Low temperature scaling of linear response coefficients in strongly disordered systems

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Motivations

- Low temperature electron transport in strongly disordered media
- Strong disorder: presence of many (infinite) relevant energetic scales

Message: Linear response coefficients are not explicit and are given as solutions of variational problems on infinite dimensional spaces. Tuning a parameter (e.g. temperature going to zero) can amplify the separation of the energetic scales and a proper universal scaling behavior can emerge

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Random walk X_t on the discrete torus

- $\mathbb{T}_N^d = \mathbb{Z}^d / N \mathbb{Z}^d$
- $(X_t)_{t\geq 0}$: continuous time random walk on \mathbb{T}_N^d
- c(x,y): probability rate for a jump $x \sim y$
- c(x,y) = 0 if $|x y| \neq 1$
- $\mathbb{P}(X_{t+dt} = y|X_t = x) = c(x, y)dt + o(dt)$

Random walk Y_t on \mathbb{Z}^d

- $\pi: \mathbb{Z}^d \to \mathbb{T}^d_N$ canonical projection
- $(Y_t)_{t\geq 0}$ random walk on \mathbb{Z}^d with N-periodic jump probability rates c(x, y)
- $\pi(Y_t) = X_t$



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Assumption

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 $(X_t)_{t\geq 0}$ is **irreducible** and its unique invariant distribution μ is **reversible**, *i.e.* μ satisfies the detailed balance condition

 $\mu(x)c(x,y) = \mu(y)c(y,x) \qquad \forall x,y \in \mathbb{T}_N^d$.

Reversibility: if X_0 has law μ , then $\forall T > 0$ the random trajectories

$$(X_t)_{0 \le t \le T}$$
 and $(X_{T-t})_{0 \le t \le T}$

have the same law.

External field

• External field = λw , $\lambda > 0$ tuning parameter, $w \in \mathbb{R}^d$

- $(X_t^{\lambda})_{t \geq 0}$: perturbed random walk on \mathbb{T}_N^d
- $(Y_t^{\lambda})_{t \geq 0}$: perturbed random walk on \mathbb{Z}_N^d
- $c_{\lambda}(x, y)$: perturbed jump probability rate

Local detailed balance

• Local detailed balance:

$$\frac{\mathbf{c}_{\lambda}(\mathbf{x},\mathbf{y})}{\mathbf{c}_{\lambda}(\mathbf{y},\mathbf{x})} = \frac{\mathbf{c}(\mathbf{x},\mathbf{y})}{\mathbf{c}(\mathbf{y},\mathbf{x})} \mathbf{e}^{\beta \mathbf{\Delta}(\mathbf{x},\mathbf{y})} \,,$$

- $\beta = 1/kT$: inverse temperature
- $\Delta(x, y)$: work done by the field on the particle jumping $x \sim y$
- $\Delta(x,y) = \lambda w \cdot (y-x)$
- Example: $c_{\lambda}(x,y) = e^{\lambda \frac{\beta}{2} w \cdot (y-x)} c(x,y)$

Asymptotic velocity

- External field= $\lambda w, \lambda > 0, w \in \mathbb{R}^d$
- μ_{λ} : unique invariant distribution of $(X_t^{\lambda})_{t\geq 0}$
- $\psi_{\lambda}(x) := \sum_{|e|=1} c_{\lambda}(x, x+e)e$ instantaneous local drift
- $v_{\lambda}(w) := \mu_{\lambda}(\psi_{\lambda})$

Fact

 $v_{\lambda}(w)$ is the asymptotic velocity:

$$\begin{aligned} v_{\lambda}(w) &= \lim_{t \to \infty} \frac{d}{dt} \mathbb{E}[X_t^{\lambda}] = \lim_{t \to \infty} \frac{d}{dt} \mathbb{E}[Y_t^{\lambda}], \\ v_{\lambda}(w) &= \lim_{t \to \infty} \frac{Y_t^{\lambda}}{t} \qquad a.s. \end{aligned}$$

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Mobility matrix

- $\psi(x) := \sum_{|e|=1} c(x, x + e)e$ instantaneous local drift at equilibrium
- $\psi(x) = (\psi_1(x), \dots, \psi_d(x))$
- $\mathcal{L}f(x) = \sum_{|e|=1} c_{x,x+e} \left(f(x+e) f(x) \right)$ Markov generator
- \mathcal{L} : symmetric operator in $L^2(\mu)$ (positive spectral gap)

