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Towards the quantum Brownian motion

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Summary. We consider random Schrödinger equations on \mathbf{R}^d or \mathbf{Z}^d for $d \geq 3$ with uncorrelated, identically distributed random potential. Denote by λ the coupling constant and ψ_t the solution with initial data ψ_0 . Suppose that the space and time variables scale as $x \sim \lambda^{-2-\kappa/2}$, $t \sim \lambda^{-2-\kappa}$ with $0 < \kappa \leq \kappa_0$, where κ_0 is a sufficiently small universal constant. We prove that the expectation value of the Wigner distribution of ψ_t , $\mathbf{E}W_{\psi_t}(x, v)$, converges weakly to a solution of a heat equation in the space variable x for arbitrary L^2 initial data in the weak coupling limit $\lambda \rightarrow 0$. The diffusion coefficient is uniquely determined by the kinetic energy associated to the momentum v .

1 Introduction

Brown observed almost two centuries ago that the motion of a pollen suspended in water was erratic. This led to the kinetic explanation by Einstein in 1905 that Brownian motion was created by the constant “kicks” on the relatively heavy pollen by the light water molecules. Einstein’s theory, based upon Newtonian dynamics of the particles, in fact postulated the emergence of the Brownian motion from a classical non-dissipative reversible dynamics. Einstein’s theory became universally accepted after the experimental verification by Perrin in 1908, but it was far from being mathematically rigorous.

The key difficulty is similar to the justification of Boltzmann’s molecular chaos assumption (Stoßzahlansatz) standing behind Boltzmann’s derivation of the Boltzmann equation. The point is that the dissipative character emerges only in a scaling limit, as the number of degrees of freedom goes to infinity.

The first mathematical definition of the Brownian motion was given in 1923 by Wiener, who constructed the Brownian motion as a scaling limit of random walks. This construction was built upon a stochastic microscopic dynamics which by itself are dissipative.

The derivation of the Brownian motion from a Hamiltonian dynamics was not seriously investigated until the end of the seventies, when several results came out

almost simultaneously. Kesten and Papanicolaou [16] proved that the velocity distribution of a particle moving in a random scatterer environment (so-called Lorenz gas with random scatterers) converges to the Brownian motion in a weak coupling limit for $d \geq 3$. The same result was obtained in $d = 2$ dimensions by Dürr, Goldstein and Lebowitz [8]. In this model the bath of light particles is replaced with random static impurities. In a very recent work [18], Komorowski and Ryzhik have controlled the same evolution on a longer time scale and proved the convergence to Brownian motion of the position process as well.

Bunimovich-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-Lebowitz [7] proved that the velocity process of a heavy particle in a light ideal gas converges to the Ornstein-Uhlenbeck process that is a version of the Brownian motion. This model is the closest to the one in Einstein's kinetic argument.

An analogous development happened around the same time towards the rigorous derivation of the Boltzmann equation. It was proved by Gallavotti [14], Spohn [26] and Boldrighini, Bunimovich and Sinai [3] that the dynamics of the Lorenz gas with random scatterers converges to the linear Boltzmann equation at low density on the kinetic time scale. Lanford [19] has proved that a truly many-body classical system, a low density gas with hard-core interaction, converges to the nonlinear Boltzmann equation for short macroscopic times.

Brownian motion was discovered and theorized in the context of classical dynamics. Since it postulates a microscopic Newtonian model for atoms and molecules, it is natural to replace the Newtonian dynamics with the Schrödinger dynamics and investigate if Brownian motion correctly describes the motion of a quantum particle in a random environment as well. One may of course take first the semiclassical limit, reduce the problem to the classical dynamics and then consider the scaling limit. This argument, however, does not apply to particles (or Lorenz scatterers) of size comparable with the Planck scale. It is physically more realistic and technically considerably more challenging to investigate the scaling limit of the quantum dynamics directly *without any semiclassical limit*. We shall prove that Brownian motion also describes the motion of a quantum particle in this situation. It is remarkable that the Schrödinger evolution, which is time reversible and describes wave phenomena, converges to a Brownian motion.

The random Schrödinger equation, or the quantum Lorentz model, is given by the evolution equation:

$$i\partial_t\psi_t(x) = H\psi_t(x), \quad H = H_\omega = -\frac{1}{2}\Delta_x + \lambda V_\omega(x) \quad (1)$$

where $\lambda > 0$ is the coupling constant and V_ω is the random potential.

The first time scale with a non-trivial limiting dynamics is the weak coupling limit, $\lambda \rightarrow 0$, where space and time are subject to kinetic scaling and the coupling constant scales as

$$t \rightarrow t\varepsilon^{-1}, \quad x \rightarrow x\varepsilon^{-1}, \quad \lambda = \sqrt{\varepsilon}. \quad (2)$$

Under this limit, the appropriately rescaled phase space density (Wigner distribution, see (10) later) of the solution to the Schrödinger evolution (1) converges weakly to a linear Boltzmann equation. This was first established by Spohn (1977) [25] if the random potential is a Gaussian random field and the macroscopic time is small.

This method was extended to study higher order correlations by Ho, Landau and Wilkins [13]. A different method was developed in [10] where the short time restriction was removed. This method was also extended to the phonon case in [9] and to the lattice case in [6].

For longer time scales, one expects a diffusive dynamics since the long time limit of a Boltzmann equation is a heat equation. We shall therefore take a time scale longer than in the weak coupling limit (2), i.e. we set $t \sim \lambda^{-2-\kappa}$, $\kappa > 0$. Our aim is to prove that the limiting dynamics of the Schrödinger evolution in a random potential under this scaling is governed by a heat equation. This problem requires to control the Schrödinger dynamics up to a time scale $\lambda^{-2-\kappa}$. This is a much harder task than first deriving the Boltzmann equation from Schrödinger dynamics on the kinetic scale and then showing that Boltzmann equation converges to a diffusive equation under a different limiting procedure. Quantum correlations that are small on the kinetic scale and are neglected in the first limit, may contribute on the longer time scale.

We consider two models in parallel. In the discrete setup we put the Schrödinger equation (1) on \mathbf{Z}^d , i.e. we work with the Anderson model [2]. Thus the kinetic energy operator on $\ell^2(\mathbf{Z}^d)$ is given by

$$(\Delta f)(x) := 2d f(x) - \sum_{|e|=1} f(x+e) \quad (3)$$

and the random potential is given by

$$V_\omega(x) = \sum_{\gamma \in \mathbf{Z}^d} V_\gamma(x), \quad V_\gamma(x) := v_\gamma \delta(x - \gamma) \quad (4)$$

where v_γ are real i.i.d. random variables and δ is the lattice delta function, $\delta(0) = 1$ and $\delta(y) = 0$, $y \neq 0$.

In the continuum model we consider the usual Laplacian, $-\frac{1}{2}\Delta_x$, as the kinetic energy operator on $L^2(\mathbf{R}^d)$. The random potential is given by

$$V_\omega(x) = \int_{\mathbf{R}^d} B(x-y) d\mu_\omega(y), \quad (5)$$

where μ_ω is a Poisson process $\{y_\gamma : \gamma = 1, 2, \dots\}$ on \mathbf{R}^d with unit density and i.i.d. random masses, v_γ , i.e. $\mu_\omega = \sum_\gamma v_\gamma \delta(\cdot - y_\gamma)$, and $B : \mathbf{R}^d \rightarrow \mathbf{R}$ is a smooth, radially symmetric function with rapid decay, with 0 in the support of \widehat{B} .

Since we investigate large distance phenomena, there should be no physical difference between the continuum and discrete models. On the technical level, the discrete model is more complicated due to the non-convexity of the energy surfaces of the discrete Laplacian in momentum space. However, the continuum model also has an additional technical difficulty: the large momentum regime needs a separate treatment.

Our proof builds upon the method initiated in [10]. In that paper the continuum model with a Gaussian random field was considered. Here we also consider the discrete model and non-Gaussian randomness, in order to demonstrate that these restrictions are not essential. On the Boltzmann scale this extension has also been achieved by Chen [6]. The other reason for working on the lattice as well is to make a connection with the extended state conjecture in the Anderson model.

We recall that the Anderson model was invented to describe the electric conduction properties of disordered metals. It was postulated by Anderson that for localized initial data the wave functions for large time are localized for large coupling constant λ and are extended for small coupling constant (away from the band edges and in dimension $d \geq 3$). The localization conjecture was first established rigorously by Goldsheid, Molchanov and Pastur [15] in one dimension, by Fröhlich-Spencer [12], and later by Aizenman-Molchanov [1] in several dimensions, and many other works have since contributed to this field. The extended state conjecture, however, has remained a difficult open problem and only very limited progress has been made.

