Nonequilibrium version of the Einstein relation

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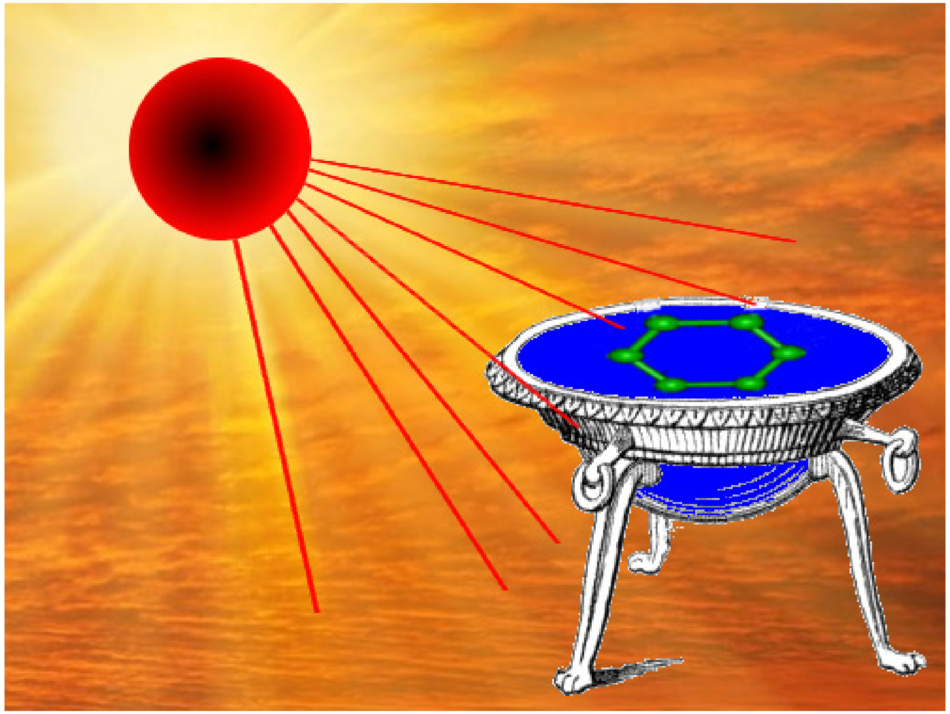


D. Hurowitz and D. Cohen, Phys. Rev. E 90, 032129 (2014)

Brownian motion

The Einstein-Smoluchowski Relation (ESR):

$$D = \mu k_B T, \qquad k_B = 1$$

Relation between mobility (μ) and diffusion (D) reflecting microscopics (k_B) in universal way.

This is a special case of a fluctuation-dissipation relation between first and second moments.

$$\begin{aligned}
\text{Drift:} \quad & \langle x \rangle \;=\; vt \;, \qquad v \;=\; \mu F \\
\text{Diffusion:} \quad & \mathrm{Var}(x) \;=\; 2Dt \\
\text{ESR:} \quad & \frac{v}{D} \;=\; \frac{F}{T} \;\equiv\; s \;=\; \text{affinity (linear response)}
\end{aligned}$$

$s \;\equiv\;$ entropy-production-per-distance

FDT is valid close to equilibrium.

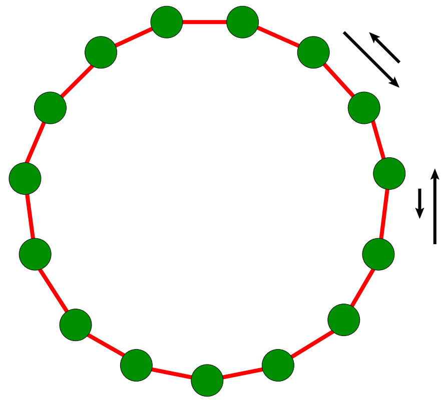
To what extent does the ESR hold?

Can it be derived from the NFT?

Non-equilibrium version?

