differences. First, because we analyze the time evolution at real time, the (near-)singularities of the propagators are located on hypersurfaces, and not at points, as would be the case in Euclidean field theories. The singularity structure is to some extent similar to that in real time Fermi surface problems, although there is no fixed Fermi surface here – the integrals over α and β "test" all possible level sets of the function e(p), and this leads to a number of serious complications. Second, we are able to control the combinatorics of a straightforward Feynman graph expansion in momentum space, while the analysis in constructive field theory (to our knowledge, always) needs to be done by cluster expansions in position space to avoid the divergence of an infinite series of Feynman graphs. The reason for this is twofold: the unitarity bound allows us to do an expansion to a finite order, and our strong improvement (38) over standard power counting bounds allows us to push this order so high that we can reach the scale where diffusion sets in, while still retaining control of the remainders.

The genuine challenge is to show diffusion without taking scaling limits, i.e. for a fixed (small) disorder λ and for any time independent of λ . With expansion techniques, this would require to renormalize not only the self–energy to arbitrary order but also the four–point functions. Refining the self–energy renormalization

poses no fundamental difficulty. The correct renormalization of all four-point functions in this problem, however, remains a widely open problem.

References

- [1] O.E. Lanford III, *On the derivation of the Boltzmann equation*. Astérisque **40**, 117-137 (1976)
- [2] H. Kesten, G. Papanicolaou: A limit theorem for stochastic acceleration. Comm. Math. Phys. 78 19-63. (1980/81)
- [3] T. Komorowski, L. Ryzhik: Diffusion in a weakly random Hamiltonian flow. Commun. Math. Phys. 263 no.2. 277-323 (2006)
- [4] D. Dürr, S. Goldstein, J. Lebowitz: Asymptotic motion of a classical particle in random potential in two dimensions: Landau model, Commun. Math. Phys. 113 (1987) no 2. 209-230.
- [5] L. Bunimovich, Y. Sinai: Statistical properties of Lorentz gas with periodic configuration of scatterers. Commun. Math. Phys. 78 no. 4, 479–497 (1980/81),
- [6] D. Dürr, S. Goldstein, J. Lebowitz: A mechanical model of Brownian motion. Commun. Math. Phys. 78 (1980/81) no. 4, 507-530.
- [7] L. Erdős, M. Salmhofer and H.-T. Yau, Quantum diffusion of the random Schrödinger evolution in the scaling limit. Advances in Mathematics (2008) DOI 10.1007/s11511-008-0027-2
- [8] L. Erdős, M. Salmhofer and H.-T. Yau, Quantum diffusion of the random Schrödinger evolution in the scaling limit II. The recollision diagrams. Commun. Math. Phys. 271, 1-53 (2007)
- [9] L. Erdős, M. Salmhofer and H.-T. Yau, Quantum diffusion for the Anderson model in scaling limit. Ann. Inst. H. Poincare 8, 621-685 (2007)
- [10] P. A. Lee, T. V. Ramakrishnan, Disordered electronic systems. Rev. Mod. Phys. 57, 287–337 (1985)
- [11] D. Vollhardt, P. Wölfle, Diagrammatic, self-consistent treatment of the Anderson localization problem in $d \le 2$ dimensions. Phys. Rev. B 22, 4666-4679 (1980)

- [12] A. Klein, Absolutely continuous spectrum in the Anderson model on the Bethe lattice, Math. Res. Lett. 1, 399–407 (1994)
- [13] M. Aizenman, R Sims, S. Warzel, Absolutely continuous spectra of quantum tree graphs with weak disorder. Commun. Math. Phys. 264 no. 2, 371-389 (2006)
- [14] R. Froese, D. Hasler, W. Spitzer, Transfer matrices, hyperbolic geometry and absolutely continuous spectrum for some discrete Schrödinger operators on graphs. J. Funct. Anal. 230 no 1, 184-221 (2006)
- [15] F. Germinet, A. Klein, J. Schenker, Dynamical delocalization in random Landau Hamiltonians. Ann. Math. 166 (2007) 215 – 344
- [16] J. Fröhlich and T. Spencer, Absence of diffusion in the Anderson tight binding model for large disorder or low energy, Commun. Math. Phys. 88, 151–184 (1983)
- [17] M. Aizenman and S. Molchanov, Localization at large disorder and at extreme energies: an elementary derivation, Commun. Math. Phys. 157, 245– 278 (1993)
- [18] I. Rodnianski, W. Schlag, Classical and quantum scattering for a class of long range random potentials. Int. Math. Res. Not. 5 243–300 (2003).
- [19] J. Bourgain, Random lattice Schrödinger operators with decaying potential: some higher dimensional phenomena. Lecture Notes in Mathematics, Vol. 1807, 70-99 (2003).
- [20] H. Spohn: Derivation of the transport equation for electrons moving through random impurities. J. Statist. Phys.**17** (1977), no. 6., 385-412.
- [21] L. Erdős and H.-T. Yau, Linear Boltzmann equation as the weak coupling limit of the random Schrödinger equation, Commun. Pure Appl. Math. LIII, 667-735, (2000).
- [22] T. Chen, Localization Lengths and Boltzmann Limit for the Anderson Model at Small Disorders in Dimension 3. J. Stat. Phys. **120** (2005), no. 1-2, 279-337.