Most approaches on extended states focused on the spectral property of the random Hamiltonian. It was proved by Klein [17] that all eigenfunctions are extended on the Bethe lattice. In Euclidean space, Schlag, Shubin and Wolff [24] proved that the eigenfunctions cannot be localized in a region smaller than $\lambda^{-2+\delta}$ for some $\delta > 0$ in $d = 2$. Chen [6], extending the method of [10] to the lattice case, proved that the eigenfunctions cannot be localized in a region smaller than λ^{-2} in any dimension $d \geq 2$ with logarithmic corrections. Lukkarinen and Spohn [21] have employed a similar technique for studying energy transport in a harmonic crystal with weakly perturbed random masses.

A special class of random Schrödinger equation was proposed to understand the dynamics in the extended region. Instead of random potential with i.i.d. random variables, one considers a random potential $V_\omega(x)$ with a power law decay, i.e.,

$$V_\omega(x) = h(x)\omega_x, \quad h(x) \sim |x|^{-\eta}$$

where ω_x are mean zero i.i.d. random variables and $\eta > 0$ is a fixed parameter.

If $\eta \geq 1$ a standard scattering argument yields that for λ small enough H_ω has absolutely continuous spectrum. Using cancellation properties of the random potential, Rodnianski and Schlag [22] have improved the same result to $\eta > 3/4$ in $d \geq 2$ and recently, J. Bourgain [4] has extended it to $\eta > 1/2$. For $\eta > 1/2$ the particle becomes essentially ballistic at large distances and there are only finitely many effective collisions.

In summary, in all known results [24, 22, 4, 6] for the Anderson model (or its modification) in Euclidean space the number of effective collisions are finite. In the scaling of the current work (13), the number of effective scatterings goes to infinity in the scaling limit, as it should be the case if we aim to obtain a Brownian motion.

As in [6], our dynamical result also implies that the eigenfunctions cannot be localized in a region smaller than $\lambda^{-2-\delta}$ for some $\delta > 0$ and dimension $d \geq 3$ (one can choose $\delta = \kappa/2$ with κ from Theorem 1). Though this result is the strongest in the direction of eigenfunction delocalization, we do not focus on it here.

Our main result is that the time reversible Schrödinger evolution with random impurities on a time scale $\lambda^{-2-\kappa}$ is described by a dissipative dynamics. In fact, this work is the first rigorous result where a heat equation is established from a time dependent quantum dynamics without first passing through a semiclassical limit.

In this contribution we explain the result and the key ideas in an informal manner. The complete proof is given in [11].

2 Statement of main result

We consider the discrete and the continuum models in parallel, therefore we work either on the d -dimensional lattice, \mathbf{Z}^d , or on the continuous space, \mathbf{R}^d . We always assume $d \geq 3$. Let

$$H_\omega := -\frac{1}{2}\Delta + \lambda V_\omega \quad (6)$$

denote a random Schrödinger operator acting on $\mathcal{H} = l^2(\mathbf{Z}^d)$, or $\mathcal{H} = L^2(\mathbf{R}^d)$. The kinetic energy operator and the random potential are defined in (3)–(5). We assume that $\mathbf{E}v_\gamma = \mathbf{E}v_\gamma^3 = 0$, $\mathbf{E}v_\gamma^2 = 1$ and $\mathbf{E}v_\gamma^{2d} < \infty$.

In the discrete case, the Fourier transform is given by

$$\widehat{f}(p) \equiv (\mathcal{F}f)(p) := \sum_{x \in \mathbf{Z}^d} e^{-2\pi i p \cdot x} f(x),$$

where $p = (p^{(1)}, \dots, p^{(d)}) \in \mathbf{T}^d := [-\frac{1}{2}, \frac{1}{2}]^d$. Sometimes an integral notation will be used for the normalized summation over any lattice $(\delta\mathbf{Z})^d$:

$$\int (\dots) dx := \delta^d \sum_{x \in (\delta\mathbf{Z})^d} (\dots).$$

The inverse Fourier transform is given by

$$(\mathcal{F}^{-1}\widehat{g})(x) = \int_{(\mathbf{T}/\delta)^d} \widehat{g}(p) e^{2\pi i p \cdot x} dp.$$

In the continuous case the Fourier transform and its inverse are given by

$$(\mathcal{F}f)(p) := \int_{\mathbf{R}^d} e^{-2\pi i p \cdot x} f(x) dx, \quad (\mathcal{F}^{-1}\widehat{g})(x) = \int_{\mathbf{R}^d} \widehat{g}(p) e^{2\pi i p \cdot x} dp.$$

We will discuss the two cases in parallel, in particular we will use the unified integral notations $\int (\dots) dx$ and $\int (\dots) dp$. The letters x, y, z will always be used for position space coordinates (hence elements of $(\delta\mathbf{Z})^d$ or \mathbf{R}^d). The letters p, q, r, u, v, w denote for d -dimensional momentum variables (elements of $(\mathbf{T}/\delta)^d$ or \mathbf{R}^d).

The Fourier transform of the kinetic energy operator is given by

$$\left(\mathcal{F} \left[-\frac{1}{2}\Delta \right] f \right) (p) = e(p) \widehat{f}(p).$$

The dispersion law, $e(p)$, is given by

$$e(p) := \sum_{i=1}^d (1 - \cos(2\pi p^{(i)})), \quad \text{and} \quad e(p) := \frac{1}{2} p^2$$

in the discrete and in the continuous case, respectively.

For $h : \mathbf{T}^d \rightarrow \mathbf{C}$ and an energy value $e \in [0, 2d]$ we introduce the notation

$$[h](e) := \int h(v) \delta(e - e(v)) dv := \int_{\Sigma_e} h(q) \frac{d\nu(q)}{|\nabla e(q)|} \quad (7)$$

where $d\nu(q) = d\nu_e(q)$ is the restriction of the d -dimensional Lebesgue measure to the level surface $\Sigma_e := \{q : e(q) = e\} \subset \mathbf{T}^d$. By the co-area formula it holds that

$$\int_0^{2d} [h](e) de = \int h(v) dv. \quad (8)$$

We define the projection onto the energy space of the free Laplacian by

$$\langle h(v) \rangle_e := \frac{[h](e)}{\Phi(e)}, \quad \text{where} \quad \Phi(e) := [1](e) = \int \delta(e - e(u)) du. \quad (9)$$

In the continuous case we define analogous formulas for any function $h : \mathbf{R}^d \rightarrow \mathbf{C}$ and energy value $e \geq 0$.

Define the *Wigner transform* of a function $\psi \in L^2(\mathbf{Z}^d)$ or $\psi \in L^2(\mathbf{R}^d)$ via its Fourier transform by

$$W_\psi(x, v) := \int e^{2\pi i w \cdot x} \overline{\widehat{\psi}\left(v - \frac{w}{2}\right)} \widehat{\psi}\left(v + \frac{w}{2}\right) dw.$$

In the lattice case the integration domain is the double torus $(2\mathbf{T})^d$ and x runs over the refined lattice, $x \in (\mathbf{Z}/2)^d$. For $\varepsilon > 0$ define the rescaled Wigner distribution as

$$W_\psi^\varepsilon(X, V) := \varepsilon^{-d} W_\psi\left(\frac{X}{\varepsilon}, V\right). \quad (10)$$

(with $X \in (\varepsilon\mathbf{Z}/2)^d$ in the lattice case).

The weak coupling limit is defined by the following scaling:

$$\mathcal{T} := \varepsilon t, \quad \mathcal{X} := \varepsilon x, \quad \varepsilon = \lambda^2. \quad (11)$$

In the limit $\varepsilon \rightarrow 0$ the Wigner distribution $W_{\psi_{\varepsilon^{-1}\mathcal{T}}}^\varepsilon(\mathcal{X}, \mathcal{V})$ converges weakly to the Boltzmann equation ([10], [6])

$$\left(\partial_{\mathcal{T}} + \frac{1}{2\pi} \nabla e(V) \cdot \nabla_{\mathcal{X}}\right) F_{\mathcal{T}}(\mathcal{X}, V) = \int dU \sigma(U, V) \left[F_{\mathcal{T}}(\mathcal{X}, U) - F_{\mathcal{T}}(\mathcal{X}, V) \right] \quad (12)$$

where $\frac{1}{2\pi} \nabla e(V)$ is the velocity. The collision kernel is given by

$$\sigma(U, V) := 2\pi \delta(e(U) - e(V)) \quad \text{discrete case}$$

$$\sigma(U, V) := 2\pi |\widehat{B}(U - V)|^2 \delta(e(U) - e(V)) \quad \text{continuous case}.$$

Note that the Boltzmann equation can be viewed as the generator of a Markovian semigroup on phase space. In particular, the validity of the Boltzmann equation shows that all correlation effects become negligible in this scaling limit.

