Ballisticity and Einstein relation in 1d Mott variable range hopping

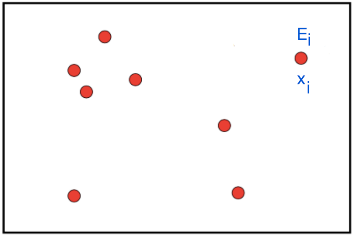
Alessandra Faggionato

Department of Mathematics
University La Sapienza

Joint work with N. Gantert and M. Salvi

Physical motivations

Phonon–assisted **electron transport in disordered solids** in the regime of strong Anderson localization (e.g. doped semiconductors)

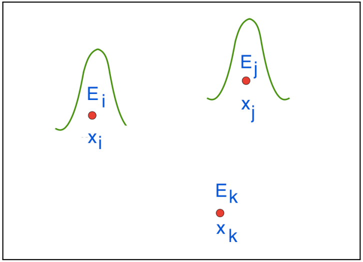


●: impurities located at x_i

E_i: energy mark associated to x_i

$\{x_i\}$ and $\{E_i\}$ are random

Physical motivations



- Electrons are localized around impurities
- E_i= energy of electron around x_i
- $\eta \in \{0,1\}^{\mathbb{N}}$
- $\eta_i = \begin{cases} 1 & \text{there is electron around } x_i \\ 0 & \text{otherwise} \end{cases}$

Simple exclusion process with site disorder

- Probability rate for an electron to hop from x_i to x_j:

$$\exp\{-|x_i - x_j| - \beta\{E_j - E_i\}_+\}$$

- μ_λ: reversible product probability, $\mu_\lambda(\eta_i) = \frac{e^{-\beta(E_i-\lambda)}}{1+e^{-\beta(E_i-\lambda)}}$
- Interesting regime: $\beta \to \infty$
- **Independent particle approximation**:
  probability rate for a jump $x_i \curvearrowright x_j$

$$\mu_\lambda(\eta_i = 1,\ \eta_j = 0) \exp\{-|x_i - x_j| - \beta\{E_j - E_i\}_+\}$$
$$\approx \exp\{-|x_i - x_j| - \frac{\beta}{2}(|E_i - \lambda| + |E_j - \lambda| + |E_i - E_j|)\}$$

- A. Miller, E. Abrahams, *Impurity Conduction at Low Concentrations*. Phys. Rev. **120**, 745-755 (1960)
- V. Ambegoakar, B. Halperin, J.S. Langer, *Hopping conductivity in disordered systems*. Phys. Rev. B **4**, 2612–2620 (1971).

- $\{x_i\} = \mathbb{Z}^d$, nearest–neighbor jumps
- Hydrodynamic limit:
  F., Martinelli (PTRF 2003); Quastel (AP 2006)
- $\partial_t m = \nabla(D(m)\nabla m)$
- Quastel (AP 2006): $\lim_{m\to 0} D(m) = D(0)$, $D(0)$ diffusion matrix random walk with jump rates obtained by a similar procedure

Continuous–time random walk $\mathbf{X}_t^\xi$

Environment: $\xi = (\{x_i\}, \{E_i\})$

- $X_t^\xi \in \{x_i\}$,
- $X_0^\xi = 0$,
- Given $x_i \neq x_j$, probability rate for a jump $x_i \curvearrowright x_j$ is

$$\mathbf{r}_{\mathbf{x_i},\mathbf{x_j}}(\xi) = \exp\left\{-|\mathbf{x_i} - \mathbf{x_j}| - \beta(|\mathbf{E_i}| + |\mathbf{E_j}| + |\mathbf{E_i} - \mathbf{E_j}|)\right\}$$

Variable range hopping

$$\mathbf{r}_{\mathbf{x_i},\mathbf{x_j}}(\xi) = \exp\left\{-|\mathbf{x_i} - \mathbf{x_j}| - \beta(|\mathbf{E_i}| + |\mathbf{E_j}| + |\mathbf{E_i} - \mathbf{E_j}|)\right\}$$

- Low temperature regime: $\beta \to \infty$.
- Long jumps can become convenient if energetically nice

Mott–Efros–Shklovskii law

In $d \geq 2$ the contribution of long jumps dominates as $\beta \to \infty$

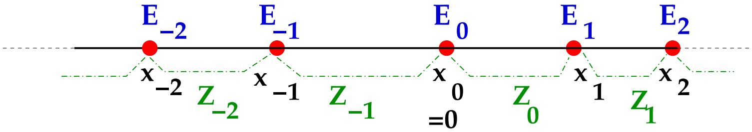
- For genuinely nearest neighbor random walk diffusion matrix $D(\beta) = O(e^{-c\beta})$
- Mott–Efros–Shklovskii law (for isotropic environment):

$$D(\beta) \sim \exp\left(-c\,\beta^{\frac{\alpha+1}{\alpha+1+d}}\right) \mathbb{1}$$

  if $P(E_i \in [E, E + dE)) = c|E|^\alpha dE$, $\alpha \geq 0$.