Fact

It holds

$$\partial_{\lambda=0} v_{\lambda}(w) = \sigma w \qquad \forall w \in \mathbb{R}^d \,,$$

where σ is the $d \times d$ symmetric matrix

$$\sigma_{ij} := \beta \mu \big(c(\cdot, \cdot + e_i) \big) \delta_{i,j} - \beta \int_0^\infty \langle \psi_i, e^{s\mathcal{L}} \psi_j \rangle_{L^2(\mu)} ds$$

σ : mobility matrix

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Diffusion matrix and Einstein's relation

Fact

As $\varepsilon \downarrow 0$ the diffusively rescaled random walk $(\varepsilon Y_{\varepsilon^{-2t}})_{t\geq 0}$ converges to a Brownian motion with diffusion matrix D, satisfying the Einstein relation:

$$\sigma = \frac{\beta}{2}D$$

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 $D_{\rm phys} = D/2$, hence $\sigma = \beta D_{\rm phys}$

In what follows, we add the subindex N: σ_N, D_N

Disordered systems: random conductance model

- $\mathbb{E}^d = \{ \text{unoriented edges of } \mathbb{Z}^d \}$
- $\omega = (\omega(x, y) : \{x, y\} \in \mathbb{E}^d)$ stationary ergodic random field
- $\omega(x,y) > 0$ and $\mathbb{E}[\omega(x,y)] < +\infty$
- Fixed ω and N, $\omega^{(N)}$ is the N-periodization of ω



Figure: Left: ω . Right: $\omega^{(N)}$. N = 3

N–mobility and N–diffusion matrix

• Given ω, N , let $X_t, X_t^{\lambda}, Y_t, Y_t^{\lambda}$ as before, where

 $c(x,y) := \omega^{(N)}(x,y) \,.$

- $\sigma_N(\omega)$: mobility matrix
- $D_N(\omega)$: diffusion matrix
- Recall: $\sigma_N(\omega) = \frac{\beta}{2} D_N(\omega)$
- \mathbb{P} : law of the random field ω

Infinite volume limit

Theorem (Homogenization)

For \mathbb{P} -a.a. ω ,

$$\begin{cases} \lim_{N \to \infty} \sigma_N(\omega) = \sigma ,\\ \lim_{N \to \infty} D(\omega) = D , \end{cases}$$

where $\sigma = \frac{\beta}{2}D$ and D is the $d \times d$ symmetric matrix

$$a \cdot Da = \inf_{f \in L^{\infty}(\mathbb{P})} \frac{1}{2} \sum_{e:|e|=1} \int d\mathbb{P}(\omega) \omega(0, e) \left(a \cdot e - \nabla_e f(\omega)\right)^2$$

 $\forall a \in \mathbb{R}^d$, where $\nabla_e f(\omega) := f(\tau_e \omega) - f(\omega)$.

σ, D enter into play in other problems

- Random walk on \mathbb{Z}^d
- $\omega(x, y)$ =probability rate for a jump $x \frown y$
- $\omega(x, y)$ bounded from above.

Fact (P. Mathieu, JSP 2008)

Diffusion behavior: For \mathbb{P} -a.a. ω the diffusively rescaled random walk converges to a Brownian motion with diffusion matrix D

Fact (d = 1 H.C. Lam, J Depauw, SPA 2016; $d \ge 2$ N.Gantert, X.Guo, J.Nagel, AP 2017)

Linear response: Under the field λw , for \mathbb{P} -a.a. ω the asymptotic velocity $v_{\lambda}(w)$ of the perturbed random walk is ω -independent and satisfies $\partial_{\lambda=0}v_{\lambda}(w) = \sigma w$.

Random resistor network

- Fix *ω*
- node set: $\Lambda_L := [-L, L]^d \cap \mathbb{Z}^d$
- filaments: each edge $\{x, y\}$, with $x, y \in \Lambda_L$, has conductivity $\omega(x, y)$
- $C_L(\omega)$: effective conductivity along 1st direction (V=electrical potential)



Limit behavior of $C_L(\omega)$

For simplicity let D be diagonal

Theorem (A.F. 2019+) Let $\mathbb{E}[\omega(0, e_i)^2] < +\infty$ for all i = 1, 2, ..., d. Then, \mathbb{P} -a.a. ω , $\lim_{L \to \infty} L^{2-d} C_L(\omega) = D_{1,1}.$

Strongly disordered systems

- $\omega(x,y) = e^{-\beta A(x,y)}$
- $(A(x,y): \{x,y\} \in \mathbb{E}^d)$: β -independent i.i.d. random variables

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- Energetic barriers
- Interesting regime: $T \ll 1$, i.e. $\beta \gg 1$
- $D = D(\beta)$