Now we consider the long time scaling, i.e. with some $\kappa > 0$,

$$x = \lambda^{-\kappa/2-2} X = \varepsilon^{-1} X, \quad t = \lambda^{-\kappa-2} T = \varepsilon^{-1} \lambda^{-\kappa/2} T, \quad \varepsilon = \lambda^{\kappa/2+2} \quad (13)$$

Theorem 1. [Quantum Diffusion on Lattice] Let $d = 3$ and $\psi_0 \in \ell^2(\mathbf{Z}^d)$ be an initial wave function with $\widehat{\psi}_0 \in C^1(\mathbf{T}^d)$. Let $\psi(t) = \psi_{t,\omega}^\lambda$ solve the Schrödinger equation (1). Let $\widetilde{\mathcal{O}}(x, v)$ be a function on $\mathbf{R}^d \times \mathbf{T}^d$ whose Fourier transform in the first variable, denoted by $\mathcal{O}(\xi, v)$, is a C^1 function on $\mathbf{R}^d \times \mathbf{T}^d$ and

$$\int_{\mathbf{R}^d} d\xi \int dv |\mathcal{O}(\xi, v)| |\xi| \leq C. \quad (14)$$

Fix $e \in [0, 2d]$. Let f be the solution to the heat equation

$$\partial_T f(T, X, e) = \nabla_X \cdot D(e) \nabla_X f(T, X, e) \quad (15)$$

with the initial condition

$$f(0, X, e) := \delta(X) \left[|\widehat{\psi}_0(v)|^2 \right]_e$$

and the diffusion matrix D

$$D_{ij}(e) := \frac{\langle \sin(2\pi v^{(i)}) \cdot \sin(2\pi v^{(j)}) \rangle_e}{2\pi \Phi(e)} \quad i, j = 1, 2, 3. \quad (16)$$

Then for $\kappa < 1/2000$ and ε and λ related by (13), the Wigner distribution satisfies

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \int_{(\varepsilon \mathbf{Z})^d} dX \int_{\mathbf{R}^d} dv \widetilde{\mathcal{O}}(X, v) \mathbf{E} W_{\psi(\lambda - \kappa - 2T)}^\varepsilon(X, v) \\ = \int_{\mathbf{R}^d} dX \int_{\mathbf{R}^d} dv \widetilde{\mathcal{O}}(X, v) f(T, X, e(v)). \end{aligned} \quad (17)$$

By the symmetry of the measure $\langle \cdot \rangle_e$ under each sign flip $v_j \rightarrow -v_j$ we see that $D(e)$ is a constant times the identity matrix:

$$D_{ij}(e) = D_e \delta_{ij}, \quad D_e := \frac{\langle \sin^2(2\pi v^{(1)}) \rangle_e}{2\pi \Phi(e)},$$

in particular we see that the diffusion is nondegenerate.

The diffusion matrix can also be obtained from the long time limit of the Boltzmann equation (12). For any fixed energy e , let

$$L_e f(v) := \int du \sigma(u, v) [f(u) - f(v)], \quad e(v) = e, \quad (18)$$

be the generator of the momentum jump process on Σ_e with the uniform stationary measure $\langle \cdot \rangle_e$. The diffusion matrix in general is given by the velocity autocorrelation function

$$D_{ij}(e) = \int_0^\infty dt \langle \sin(2\pi v^{(i)}(t)) \cdot \sin(2\pi v^{(j)}(0)) \rangle_e, \quad (19)$$

where $v(t)$ is the process generated by L_e . Since the collision kernel $\sigma(U, V)$ is uniform, the correlation between $v(t)$ and $v(0)$ vanishes after the first jump and we obtain (16), using

$$\int du \sigma(u, v) = 2\pi\Phi(e), \quad e(v) = e.$$

The result in the continuum case is analogous. The diffusion matrix is again a constant times the identity matrix, $D_{ij}(e) = D_e\delta_{ij}$, and D_e is again given by the velocity autocorrelation function

$$D_e := \frac{1}{3(2\pi)^2} \int_0^\infty dt \langle v(t) \cdot v(0) \rangle_e \quad (20)$$

using the spatial isotropy. In this case D_e cannot be computed as a simple integral since the outgoing velocity u in the transition kernel $\sigma(u, v)$ of the momentum process depends on the direction of v .

Theorem 2. [Quantum Diffusion on \mathbf{R}^d] Let $d = 3$ and $\psi_0 \in L^2(\mathbf{R}^d)$ be an initial wave function with $|\widehat{\psi}_0(v)|^2|v|^N \in L^2$ for a sufficiently large N .

Let $\psi(t) = \psi_{t,\omega}^\lambda$ solve the Schrödinger equation (1). Let $\tilde{\mathcal{O}}(x, v)$ be a function whose Fourier transform in x , denoted by $\mathcal{O}(\xi, v)$, is a C^1 function on $\mathbf{R}^d \times \mathbf{R}^d$ and

$$\iint d\xi dv |\mathcal{O}(\xi, v)| |\xi| \leq C. \quad (21)$$

Let $e > 0$ and let f be the solution to the heat equation

$$\partial_T f(T, X, e) = D_e \Delta_X f(T, X, e) \quad (22)$$

with diffusion constant D_e given in (20) and with the initial condition

$$f(0, X, e) := \delta(X) \left[|\widehat{\psi}_0(v)|^2 \right] (e).$$

Then for $\kappa < 1/500$ and ε and λ related by (13), the Wigner distribution satisfies

$$\begin{aligned} \lim_{\varepsilon \rightarrow 0} \iint_{\mathbf{R}^d \times \mathbf{R}^d} dX dv \tilde{\mathcal{O}}(X, v) \mathbf{E} W_{\psi(\lambda^{-\kappa-2T})}^\varepsilon(X, v) \\ = \iint_{\mathbf{R}^d \times \mathbf{R}^d} dX dv \tilde{\mathcal{O}}(X, v) f(T, X, e(v)). \end{aligned} \quad (23)$$

The main tool of our proof is to use the Duhamel expansion to decompose the wave function into elementary wavefunctions characterized by their collision histories with the random obstacles. Assume for the moment that the randomness is Gaussian and high order expectations can be computed by Wick pairing. The higher order cumulants arising from a non-Gaussian randomness turn out to be negligible by a separate argument. Therefore, when computing the expectation of a product involving ψ and $\bar{\psi}$ (e.g. $\mathbf{E} W_\psi$), we pair the obstacles in the collision histories of ψ and $\bar{\psi}$ and we thus generate Feynman graphs.

If we take only the Laplacian as the free part in the expansion, even the amplitudes of individual graphs diverge in the limit we consider. However, this can be remedied by a simple resummation of all two-legged insertions caused by the lowest order self-energy contribution. The resummation is performed by choosing an appropriate reference Hamiltonian H_0 for the expansion. After this rearrangement, all

graphs have a finite amplitude in our scaling limit, and the so-called ladder graphs give the leading contribution.

Each non-ladder graph has a vanishing amplitude as $\lambda \rightarrow 0$ due to oscillatory integrals, in contrast to the ladder graphs where no oscillation is present. However, the number of non-ladder graphs grows as $k!$, where $k \sim \lambda^2 t \sim \lambda^{-\kappa}$ is the typical number of collisions. To beat this factorial growth, we need to give a very sharp bound on the individual graphs.

We give a classification of arbitrary large graphs, based on counting the number of vertices carrying oscillatory effects. The number of these vertices is called the *degree* of the graph. For the ladder graphs, the degree is zero. For general graphs, the degree is roughly the number of vertices after removing all ladder and anti-ladder subgraphs. We thus obtain an extra λ^c power (for some $c > 0$) *per non-(anti)ladder vertex*. This strong improvement is sufficient to beat the growth of the combinatorics in the time scale we consider. To our knowledge, nothing like this has been done in a graphical expansion before.

For a comparison, the unperturbed Green functions in the perturbation expansion for the many-fermion systems for small temperature and for the random Schrödinger equation for large time are given by

$$\frac{1}{ip_0 + p^2 - \mu}, \quad \frac{1}{p^2 - \alpha + i\eta}.$$

In the many-fermion case, $p_0 \in M_F = \{\frac{\pi}{\beta}(2n+1) : n \in \mathbf{Z}\}$ where $\beta \sim T^{-1}$ is the inverse temperature. In the random Schrödinger case, $\eta \sim t^{-1}$. Their L^2 properties are different:

$$\frac{1}{\beta} \sum_{p_0 \in M_F} \int dp |ip_0 + p^2 - \mu|^{-2} \sim |\log \beta|, \quad \int dp |p^2 - \alpha + i\eta|^{-2} \sim \eta^{-1}$$

Notice the divergence is more severe for the random Schrödinger equation case.

Finally we note that the threshold $\kappa < 1/2000$ in our theorem can be significantly improved with more detailed arguments. However, one cannot go beyond $\kappa = 2$ with only improvements on estimates of the individual graphs. The Duhamel formula must be expanded at least up to $k = \lambda^2 t = \lambda^{-\kappa}$, which is the typical number of collisions up to time t . Even if one proves for most graphs the best possible estimate, λ^{2k} , it cannot beat the $k!$ combinatorics when $k \gg \lambda^{-2}$, i.e., $\lambda^{2k} k! \gg 1$ for $k \gg \lambda^{-2}$. A different resummation procedure is needed beyond this threshold to exploit cancellations among these graphs.