- Rigorous lower/upper bounds: A.F. D.Spehner, H. Schulz–Baldes CMP (2006); A.F., P.Mathieu CMP (2008)
- M-E-S law concerns conductivity $\sigma(\beta)$. If Einstein relation is not violated, then $\sigma(\beta) = \beta D(\beta)$

Diffusive/Subdiffusive behavior



Theorem (A.F., P. Caputo AAP (2009))

- *If* $\mathbb{E}\left(e^{Z_0}\right) < \infty$, *then quenched invariance principle and*

$$c_1 \exp\{-\kappa_1 \beta\} \leq D(\beta) \leq c_2 \exp\{-\kappa_2 \beta\}.$$

- *If* $\mathbb{E}\left(e^{Z_0}\right) = \infty$, *then annealed invariance principle and*

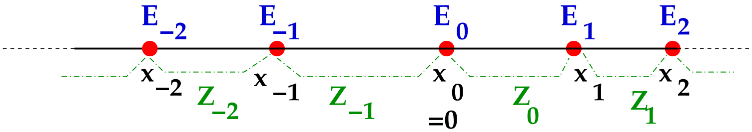
$$D(\beta) = 0\,.$$

Einstein relation for random walks in random environment

- J. Lebowitz, H. Rost (SPA 1994)
- Tagged particle in a dynamical random environment with positive spectral gap: T. Komorowski, S. Olla (JSP 2005)
- Reversible diffusion in random environment: Gantert, Mathieu, Piatnitski (CPAM 2012)
- ...

Biased 1d Mott random walk

Joint work with N. Gantert, M. Salvi (2016)



Take $\lambda \in (0,1)$ and $u(\cdot,\cdot)$ bounded, symmetric

$$r^{\lambda}_{x_i,x_j}(\xi) = \exp\{-|x_i - x_j| + \lambda(x_j - x_i) - u(E_i, E_j)\}$$

Biased random walk $(X_t^{\xi,\lambda})_{t\geq 0}$ is well defined.

Assumptions:

- (A1) The sequence $(Z_k, E_k)_{k\in\mathbb{Z}}$ is ergodic and stationary w.r.t. shifts;
- (A2) The expectation $\mathbb{E}(Z_0)$ is finite;
- (A3) There exists $\ell > 0$ satisfying $\mathbb{P}(Z_0 \geq \ell) = 1$.

Transience

Proposition

For $\mathbb{P}$–a.a. ξ the rw $X_t^{\xi,\lambda}$ is transient to the right:

- $\lim_{t\to\infty} X_t^{\xi,\lambda} = +\infty$ *a.s.*

Ballistic/Subballistic behavior

Theorem

- *If* $\mathbb{E}\left[e^{(1-\lambda)Z_0}\right] < \infty$, *then for* $\mathbb{P}$*–a.a.* ξ *it holds*

$$\lim_{t\to\infty} \frac{X_t^{\xi,\lambda}}{t} = v(\lambda) > 0 \qquad a.s.$$

- *If* $\mathbb{E}\left[e^{-(1+\lambda)Z_{-1}+(1-\lambda)Z_0}\right] = \infty$, *then for* $\mathbb{P}$*–a.a.* ξ *it holds*

$$\lim_{t\to\infty} \frac{X_t^{\xi,\lambda}}{t} = v(\lambda) = 0 \qquad a.s.$$

Comments

$$\begin{cases} \mathbb{E}\big[e^{(1-\lambda)Z_0}\big] < \infty \;\Rightarrow\; v(\lambda) > 0 \\ \mathbb{E}\big[e^{-(1+\lambda)Z_{-1}+(1-\lambda)Z_0}\big] = \infty \;\Rightarrow\; v(\lambda) = 0 \end{cases}$$