Low temperature scaling limit of $D(\beta)$

- Take isotropic medium. Hence $D(\beta) = D_{1,1}(\beta)\mathbb{I}$
- $\omega(x,y) = e^{-\beta A(x,y)}$
- $G(\theta)$: graph with edges $\{x, y\}$ such that $A(x, y) \le \theta$, i.e. $\omega(x, y) \ge e^{-\beta \theta}$

Theorem (A.F. 2019+)

Let $\theta_c := \inf\{\theta : G(\theta) \text{ percolates}\}$. Then

$$\lim_{\beta \to \infty} -\frac{1}{\beta} \ln D_{1,1}(\beta) = \theta_c \,.$$

 $D(\beta) \approx e^{-\theta_c \beta} \mathbb{I}$

Bond percolation on \mathbb{Z}^d with parameter p

- We build a random graph by keeping each edge of \mathbb{Z}^d with probability p (otherwise we erase it), independently for each edge
- $p_c(d) \in (0,1)$: critical parameter p for the existence of infinite connected component



θ_c and bond percolation

- $G(\theta)$: graph with edges $\{x, y\}$ such that $A(x, y) \leq \theta$
- $G(\theta)$: bond percolation on \mathbb{Z}^d with parameter $p(\theta) := \mathbb{P}(A(x, y) \le \theta)$
- $\theta_c := \inf\{\theta : G(\theta) \text{ percolates}\}$



$\overline{D_{1,1}(\beta)} \ge e^{-\theta_c \beta(1+o(1))}$

- $D_{1,1}(\beta) = \lim_{L \to \infty} L^{2-d} C_L(\omega)$
- $C_L(\omega) \geq \text{effective conductivity of } G(\theta_c + \varepsilon) \text{ on } \Lambda_L$
- ^③ Edges in $G(\theta_c + ε)$ have conductivity ≥ $e^{-β(\theta_c + ε)}$
- $G(\theta_c + \varepsilon)$ percolates \implies on Λ_L it has $O(L^{d-1})$ edge-disjoint left right crossings



 \implies effective conductivity of $G(\theta_c + \varepsilon) \ge O(L^{d-2})e^{-\beta(\theta_c + \varepsilon)}$

$$D_{1,1}(\beta) \le e^{-\theta_c \beta (1+o(1))}$$

Variational characterization:

$$a \cdot Da = \inf_{f \in L^{\infty}(\mathbb{P})} \frac{1}{2} \sum_{e:|e|=1} \int d\mathbb{P}(\omega) \omega(0, e) \left(a \cdot e - \nabla_e f(\omega)\right)^2$$

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Strategy: Take a clever test function f

Mott variable range hopping

- **Doped semiconductors**: crystalline solids with inserted atoms of a different type, called **impurities**
- Electron wavefunctions are **localized** around impurities and can **hop** by quantum tunneling
- In the regime of **low impurity density**, one considers independent random walks and encodes the electron interactions into the jump rates.
- Final object: random walk on a marked simple point process

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Marked point process



- $\{\bullet\} = \{x_i\}$: simple point process, random locally finite subset of \mathbb{R}^d
- E_i : mark of x_i , real random variable
- $\omega = \{(x_i, E_i)\}$ marked simple point process

Marked Poisson point process

- $\{x_i\}$ is Poisson point process on \mathbb{R}^d of intensity λ
 - $\bullet \ \lambda = \mathbb{E}\left[\left|\{x_i\} \cap [0,1]^d\right|\right]$
 - $\textcircled{2} A, B \subset \mathbb{R}^d \text{ and } A \cap B = \emptyset \Longrightarrow$

 $|\{x_i\} \cap A|$ and $|\{x_i\} \cap B|$ are independent random variables



• Points x_i are marked by i.i.d. random variables E_i

Random walk $(X_t^{\omega})_{t\geq 0}$

- $\omega = \{(x_i, E_i)\}$ marked point process
- $(X_t^{\omega})_{t\geq 0}$ continuous time random walk
- Markov chain such that

• state space =
$$\{x_i\}$$

$$\odot P(X_{t+dt}^{\omega} = x_j \mid X_t^{\omega} = x_i) = c_{x_i, x_j}(\omega)dt + o(dt), \ i \neq j$$



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Jump probability rates

$$c_{x_i,x_j}(\omega) = \exp\left\{-\frac{2}{\gamma}|x_i - x_j| - \frac{\beta}{2}(|E_i| + |E_j| + |E_i - E_j|)\right\}$$

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- $\gamma = \text{localization length}$
- $\beta = \frac{1}{kT}$
- k = Boltzmann constant
- T =absolute temperature

Group of translations

Given $x \in \mathbb{R}^d$ and $\omega = \{(x_i, E_i)\},\$ define the *x*-translated configuration as

$$\tau_x \omega := \{ (x_i - x, E_i) \}$$



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 \mathbb{P} : law of $\omega = \{(x_i, E_i)\}$. \mathbb{P} stationary and ergodic.