3 Sketch of the proof

We present the main ideas of the proof for the lattice case and comment on the modifications for the continuous case.

3.1 Renormalization

Before expanding the solution of the Schrödinger equation (1) via the Duhamel formula, we perform a renormalization of the "one-particle propagator" by splitting

the Hamiltonian as $H = H_0 + \tilde{V}$, with H_0 already containing the part of the self-energy produced by immediate recollisions with the same obstacle. This effectively resums all such immediate recollisions.

Let $\theta(p) := \Theta(e(p))$, where $\Theta(\alpha) := \lim_{\varepsilon \rightarrow 0^+} \Theta_\varepsilon(\alpha)$ and

$$\Theta_\varepsilon(\alpha) := \int \frac{1}{\alpha - e(q) + i\varepsilon} dq. \quad (24)$$

We have

$$\text{Im } \Theta(\alpha) = -\pi\Phi(\alpha) \quad (25)$$

with Φ defined in (9).

We rewrite the Hamiltonian as $H = H_0 + \tilde{V}$ with

$$H_0 := \omega(p) := e(p) + \lambda^2\theta(p), \quad \tilde{V} := \lambda V - \lambda^2\theta(p). \quad (26)$$

Our renormalization includes only the lowest order self-energy. This suffices on the time scales we consider.

3.2 The Expansion and the Stopping Rules

Iterating the Duhamel formula

$$e^{-itH} = e^{-itH_0} - i \int_0^t ds e^{-i(t-s)H} \tilde{V} e^{-isH_0} \quad (27)$$

gives for any fixed integer $N \geq 1$

$$\psi_t := e^{-itH} \psi_0 = \sum_{n=0}^{N-1} \psi_n(t) + \Psi_N(t), \quad (28)$$

with

$$\psi_n(t) := (-i)^n \int_0^t [ds_j]_1^{n+1} e^{-is_{n+1}H_0} \tilde{V} e^{-is_n H_0} \tilde{V} \dots \tilde{V} e^{-is_1 H_0} \psi_0 \quad (29)$$

being the fully expanded terms and

$$\Psi_N(t) := (-i) \int_0^t ds e^{-i(t-s)H} \tilde{V} \psi_{N-1}(s) \quad (30)$$

is the non-fully expanded or error term. We used the shorthand notation

$$\int_0^t [ds_j]_1^n := \int_0^t \dots \int_0^t \left(\prod_{j=1}^n ds_j \right) \delta\left(t - \sum_{j=1}^n s_j\right).$$

Since each potential \tilde{V} in (29), (30) is a summation itself, $\tilde{V} = -\lambda^2\theta(p) + \lambda \sum_\gamma V_\gamma$, both of these terms in (29) and (30) are actually big summations over so-called elementary wavefunctions, which are characterized by their collision history, i.e. by a sequence of obstacles labelled by $\gamma \in \mathbf{Z}^d$ and a label ϑ corresponding to an insertion of $-\lambda^2\theta(p)$.

Because this expansion is generated by iteration of (27), the sequences defining collision histories can be obtained recursively. This allows us to refine the Duhamel expansion by using stopping rules that depend on the type of collision history. We call a sequence *nonrepetitive* if the only repetitions in potential labels γ occur in gates (immediate recollisions). The iteration of (27) is stopped when adding a new entry to the sequence makes it violate this condition. This can happen because of a recollision, a nested recollision, or a triple collision. The precise definition of these recollision types is given in [11]. The iteration is also stopped when the last entry in the sequence causes the total number of gates and ϑ 's to reach 2. If the sequence stays nonrepetitive and the total number of gates and ϑ 's stays below 2, the iteration is stopped when the number of non-gate potential labels reaches

$$K = \lambda^{-\delta}(\lambda^2 t). \quad (31)$$

Note that K is much bigger than the expected typical number of collisions, $\lambda^2 t$.

We denote the sum of the truncated elementary non-repetitive wave functions with at most one λ^2 power from the non-skeleton indices or ϑ 's and with K skeleton indices by $\psi_{*s,K}^{(\leq 1),nr}$. The superscript (≤ 1) refers to the number of gates and ϑ 's, each of which gives a factor λ^2 . By this splitting, we arrive at the following modified Duhamel formula, in which all non-error terms are nonrepetitive.

Proposition 1. [Duhamel formula] *For any $K \geq 1$ we have*

$$\begin{aligned} \psi_t = e^{-itH} \psi_0 &= \sum_{k=0}^{K-1} \psi_{t,k}^{(\leq 1),nr} \\ &+ \int_0^t ds e^{-i(t-s)H} \left\{ \psi_{*s,K}^{(\leq 1),nr} + \sum_{k=0}^K \left(\psi_{*s,k}^{(2),last} + \psi_{*s,k}^{(\leq 1),rec} + \psi_{*s,k}^{(\leq 1),nest} + \psi_{*s,k}^{(\leq 1),tri} \right) \right\} \end{aligned} \quad (32)$$

The terms under the integral correspond to the various stopping criteria indicated above. For the precise definition of the corresponding wave functions, see [11].

The main contribution comes from the non-repetitive sequences with $k < K$, i.e. from the first term in (32). The estimate of the terms in the second line (32) first uses the unitarity of the full evolution

$$\left\| \int_0^t ds e^{-i(t-s)H} \psi_s^\# \right\| \leq t \cdot \sup_{s \leq t} \|\psi_s^\#\|. \quad (33)$$

For $\# = rec, nest, tri$ we will use the fact the Feynman graphs arising in the expectation $\mathbf{E} \|\psi_s^\#\|^2$ contain an additional oscillatory factor, which renders them smaller than the corresponding non-repetitive term. It turns out that the oscillation effect from one single recollision, nest or triple collision is already sufficient to overcome the additional factor t arising from the crude bound (33). This fact relies on estimates on singular integrals concentrating on the energy level sets Σ_e . It is a well-known fact from harmonic analysis, that such singular integrals can more effectively be estimated for convex level sets. This is why the non-convexity of the energy shells is a major technical complication for the discrete model in comparison with the continuous case, where the level sets are spheres.

Non-skeleton labels also give rise to a smallness effect due to a cancellation between gates and ϑ 's, however, one such cancellation would not be sufficient to beat

the t -factor. This is why at least two such cancellations are necessary in $\psi_{*s,k}^{(2),last}$. Finally, the term $\psi_{*s,K}^{(\leq 1),nr}$ is small because it has unusually many collisions, thanks to the additional factor $\lambda^{-\delta}$ in the definition of K .

In this exposition we focus only on the non-repetitive terms, $\psi_{t,k}^{(\leq 1),nr}$, because estimating them involves the main new ideas. The error terms are estimated by laborious technical modifications of these ideas.

3.3 The L^2 norm of the non-repetitive wavefunction

We first estimate the L^2 norm of the fully expanded wave function with no gates or ϑ , $\psi_{t,k}^{(0),nr}$. This is the core of our analysis.

Feynman Graphs

The wavefunction

$$\psi_{t,k}^{(0),nr} = \sum_{\gamma} \int_0^t [ds_j]_1^{k+1} e^{-is_{k+1}H_0} V_{\gamma_k} e^{-is_k H_0} V_{\gamma_{k-1}} \dots e^{-is_2 H_0} V_{\gamma_1} e^{-is_1 H_0} \psi_0$$

where the summation is over all sequences for which the potential labels γ_i are all different. Therefore every term in

$$\mathbf{E} \|\psi_{t,k}^{(0),nr}\|^2 = \sum_{\gamma, \gamma'} \mathbf{E} \int \overline{\psi_{t,\gamma}} \psi_{t,\gamma'}$$

has $2k$ potential terms, and their expectation,

$$\mathbf{E} \overline{V_{\gamma_1} V_{\gamma_2} \dots V_{\gamma_k} V_{\gamma'_1} V_{\gamma'_2} \dots V_{\gamma'_k}},$$

is zero, using $\mathbf{E} V_{\gamma} = 0$, unless the potentials are paired. Since there is no repetition within γ and γ' , all these pairings occur between γ and γ' , therefore every pairing corresponds to a permutation on $\{1, 2, \dots, k\}$. The set of such permutations is denoted by \mathcal{P}_k and they can be considered as a map between the indices of the γ and γ' labels.