- If $(Z_k)_{k\in\mathbb{Z}}$ are i.i.d., or in general if $\|\mathbb{E}(Z_{-1}|Z_0)\|_\infty < \infty$, then

$$\mathbb{E}\big[e^{(1-\lambda)Z_0}\big] < \infty \iff v(\lambda) > 0$$

- Previous theorem holds for $\mathbf{Y}_{\mathbf{n}}^{\xi,\lambda}$= jump process of $X_t^{\xi,\lambda}$

$p^\lambda_{x_i,x_k}(\xi) = \frac{r^\lambda_{x_i,x_j}(\xi)}{\sum_k r^\lambda_{x_i,x_k}(\xi)}$ probability for $Y_n^{\xi,\lambda}$ to $x_i \curvearrowright x_j$

- $\mathbf{Y}_{\mathbf{n}}^{\xi,\lambda}$: discrete time random walk
- $p^{\lambda}_{x_i,x_k}(\xi)$: probability to jump from x_i to x_k
- $\varphi_\lambda(\xi) = \sum_k x_k p^{\lambda}_{0,x_k}(\xi)$ local drift

Theorem

Suppose that $\mathbb{E}\left[e^{(1-\lambda)Z_0}\right] < \infty$. The environment viewed from $Y_n^{\xi,\lambda}$ has an invariant ergodic distribution $\mathbb{Q}_\lambda$ mutually absolutely continuous w.r.t. $\mathbb{P}$,

$$v_Y(\lambda) = \mathbb{Q}_\lambda\left[\varphi_\lambda\right] \quad \textit{and} \quad v_X(\lambda) = \frac{v_Y(\lambda)}{\mathbb{Q}_\lambda\left[1/(\sum_k r^{\lambda}_{0,x_k})\right]}$$

True also for $\lambda = 0$:
$d\mathbb{Q}_0 = \frac{\sum_k r_{0,x_k}}{\mathbb{E}[\sum_k r_{0,x_k}]} d\mathbb{P}$ reversible, $v_Y(0) = v_X(0) = 0$

Warning

When $\lambda = 0$, λ is understood: $r_{x_i,x_j}(\xi)$, $p_{x_i,x_k}(\xi)$, X_t^ξ, Y_n^ξ

Cut-off

- ρ: positive integer
- Consider $Y_n^{\xi,\lambda}$, and suppress jumps of length larger than ρ.
- $\mathbb{Q}_\lambda^{(\rho)}$: invariant ergodic distribution for the new random walk, absolutely continuous w.r.t. $\mathbb{P}$.
- Probabilistic representation of $\frac{d\mathbb{Q}_\lambda^{(\rho)}}{d\mathbb{P}}$.
- $\mathbb{Q}_\lambda^{(\rho)}$ weakly converges to $\mathbb{Q}_\lambda$.
- F. Comets, S. Popov, AIHP **48**, 721–744 (2012)

Estimates on the Radon–Nykodim derivative $\frac{d\mathbb{Q}_\lambda}{d\mathbb{Q}_0}$

Proposition

Suppose that for some $p \geq 2$ *it holds* $\mathbb{E}\left[e^{pZ_0}\right] < +\infty$. *Fix* $\lambda_0 \in (0,1)$. *Then*

$$\sup_{\lambda \in (0,\lambda_0)} \left\| \frac{d\mathbb{Q}_\lambda}{d\mathbb{Q}_0} \right\|_{L^p(\mathbb{Q}_0)} < \infty$$

Continuity of $\mathbb{Q}_\lambda(f)$ at $\lambda = 0$

Theorem

Suppose that $\mathbb{E}(e^{pZ_0}) < \infty$ *for some* $p \geq 2$ *and let* q *be the coniugate exponent, i.e.* q *satisfies* $\frac{1}{p} + \frac{1}{q} = 1$.
If $f \in L^q(\mathbb{Q}_0)$, *then* $f \in L^1(\mathbb{Q}_\lambda)$ *for* $\lambda \in (0,1)$ *and*

$$\lim_{\lambda \to 0} \mathbb{Q}_\lambda(f) = \mathbb{Q}_0(f)$$

$\partial_{\lambda=0}\mathbb{Q}_\lambda(f)$

- $\tau_{x_k}\xi$: environment translated to make x_k the new origin
- $\mathbb{L}_0 f(\xi) = \sum_k p_{0,x_k}[f(\tau_{x_k}\xi) - f(\xi)]$ for $f \in L^2(\mathbb{Q}_0)$
- $f \in L^2(\mathbb{Q}_0) \cap H_{-1}$: there exists $C > 0$ such that

$$|\langle f, g\rangle| \leq C\langle g, -\mathbb{L}_0 g\rangle^{1/2} \quad \forall g \in \mathcal{D}(\mathbb{L}_0)$$

Above $\langle \cdot, \cdot \rangle$ is the scalar product in $L^2(\mathbb{Q}_0)$.