Palm distribution

\mathbb{P}_0 : Palm distribution associated to \mathbb{P}

- Probability measure with support $\{\omega : 0 \in \{x_i\}\},\$
- Roughly, $\mathbb{P}_0 = \mathbb{P}(\cdot | 0 \in \{x_i\})$
- By ergodicity,

$$\mathbb{P}_0 = \lim_{k \to \infty} \operatorname{Av}_{\substack{x: |x| \le k \\ x \in \{x_i\}}} \delta_{\tau_x \omega} \,.$$

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Effective diffusion matrix D

- Given $x \in \mathbb{R}^d$, $\nabla_x f(\omega) := f(\tau_x \omega) f(\omega)$
- $D: d \times d$ symmetric matrix such that, $\forall a \in \mathbb{R}^d$,

$$a \cdot Da = \inf_{f \in L^{\infty}(\mathbb{P}_0)} \frac{1}{2} \int d\mathbb{P}_0(\omega) \sum_i c_{0,x_i}(\omega) \left(a \cdot x_i + \nabla_{x_i} f\right)^2$$

• \mathbb{P}_0 : Palm distribution

Under very general assumptions:

Theorem (A.F., P.Caputo, T. Prescotti, AIHP 2013) For \mathbb{P} -a.a. ω , as $\varepsilon \downarrow 0$ the diffusively rescaled random walk $\left(\varepsilon X_{\varepsilon^{-1/2}t}^{\omega}\right)_{t\geq 0}$ converges to a Brownian motion with diffusion matrix D.

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Linear response

One expects that, when applying an external field λw , the perturbed random walk $X_t^{\omega,\lambda}$ has asymptotic velocity $v_{\lambda}(w)$ satisfying

$$\begin{cases} \partial_{\lambda=0} v_{\lambda}(w) = \sigma w \,, \\ \sigma = \frac{\beta}{2} D \,. \end{cases}$$

For d = 1 it is proved (A.F., N. Gantert, M. Salvi AIHP, 2019)

Miller-Abrahams random resistor network





Electrical filament with conductivity $c_{x_i,x_j}(\omega)$

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Infinite volume effective conductivity

For simplicity: take D diagonal



 $C_L(\omega)$: conductivity along the first coordinate (electrical current in the box, along first direction)

Theorem (A.F. 2019+)

For \mathbb{P} -a.a. ω we have

$$\lim_{L \to \infty} L^{2-d} C_L(\omega) = D_{1,1} \,.$$

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Mott law

Mott variable range hopping:

$$c_{x_i,x_j}(\omega) = \exp\left\{-\frac{2}{\gamma}|x_i - x_j| - \frac{\beta}{2}(|E_i| + |E_j| + |E_i - E_j|)\right\}$$
$$D_{1,1} = D_{1,1}(\beta)$$
Physics:

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{E_i} i.i.d. random variables, law c|E|^αdE around zero, α ≥ 0
Mott law: D_{1,1}(β) ≈ e^{-Cβ^{α+1}/α+1+d}, β ≫ 1
C=?

Mott law

Homogenization + Percolation results (with A.H.Mimun):

Theorem (A.F. 2019+)

Let ω be a marked Poisson point process of intensity λ and let $E_i \geq 0$, then

$$\lim_{\beta \to +\infty} -\beta^{-\frac{\alpha+1}{\alpha+1+d}} \ln D_{1,1}(\beta) = (c_0/\lambda)^{\frac{1}{\alpha+1+d}}$$

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where c_0 admits a percolative characterization

- $E_i \ge 0 \Longrightarrow$ FKG inequality
- Universality:

Stationary and ergodic simple point processes are in the domain of attraction of PPP by thinning+rescaling

- $E_i \ge 0 \Longrightarrow$ FKG inequality
- Universality:
 - ⊙ Let ξ be a stationary ergodic simple point process of intensity $\lambda = \mathbb{E}[|\xi \cap [0, 1]^d|]$
 - \odot Given p > 0, let

 $[\xi]_p := p$ -thinning of ξ

i.e. $[\xi]_p =$ site percolation on ξ with parameter p

• Then

 $\lim_{p \downarrow 0} p^{-1/d} [\xi]_p = \text{ PPP with intensity } \lambda$