We recall the following identity from Lemma 3.1 of [10]

$$\int_0^t [ds_j]_1^{k+1} \prod_{j=1}^{k+1} e^{-is_j \omega(p_j)} = \frac{i e^{\eta t}}{2\pi} \int_{\mathbf{R}} d\alpha e^{-i\alpha t} \prod_{j=1}^{k+1} \frac{1}{\alpha - \omega(p_j) + i\eta}$$

for any $\eta > 0$. We will choose $\eta := t^{-1}$. Therefore, we have

$$\begin{aligned} \mathbf{E} \|\psi_{t,k}^{(0),nr}\|^2 &= \frac{\lambda^{2k} e^{2t\eta}}{(2\pi)^2} \sum_{\sigma \in \mathcal{P}_k} \sum_{\substack{\gamma_1, \dots, \gamma_k \\ \gamma_i \neq \gamma_j}} \int d\mathbf{p} d\tilde{\mathbf{p}} \delta(p_{k+1} - \tilde{p}_{k+1}) \\ &\times \mathbf{E} \prod_{j=1}^k \overline{\widehat{V}_{\gamma_j}(p_{j+1} - p_j)} \widehat{V}_{\gamma_j}(\tilde{p}_{\sigma(j)+1} - \tilde{p}_{\sigma(j)}) M(k, \mathbf{p}, \tilde{\mathbf{p}}, \eta) \overline{\widehat{\psi}_0(p_1)} \widehat{\psi}_0(\tilde{p}_1) \end{aligned} \quad (34)$$

with $\mathbf{p} = (p_1, p_2, \dots, p_{k+1})$, $\int d\mathbf{p} := \int_{(\mathbb{T}^d)^{k+1}} dp_1 dp_2 \dots dp_{k+1}$, similarly for $\tilde{\mathbf{p}}$ and $d\tilde{\mathbf{p}}$, and

$$M_\eta(k, \mathbf{p}, \tilde{\mathbf{p}}) := \int \int_{\mathbf{R}} d\alpha d\beta e^{i(\alpha-\beta)t} \left(\prod_{j=1}^{k+1} \frac{1}{\alpha - \bar{\omega}(p_j) - i\eta} \frac{1}{\beta - \omega(\tilde{p}_j) + i\eta} \right). \quad (35)$$

We compute the expectation:

$$\mathbf{E} \prod_{j=1}^k \overline{\widehat{V}_{\gamma_j}(p_{j+1} - p_j)} \widehat{V}_{\gamma_j}(\tilde{p}_{\sigma(j)+1} - \tilde{p}_{\sigma(j)}) = \sum_{\substack{\gamma_1, \dots, \gamma_k \\ \gamma_i \neq \gamma_j}} \prod_{j=1}^k e^{i\gamma_j(p_{j+1} - p_j - (\tilde{p}_{\sigma(j)+1} - \tilde{p}_{\sigma(j)})}. \quad (36)$$

In the continuous model this formula also contains a product of \widehat{B} -terms, where B was the single site potential function in (5). These factors are included into the definition of M_η . Most importantly, they provide the necessary decay in the momentum variables in the case of non-compact momentum space. A similar idea was used in [10].

Due to the restriction $\gamma_i \neq \gamma_j$, (36) is not a simple product of delta functions in the momenta. We have to use a connected graph expansion that is well known in the polymer expansions of field theory (see, e.g. [23]). We do not give the details here, we only note that the result is a weighted sum over partitions of the index set $\{1, \dots, k\}$. Each term in the sum is a product of delta functions labelled by the lumps of the partition and each delta function imposes the Kirchoff Law for the incoming and outgoing momenta of the lump and its σ -image. The trivial partition, where each lump has a single element, carries the main contribution. Estimating the terms with nontrivial partitions can be reduced to estimates for the trivial partition [11]. We therefore discuss only the contribution from the trivial partition to $\mathbf{E} \|\psi_{t,k}^{(0),nr}\|^2$, given by $\sum_{\sigma \in \mathcal{P}_k} V_\eta(k, \sigma)$, where

$$V_\eta(k, \sigma) := \frac{\lambda^{2k} e^{2t\eta}}{(2\pi)^2} \int d\mathbf{p} d\tilde{\mathbf{p}} M_\eta(k, \mathbf{p}, \tilde{\mathbf{p}}) \delta(\tilde{p}_{k+1} - p_{k+1}) \overline{\widehat{\psi}_0(p_1)} \widehat{\psi}_0(\tilde{p}_1) \\ \times \prod_{i=1}^k \delta(p_{i+1} - p_i - (\tilde{p}_{\sigma(i)+1} - \tilde{p}_{\sigma(i)})) \quad (37)$$

This complicated formula can be encoded by a Feynman graph and $V_\eta(k, \sigma)$ is called the value or amplitude of the graph. The Feynman graph for the trivial partition corresponds to the usual Feynman graphs for the Gaussian case discussed in [10] and we briefly describe their construction. A Feynman graph consists of two directed horizontal lines (upper and lower) with k collision vertices on each that represent the collision histories of $\bar{\psi}$ and ψ , respectively. These two lines are joined at the two ends. This corresponds to evaluating the L^2 -norm on one end and inserting the initial wavefunction ψ_0 on the other end. Each horizontal segment carries a momentum, p_1, p_2, \dots, p_{k+1} and $\tilde{p}_1, \tilde{p}_2, \dots, \tilde{p}_{k+1}$ and a corresponding (renormalized) propagator, $(\alpha - \bar{\omega}(p_j) - i\eta)^{-1}$ and $(\beta - \omega(\tilde{p}_j) + i\eta)^{-1}$. Here α and β are the dual variables to the time on each line and they will be integrated out, see (35). Finally, the collision vertices are paired. Each pairing line joins an upper and a lower vertex and thus can be encoded with a permutation $\sigma \in \mathcal{P}_k$. It is useful to think of the

momenta as flowing through the lines of the graph. The delta function associated to each pairing line in the value of the graph (37) then expresses the Kirchoff Law for the flow of momenta adjacent to the two vertices.

A typical graph with trivial partition is shown on Fig. 1. For the special case of

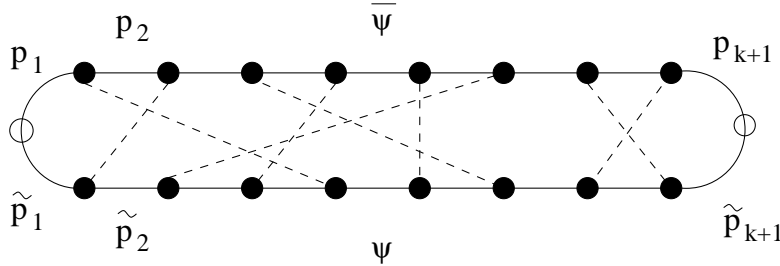


Fig. 1. Typical Feynman graph with no lumps

the identity permutation $\sigma = id$ we obtain the so-called ladder graph (Fig. 2). The following proposition shows that the ladder gives the main contribution.

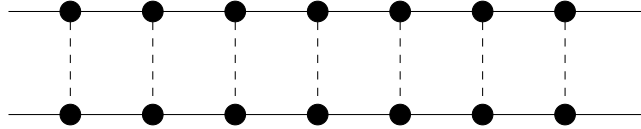


Fig. 2. Ladder graph

The Main Contribution is the Ladder

Proposition 2 (L^2 -estimate). *Let $\eta^{-1} := t$, $t = O(\lambda^{2+\kappa})$ and $k \leq K := \lambda^{-\delta}(\lambda^2 t)$. For sufficiently small λ , κ and δ there exists a positive number $c_1(\kappa, \delta)$ such that*

$$\mathbf{E} \|\psi_{t,k}^{(0),nr}\|^2 = V_\eta(k, id) + O_\delta\left(\lambda^{c_1(\kappa, \delta)}\right). \tag{38}$$

The threshold values for κ, δ and the explicit form of $c_1(\kappa, \delta)$ are found in [11].

Sketch of the proof. As mentioned above, we discuss only how to estimate the contributions from the trivial partition, but for an arbitrary permutation σ .

Given a permutation $\sigma \in \mathcal{P}_k$, we define a $(k+1) \times (k+1)$ matrix $M = M(\sigma)$ as follows

$$M_{ij}(\sigma) := \begin{cases} 1 & \text{if } \tilde{\sigma}(j-1) < i \leq \tilde{\sigma}(j) \\ -1 & \text{if } \tilde{\sigma}(j) < i \leq \tilde{\sigma}(j-1) \\ 0 & \text{otherwise} \end{cases} \tag{39}$$

where, by definition, $\tilde{\sigma}$ is the extension of σ to a permutation of $\{0, 1, \dots, k+1\}$ by $\tilde{\sigma}(0) := 0$ and $\tilde{\sigma}(k+1) := k+1$. It is easy to check that

$$V_\eta(k, \sigma) := \frac{\lambda^{2k} e^{2t\eta}}{(2\pi)^2} \int d\mathbf{p} d\tilde{\mathbf{p}} M_\eta(k, \mathbf{p}, \tilde{\mathbf{p}}) \prod_{i=1}^{k+1} \delta\left(\tilde{p}_i - \sum_{j=1}^{k+1} M_{ij} p_j\right), \quad (40)$$

in other words, the matrix M encodes the dependence of the \tilde{p} -momenta on the p -momenta. This rule is transparent in the graphical representation of the Feynman graph: the momentum p_j appears in those \tilde{p}_i 's which fall into its "domain of dependence", i.e. the section between the image of the two endpoints of p_j , and the sign depends on the ordering of these images (see Fig. 3)

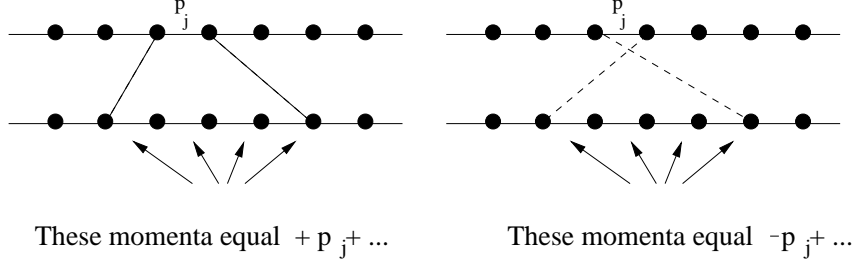


Fig. 3. Domain of momenta dependencies

The matrix $M(\sigma)$ has several properties that follow easily from this structure:

Lemma 1. *For any permutation $\sigma \in \mathcal{P}_k$ the matrix $M(\sigma)$ is*

- (i) invertible;
- (ii) totally unimodular, i.e. any subdeterminant is 0 or ± 1 .