$\partial_{\lambda=0}\mathbb{Q}_\lambda(f)$

Theorem

Suppose $\mathbb{E}(\mathrm{e}^{pZ_0}) < \infty$ *for some* $p > 2$.
Then, for any $f \in H_{-1} \cap L^2(\mathbb{Q}_0)$, $\partial_{\lambda=0}\mathbb{Q}_\lambda(f)$ *exists.*
Moreover:

$$\partial_{\lambda=0}\mathbb{Q}_\lambda(f) = \begin{cases} \mathbb{Q}_0\left[\sum_{k\in\mathbb{Z}} p_{0,x_k}(x_k - \varphi)h\right] \\ -\mathrm{Cov}(N^f, N^\varphi) \end{cases}$$

Representation of $\partial_{\lambda=0}\mathbb{Q}_\lambda(f)$ by forms

- Homogenization theory
- M measure on $\Omega \times \mathbb{Z}$

$$M(u) = \mathbb{Q}_0\Big[\sum_k p_{0,x_k} u(\xi,k)\Big]\,, \qquad u(\xi,k) \text{ Borel, bounded}$$

- $L^2(M)$: square integrable forms
- Potential form:

$$\nabla g(\xi,k) := g(\tau_k \xi) - g(\xi)\,, \qquad g \in L^2(\mathbb{Q}_0)$$

- Given $\varepsilon > 0$ let $g_\varepsilon \in L^2(\mathbb{Q}_0)$ solve $(\varepsilon - \mathbb{L}_0) g_\varepsilon = f$
- Kipnis–Varadhan [CMP, 1986]: $\nabla g_\varepsilon \to h$ in $L^2(M)$

Representation of $\partial_{\lambda=0}\mathbb{Q}_\lambda(f)$ by forms

- Given $\varepsilon > 0$ let $g_\varepsilon \in L^2(\mathbb{Q}_0)$ solve $(\varepsilon - \mathbb{L}_0)g_\varepsilon = f$
- Kipnis–Varadhan: $\nabla g_\varepsilon \to h$ in $L^2(M)$

$$\partial_{\lambda=0}\mathbb{Q}_\lambda(f) = \mathbb{Q}_0\Big[\sum_{k\in\mathbb{Z}} p_{0,x_k}(x_k - \varphi)h\Big]$$

Representation of $\partial_{\lambda=0}\mathbb{Q}_\lambda(f)$ as covariance

$(\xi_n)_{n=0,1,2,\dots}$ environment viewed from Y_n^ξ
By Kipnis–Varadhan

$$\frac{1}{\sqrt{n}}\Big(\sum_{j=0}^{n-1} f(\xi_j), \sum_{j=0}^{n-1}\varphi(\xi_j)\Big) \stackrel{n\to\infty}{\to} (N^f, N^\varphi)$$

(N^f, N^φ) gaussian 2d vector

$$\partial_{\lambda=0}\mathbb{Q}_\lambda(f) = -\mathrm{Cov}(N^f, N^\varphi)$$

- N. Gantert, X. Guo, J. Nagel; *Einstein relation and steady states for the random conductance model.*
- P. Mathieu, A. Piatnitski; *Steady states, fluctuation-dissipation theorems and homogenization for diffusions in a random environment with finite range of dependence*

- D_X: diffusion coefficient of X_t^ξ
- D_Y: diffusion coefficient of Y_n^ξ

Theorem

Suppose $\mathbb{E}(e^{pZ_0}) < \infty$ *for some* $p > 2$. *Then the Einstein relation holds:*

$$\partial_{\lambda=0} v_Y(\lambda) = D_Y \qquad \text{and} \qquad \partial_{\lambda=0} v_X(\lambda) = D_X$$

Workshop "Random motion in random media". Eurandom 2015. S. Olla's talk

Most recent papers

A. Faggionato, M. Salvi, N. Gantert

- *The velocity of 1d Mott varaible–range hopping with external field.* AIHP. To appear. Available online
- *Einstein relation for 1d Mott variable range hopping.* Forthcoming