The following definition is crucial. It establishes the necessary concepts to measure the complexity of a permutation.

Definition 1 (Valley, peak and slope). *Given a permutation $\sigma \in \mathcal{P}_k$ let $\tilde{\sigma}$ be its extension. A point $(j, \sigma(j))$, $j \in I_k := \{1, 2, \dots, k\}$, on the graph of σ is called **peak** if $\tilde{\sigma}(j-1) > \sigma(j) < \tilde{\sigma}(j+1)$, it is called **valley** if $\tilde{\sigma}(j-1) < \sigma(j) > \tilde{\sigma}(j+1)$, otherwise it is called **slope**. Additionally, the point $(k+1, k+1)$ is also called valley. The set $I = \{1, 2, \dots, k+1\}$ is partitioned into three disjoint subsets, $I = I_v \cup I_p \cup I_s$, such that $i \in I_v, I_p$ or I_s depending on whether $(\tilde{\sigma}^{-1}(i), i)$ is a valley, peak or slope, respectively. Finally, an index $i \in I_v \cup I_s$ is called **ladder index** if $|\tilde{\sigma}^{-1}(i) - \tilde{\sigma}^{-1}(i-1)| = 1$. The set of ladder indices is denoted by $I_\ell \subset I$ and their cardinality is denoted by $\ell = \ell(\sigma) := |I_\ell|$. The number of non-ladder indices, $d(\sigma) := k+1 - \ell(\sigma)$ is called the **degree** of the permutation σ .*

Remarks: (i) The terminology of peak, valley, slope, ladder comes from the graph of the permutation $\tilde{\sigma}$ viewed as a function on $\{0, 1, \dots, k+1\}$ in a coordinate system where the vertical axis is oriented downward.

(ii) For $\sigma = id$ we have $I_p = \emptyset$, $I_s = \{1, 2, \dots, k\}$, $I_v = \{k+1\}$ and $I_\ell = \{1, 2, \dots, k+1\}$. In particular, $d(id) = 0$ and $d(\sigma) > 0$ for any other permutation $\sigma \neq id$.

The following theorem shows that the degree of the permutation $d(\sigma)$ measures the size of $V_\eta(k, \sigma)$. This is the key theorem in our method and we will sketch its proof separately in Section 3.4.

Theorem 3. *Let $\eta^{-1} := t$, $t = O(\lambda^{2+\kappa})$ with a sufficiently small κ . Let $\sigma \in \mathcal{P}_k$ and assume that $k \leq K = \lambda^{-\delta}(\lambda^2 t)$. For sufficiently small κ and δ there exists $c_2(\kappa, \delta) > 0$ such that*

$$|V_\eta(k, \sigma)| \leq \left(C \lambda^{c_2(\kappa, \delta)} \right)^{d(\sigma)}, \quad \lambda \ll 1. \quad (41)$$

This theorem is complemented by the following lemma:

Lemma 2. *Let $k = O(\lambda^{-\kappa-\delta})$, $d > 0$ integer and let $\gamma > \kappa + \delta$. Then*

$$\sum_{\substack{\sigma \in \mathcal{P}_k \\ d(\sigma) \geq d}} \lambda^{\gamma d(\sigma)} \leq O\left(\lambda^{d(\gamma - \kappa - \delta)} \right) \quad (42)$$

for all sufficiently small λ .

The proof follows from the combinatorial estimate on the number of permutations with a given degree:

$$\#\{\sigma \in \mathcal{P}_k : d(\sigma) = d\} \leq (Ck)^d.$$

From Theorem 3 and Lemma 2 we immediately obtain an estimate on the contribution of the trivial lumps to $\mathbf{E} \|\psi_{t,k}^{(0),nr}\|^2$ if κ and δ are sufficiently small:

$$\sum_{\substack{\sigma \in \mathcal{P}_k \\ \sigma \neq id}} |V_\eta(k, \sigma)| \leq O_\delta \left(\lambda^{c_3(\kappa, \delta)} \right) \quad (43)$$

with some appropriate $c_3(\kappa, \delta) > 0$.

3.4 Sketch of the proof of the main technical theorem

In this section we explain the proof of Theorem 3. We set

$$E_\eta(M) := \lambda^{2k} \int \int_{-4d}^{4d} d\alpha d\beta \int d\mathbf{p} \prod_{i=1}^{k+1} \frac{1}{|\alpha - \bar{\omega}(p_i) - i\eta|} \prod_{j=1}^{k+1} \frac{1}{|\beta - \omega(\sum_{\ell=1}^{k+1} M_{j\ell} p_\ell) + i\eta|}. \quad (44)$$

For the continuous model, the definition includes the \widehat{B} factors to ensure the integrability for the large momentum regime. It is easy to check that $V_\eta(k, \sigma)$ is estimated by $E_\eta(M(\sigma))$ modulo constant factors and negligible additive terms coming from the regime where α or β is big.

The denominators in this multiple integral are almost singular in certain regimes of the high dimensional space of all momenta. The main contribution comes from the overlap of these singularities. The overlap structure is encoded in the matrix M , hence in the permutation σ , in a very complicated entangled way. Each variable p_j may appear in many denominators in (44), so successive integration seems very difficult. We could not find the exact order (as a power of λ) of this multiple integral but we conjecture that true order is essentially $\lambda^{2d(\sigma)}$. Our goal in Theorem 3 is to

give a weaker bound of order $\lambda^{cd(\sigma)}$, i.e. that is still a λ -power linear in the degree, but the coefficient considerably smaller than 2.

Notice that the α -denominators in (44) correspond to the columns of M and the β -denominators corresponds to the rows. For this presentation we will use j to label row indices and i to label column indices. We recall the sets I_v, I_p, I_ℓ from Definition 1 and we will view these sets as subsets of the row indices of M .

First we notice that if $j \in (I_\ell \setminus I_v)$, i.e. j is a non-valley ladder row, then there exists a column index $i = c(j)$ such that the momentum p_i appears only in the j -th β -denominator. In other words, the i -th column of M has a single nonzero element (that is actually ± 1) and it is in the j -th row. Therefore the dp_i integral can be performed independently of the rest of the integrand by using the following elementary but quite involved bound for small κ :

$$\sup_{w, \alpha, \beta} \int_{\mathbb{T}^d} dp_i \frac{\lambda^2}{|\alpha - \bar{\omega}(p_i) - i\eta| |\beta - \omega(\pm p_i + w) + i\eta|} \leq 1 + O(\lambda^{1/4}). \quad (45)$$

Note that the constant of the main term is exactly 1. This fact is important, since in graphs with low degree this estimate has to be raised to a power $|I_\ell \setminus I_v|$ that may be comparable with k . Clearly for $k \leq K \sim \lambda^{-\kappa-\delta}$ and $\kappa + \delta < 1/4$ we have

$$\left(1 + O(\lambda^{1/4})\right)^k \leq \text{const}, \quad (46)$$

but had 1 been replaced with a bigger constant in (45), we would obtain an exponentially big factor $(\text{const})^k$ that would not be affordable. The precise constant 1 in the estimate (45) is related to the appropriate choice of the renormalization $\theta(p)$ in $\omega(p)$.

After the non-valley ladder rows are integrated out, and the corresponding rows and columns are removed from the matrix M , we obtain a smaller matrix $M^{(1)}$ describing the remaining denominators. In $M^{(1)}$ we keep the original labelling of the rows from M .

Now we estimate some of the β -denominators in (44) by L^∞ norm, i.e. by η^{-1} . This is a major overestimate, but these denominators are chosen in such a way that the entangled structure imposed by M becomes much simpler and many other denominators can be integrated out by L^1 -bounds that are only logarithmic in λ .

We start with estimating all β -denominators in rows $j \in I_p$ by the trivial L^∞ -norm. The corresponding rows are removed from $M^{(1)}$, in this way we obtain a matrix $M^{(2)}$. Let

$$I^* := I \setminus \left(I_p \cup (I_\ell \setminus I_v) \right)$$

be the remaining row indices after removing the peaks and the non-valley ladders.

Then we inspect the remaining rows $j \in I^*$ of $M^{(2)}$ in increasing order. The key observation is that for each $j \in I^*$ there exists a column index, $i = c(j)$, such that the variable p_i appears **only** in the j -th β -denominator, provided that all β -denominators with $j' < j$ have already been integrated out. In view of the structure of $M^{(1)}$, it means that for any $j \in I^*$ there exists a column $i = c(j)$ such that the only nonzero element among $\{M_{ij'}^{(2)} : j' \geq j\}$ is $M_{ij}^{(2)}$. This fact follows from the structure of $M(\sigma)$ and from the fact that all rows with $j \in I_p$ have been removed.

This property allows us to remove each remaining β -denominator, one by one, by estimating integrals of the type

$$\int_{\mathbf{T}^d} dp_i \frac{1}{|\alpha - \bar{\omega}(p_i) - i\eta|} \frac{1}{|\beta - \omega(\pm p_i + w) + i\eta|} \leq \frac{C\eta^{-\tau}}{|w|}, \quad (47)$$

where w is a linear combination of momenta other than p_i . The absolute value $|w|$ is interpreted as the distance of w from the nearest critical point of the dispersion relation $e(p)$. The variable p_i at this stage of the procedure appears only in these two denominators.

The exponent τ can be chosen zero (with logarithmic corrections) for the continuous model and this fact has already been used in [10]. For the discrete model we can prove (47) with $\tau = 3/4 + 2\kappa$ and we know that the exponent cannot be better than $1/2$. The reason for the weaker estimate is the lack of convexity of the level set Σ_e . Replacing $\omega(p)$ with $e(p)$ for a moment, the inequality (47) with $\tau = 0$ essentially states that the level set $\{\alpha = e(p)\}$ and its shifted version $\{\beta = e(p+w)\}$ intersect each other transversally, unless w is close to zero. Indeed, the transversal intersection guarantees that the volume of the p values, where *both* denominators are of order η , is of order η^2 . Then a standard argument with dyadic decomposition gives the result with a logarithmic factor. For translates of spheres the transversal intersection property holds, unless $w \sim 0$. However, in certain points of the level sets Σ_e of the discrete dispersion relation the curvature vanishes, in fact Σ_e even contains straight lines for $2 \leq e \leq 4$. The transversal intersection fails in certain regions and results in a weaker bound.

Neglecting the point singularity $|w|^{-1}$ in (47) for a moment (see Section 3.5 later), we easily see that with this algorithm one can bound $E_\eta(M(\sigma))$ by $\lambda^{2(k-q)}\eta^{-p}\eta^{-\tau(k-p-q)}$, modulo logarithmic factors, where $p = |I_p|$ is the number of peak indices and $q := |I_\ell \setminus I_v|$ is the number of non-valley ladder indices. From the definitions it follows that the sets I_v , I_p and $I_\ell \setminus I_v$ are disjoint and $|I_v| = p+1$. Thus we have $2p+1+q \leq k+1$. Therefore

$$\lambda^{2(k-q)}\eta^{-p(1-\tau)-\tau(k-q)} \leq (\lambda^4 t^{\tau+1})^{(k-q)/2} \leq (\lambda^4 t^{\tau+1})^{\frac{1}{2}[d(\sigma)-1]} \quad (48)$$

since $q \leq \ell$. If $\tau < 1$, then with a sufficiently small κ we see that $\lambda^4 t^{\tau+1}$ is a positive power of λ . Thus we obtain a bound where the exponent of λ is linear in $d(\sigma)$. With a more careful estimate one can remove the additional -1 in the exponent. In particular, for the continuous case with $\tau = 0$ this argument works up to $\kappa < 2$.

We end this section with a remark. Apparently the bound $\kappa < 2$ (or, equivalently, $t \ll \lambda^{-4}$) shows up in two different contexts in this argument. To avoid misunderstandings, we explain briefly that neither of these two appearances is the genuine signature of the expected threshold $\kappa = 2$ for our expansion method to work. The true reason is the one mentioned in the introduction: even the best possible bound, $\lambda^{2d(\sigma)}$, on the graph with permutation σ , cannot beat the $k!$ combinatorics of the graphs beyond $\kappa = 2$.

In the argument above, on one hand, $\kappa < 2$ is related to the error term in the ladder calculation (45). This error term can be improved to $\lambda^2 |\log \lambda|$ and it is apparently due to the fact that the renormalization term $\theta(p)$ was solved only up to lowest order. An improvement may be possible by including more than the lowest order of the self-energy.

The second appearance of $\kappa < 2$, or $t \ll \lambda^{-4}$, at least for the continuous model, is in (48) and it is due to the fact that certain β -denominators are overestimated by L^∞ . This is again a weakness of our method; we did overestimate in order to simplify the integrand.

3.5 Point singularities

The argument in the previous section has neglected the point singularity arising from (47). While a point singularity is integrable in $d \geq 3$ dimensions, it may happen that exactly the same linear combinations of the independent variables keep on accumulating by the repeated use of the bound (47). In that case at some point a high negative power of $|w|$ needs to be integrated. While it is possible to improve the estimate (47) by changing the denominator on the right hand side to $|w| + \eta$, this would still yield further negative η -powers.

It is easy to see that this phenomenon does occur. Primarily this would have occurred if we had not treated the ladders separately: if p_i 's are ladder variables, then the corresponding w momenta in (47) are indeed the same. Although we have removed the ladders beforehand, the same phenomenon occurs in case of a graph which contains ladder *only as a minor but not as a subgraph*. Our separate ladder integration procedure (45) can be viewed as a very simple renormalization of the ladder subgraphs. The correct procedure should renormalize all ladder minors as well.

To cope with this difficulty, we have to follow more precisely the point singularities. To this end, we define the following generalization of $E_\eta(M)$. For any index set $I' \subset I = \{1, 2, \dots, k+1\}$, any $|I'| \times (k+1)$ matrix M , any ν integer and any $\nu \times (k+1)$ matrix \mathcal{E} we define

$$E_\eta(I', M, \mathcal{E}) := \lambda^{2k} e^{2i\eta} \int \int_{-4d}^{4d} d\alpha d\beta \int d\mathbf{p} \\ \times \left(\prod_{i \in I'} \frac{1}{|\alpha - \bar{\omega}(p_i) - i\eta|} \frac{1}{|\beta - \omega(\sum_{j=1}^{k+1} M_{ij} p_j) + i\eta|} \right) \prod_{\mu=1}^{\nu} \frac{1}{|\sum_{j=1}^{k+1} \mathcal{E}_{\mu j} p_j|} \quad (49)$$

We follow the same procedure as described in Section 3.4, but we also keep track of the evolution of the point singularity matrix \mathcal{E} . At the beginning $I' = I$, $\nu = 0$ and \mathcal{E} is not present. After the first non-ladder type integration, a point singularity will appear from (47). Some of the point singularities may get integrated out later as one of their variables become integration variable. Therefore we will need the following generalization of (47):

Lemma 3. *There exists a constant C such that for any index set A*

$$\sup_{|\alpha|, |\beta| \leq 4d} \int \frac{1}{|\alpha - \bar{\omega}(p) - i\eta|} \frac{1}{|\beta - \omega(r+p) + i\eta|} \prod_{a \in A} \frac{1}{|r_a + p|} dp \\ \leq C \eta^{-\tau'} |\log \eta|^3 \sum_{a \in A} \left(\prod_{\substack{a' \in A \\ a' \neq a}} \frac{1}{|r_a - r_{a'}|} \right) \frac{1}{|r|}. \quad \square \quad (50)$$

For the continuous model $\tau' = 0$ while for the discrete model $\tau' = \frac{7}{8} + 2\kappa$.

Using this lemma, we can keep record of the evolution of the point singularity matrix \mathcal{E} at an intermediate step of our integration algorithm. These matrices change by simple operations reminiscent to the Gaussian elimination.

Three complications occur along this procedure, we briefly describe how we resolve them:

(1) The inequality (50) does not allow higher order point singularities. Although it is possible to generalize it to include such singularities as well, we followed a technically simpler path. In addition to the indices $j \in I_p$, we select further β -denominators that we estimate by the trivial L^∞ bound. These additional indices are chosen in such a way, that (i) the number of remaining rows be at least $\frac{1}{3}d(\sigma)$; (ii) the point singularity matrix be of full rank at every step of the algorithm. This second criterion guarantees that no higher order point singularities occur. Since every \mathcal{E} can be derived from M by a procedure that is close to Gaussian elimination and M is invertible (Lemma 1), the full-rank property is relatively easy to guarantee.

(2) The full-rank property actually needs to be guaranteed in a quantitative way, at least the entries of \mathcal{E} needs to be controlled. These entries appear in the point singularity denominators of (50) and their inverses would appear in the estimate. The key observation is that each entry of every matrix \mathcal{E} along the procedure is always 0, 1 or -1 . It is actually easier to prove a stronger statement, namely that every \mathcal{E} is a *totally unimodular matrix*. The proof follows from the fact that every \mathcal{E} can be derived from M by elementary Gaussian elimination steps plus zeroing out certain rows and columns. Such steps preserve total unimodularity and M is totally unimodular by Lemma 1.

(3) After all β -denominators are eliminated, we are left with an integral of the form

$$E_\eta(J, \emptyset, \mathcal{E}) := \int_{-4d}^{4d} d\alpha \int \left(\prod_{i \in J} dp_i \right) \prod_{i \in J} \frac{1}{|\alpha - \bar{\omega}(p_i) - i\eta|} \prod_{\mu=1}^{\nu} \frac{1}{|\sum_{i \in J} \mathcal{E}_{\mu i} p_i|} \quad (51)$$

for some index set J and some point singularity matrix obtained along the integration procedure. Without the point singularities, this integral could be estimated by the $|J|$ -th power of $|\log \eta|$. Since \mathcal{E} is totally unimodular, a similar estimate can be obtained for (51) as well.

4 Computation of the main term and its convergence to a Brownian motion

Our goal is to compute the Wigner distribution $\mathbf{E}W_{\psi_t^\varepsilon}^\varepsilon(X, v)$ with $t = \lambda^{-2-\kappa}T$ and $\varepsilon = \lambda^{2+\kappa/2}$. From Proposition 2, and similar bounds on the repetitive terms in (32), we can restrict our attention to the ladder graph. The following lemma is a more precise version of the ladder integration Lemma (45) and it is crucial to this computation. We present it for the more complicated discrete case. The proof is a tedious calculation in [11].

Lemma 4. *Suppose $f(p)$ is a C^1 function on \mathbf{T}^d . Recall $0 < \kappa < 1/16$ and define $\gamma := (\alpha + \beta)/2$. Let η satisfy $\lambda^{2+4\kappa} \leq \eta \leq \lambda^{2+\kappa}$. Then for $|r| \leq \lambda^{2+\kappa/4}$ we have,*

$$\int \frac{\lambda^2 f(p)}{(\alpha - \bar{\omega}(p-r) - i\eta)(\beta - \omega(p+r) + i\eta)} dp \quad (52)$$

$$= -2\pi i \lambda^2 \int \frac{f(p) \delta(e(p) - \gamma)}{(\alpha - \beta) + 2(\nabla e)(p) \cdot r - 2i[\lambda^2 \text{Im}\Theta(\gamma) + \eta]} dp + O(\lambda^{1/2-8\kappa} |\log \lambda|).$$

Since the Boltzmann collision kernel is uniform on the energy shell, the calculation of $\mathbf{E}W_{\psi_t}^\varepsilon(X, v)$ is more straightforward for the discrete case. We present the sketch of this calculation, the continuous model requires a little more effort at this stage.

Let $\varepsilon = \lambda^{2+\kappa/2}$ be the space scale. After rescaling the Wigner function at time t , we compute $\widehat{W}(\varepsilon\xi, v)$ tested against a smooth, decaying function $\mathcal{O}(\xi, v)$. In particular ξ is of order 1. After the application of Lemma 4 (with $v = v_{k+1}$) and change of variables $a := (\alpha + \beta)/2$ and $b := \lambda^{-2}(\alpha - \beta)$, we obtain

$$\begin{aligned} \langle \mathcal{O}, \mathbf{E}\widehat{W} \rangle &:= \int dv d\xi \mathcal{O}(\xi, v) \mathbf{E}\widehat{W}(\varepsilon\xi, v) = \sum_{k \leq K} \int \int_{\mathbf{R}} \frac{d\alpha d\beta}{(2\pi)^2 \lambda^2} \int d\mathbf{v} e^{it(\alpha - \beta) + 2\eta t} \\ &\quad \times \mathcal{O}(\xi, v_{k+1}) \widehat{W}_0(\varepsilon\xi, v_1) \prod_{j=1}^{k+1} \frac{\lambda^2}{\left(\alpha - \bar{\omega}(v_j + \frac{\varepsilon\xi}{2}) - i\eta\right) \left(\beta - \omega(v_j - \frac{\varepsilon\xi}{2}) + i\eta\right)} \\ &\approx \sum_{k \leq K} \int \int_{\mathbf{R}} \frac{dadb}{(2\pi)^2} e^{it\lambda^2 b} \int \left(\prod_j \frac{-2\pi i \delta(e(v_j) - a) dv_j}{b + \lambda^{-2}\varepsilon \nabla e(v_j) \cdot \xi - 2i\mathcal{I}(a)} \right) \widehat{W}_0(\varepsilon\xi, v_1) \mathcal{O}(\xi, v_{k+1}), \end{aligned}$$

where we defined $\mathcal{I}(\gamma) := \text{Im}\Theta(\gamma)$ for brevity. We used $\eta = \lambda^{2+\kappa}$ to estimate the error terms. The main term (left hand side above) however, is independent of η , so we can choose $\eta = \lambda^{2+4\kappa}$ for the rest of the calculation and we note that Lemma 4 holds for this smaller η as well. This is the reason why the $e^{2\eta t}$ factor is negligible.

We expand the fraction up to second order in ε , we get

$$\frac{-i}{b + \lambda^{-2}\varepsilon \nabla e(v_j) \cdot \xi - 2i\mathcal{I}(a)} \approx \frac{-i}{b - 2i\mathcal{I}(a)} \left[1 - \frac{\lambda^{-2}\varepsilon \nabla e(v_j) \cdot \xi}{b - 2i\mathcal{I}(a)} + \frac{\lambda^{-4}\varepsilon^2 [\nabla e(v_j) \cdot \xi]^2}{(b - 2i\mathcal{I}(a))^2} \right]$$

By symmetry of the measure $2\pi\delta(e(v) - a)dv$ under the sign flip, $v \rightarrow -v$ and using $(\nabla e)(v) = -\nabla e(-v)$, we see that the first order term vanishes after the integration. We also define the matrix

$$D(a) := \frac{1}{2\mathcal{I}(a)} \int d\mu_a(v) \frac{\nabla e(v)}{2\pi} \otimes \frac{\nabla e(v)}{2\pi}$$

After integrating out all momenta and changing the b variable we obtain

$$\begin{aligned} \langle \mathcal{O}, \mathbf{E}\widehat{W} \rangle &\approx \sum_{k \leq K} \int d\xi \int_{\mathbf{R}} \frac{2\mathcal{I}(a) da}{2\pi} \langle \mathcal{O}(\xi, \cdot) \rangle_a \langle \widehat{W}_0(\varepsilon\xi, \cdot) \rangle_a \int_{\mathbf{R}} \frac{db}{2\pi} e^{2i\lambda^2 t b \mathcal{I}(a)} \\ &\quad \times \left(\frac{-i}{b - i} \right)^{k+1} \times \left[1 + \frac{(2\pi)^2 \varepsilon^2 \lambda^{-4} \langle \xi, D(a)\xi \rangle}{2\mathcal{I}(a)} \cdot \frac{1}{(b - i)^2} \right]^{k+1} \end{aligned}$$

We sum up the geometric series and perform a residue calculation to evaluate the db integral. We obtain that the main contribution comes from $k \sim 2\lambda^2 t \mathcal{I}(e)$, so the truncation $k \leq K$ can be neglected and the result of the db integration is

$$\int_{\mathbf{R}} \frac{db}{2\pi} (\dots) \approx \exp \left(- \frac{(2\pi)^2 \varepsilon^2 t \langle \xi, D(e)\xi \rangle}{\lambda^2} \right)$$

To obtain a nontrivial limit, $\varepsilon^2 t / \lambda^2 \sim 1$ is necessary. Noting that $t = \lambda^{-2-\kappa} T$ with $T = O(1)$, we see that indeed the space must be scaled by $\varepsilon = \lambda^{2+\kappa/2}$. Finally we obtain

$$\langle \mathcal{O}, \mathbf{E}\widehat{W} \rangle \approx \int d\xi \int_{\mathbf{R}} \frac{2\mathcal{I}(a)da}{2\pi} \langle \mathcal{O}(\xi, \cdot) \rangle_a \langle \widehat{W}_0(\varepsilon\xi, \cdot) \rangle_a \exp \left(- (2\pi)^2 T \langle \xi, D(a)\xi \rangle \right)$$

Since $\exp[-(2\pi)^2 T \langle \xi, D(a)\xi \rangle]$ is the fundamental solution to the heat equation (15), from the definition of $\langle \cdot \rangle$, and after inverse Fourier transform we obtain (17). This completes the sketch of the calculation of the main term.

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