Sinai spreading

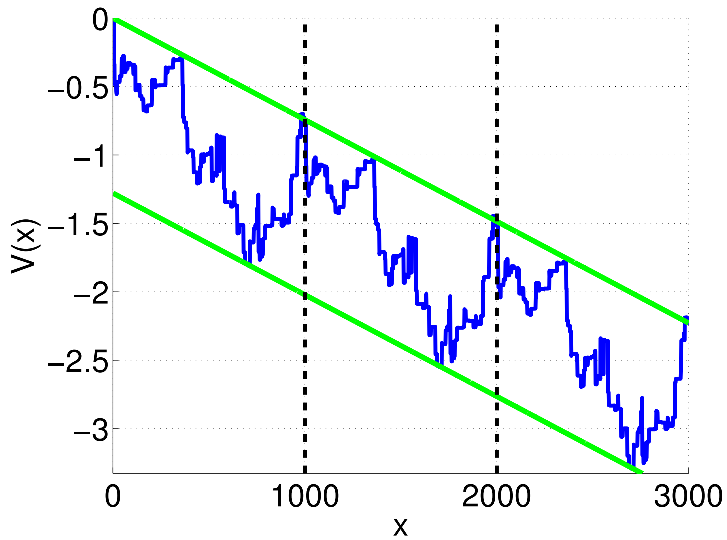
Stochastic field: $\mathcal{E}_n \equiv \ln\left[\frac{\overrightarrow{w}_n}{\overleftarrow{w}_n}\right]$, $\sigma = \sqrt{\mathrm{Var}(\mathcal{E}_n)}$



Stochastic Motive Force: $\mathcal{S}_{\circlearrowleft} = \sum_{n\in\mathrm{ring}} \ln\left[\frac{\overrightarrow{w}_n}{\overleftarrow{w}_n}\right]$

If $\frac{\overrightarrow{w}_n}{\overleftarrow{w}_n} = \exp\left[-\frac{E_n - E_{n-1}}{T}\right] \rightsquigarrow \mathcal{S}_{\circlearrowleft} = 0$

Affinity : $s = \frac{\mathcal{S}_{\circlearrowleft}}{N}$



For small s [1]:
Sub-diffusive spreading $x \sim [\log(t)]^2$,
Exponentially small drift $v \sim e^{-\sqrt{N}}$.

For arbitrary s [2,3]:
Complicated expressions for v and D.

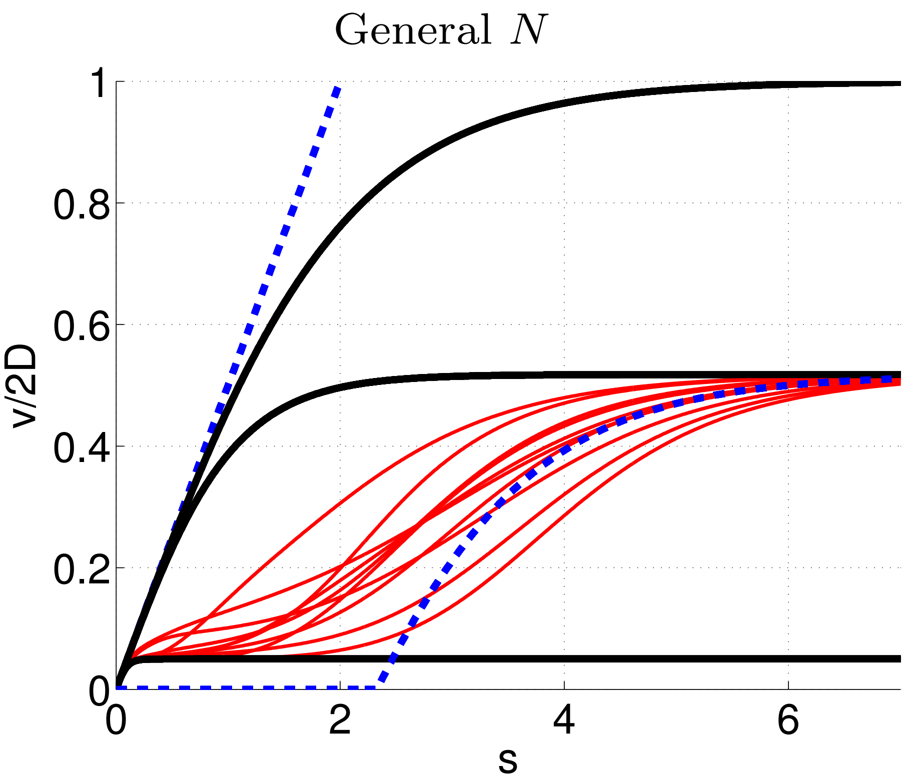
For a periodic lattice, no disorder:

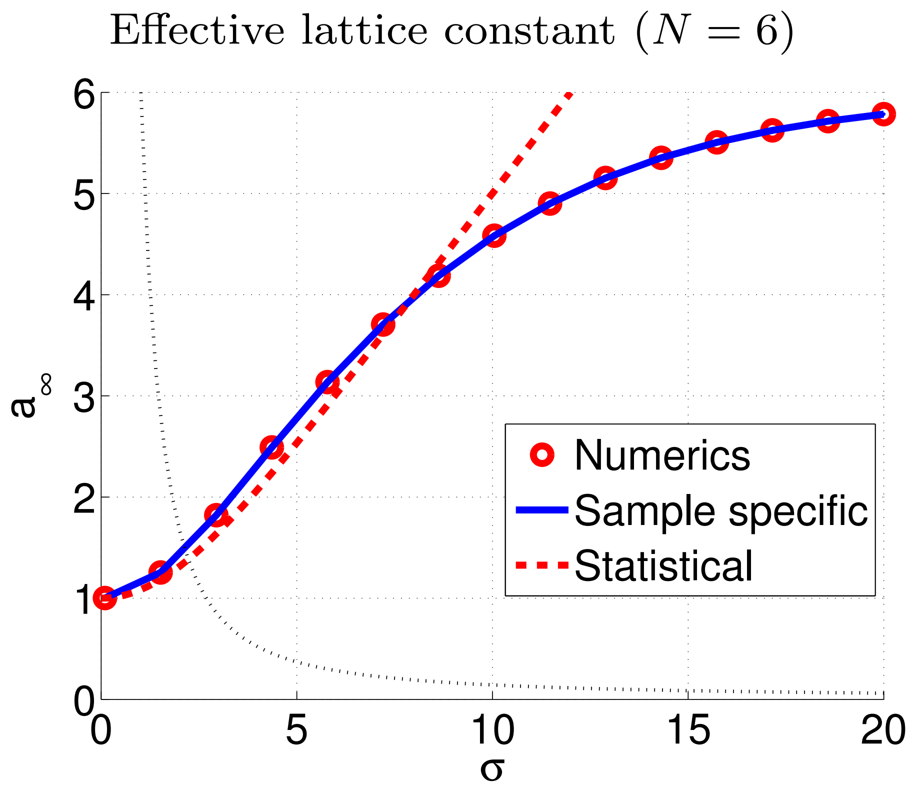
$$\frac{v}{D} = \frac{2}{a}\tanh\left(\frac{as}{2}\right)$$

[1] **Sinai** (1982)
[2] **Derrida** (1983)
[3] **Aslangul, Pottier, Saint-James** (1989)

ESR is violated for large s

Observations for finite N





Generalized ESR for a given disorder σ

$$\frac{v}{D} = \frac{2}{a_s}\tanh\frac{a_s s}{2}$$

(1) For small values of s we have $v/D = s$, in consistency with the ESR.

(2) For no disorder ($\sigma = 0$) we have $a_s = 1$, reflecting the discreteness of the lattice.

(3) For finite disorder and moderate s we have $a_s \sim N$, reflecting the length of the unit cell.

(4) For finite disorder and large s we have $a_s = a_\infty$, reflecting the disorder σ.

(5) As N becomes larger our results approach those of [2,3], which we call "Sinai step".

Outline

General s dependence $\quad \frac{v}{D} = \frac{2}{a_s} \tanh \frac{a_s s}{2} \quad a_s : \; N ... a_\infty$

Poisson $(s \to \infty)$ $\quad \frac{v}{D} = \frac{2}{a_\infty} \quad a_\infty(\sigma) : \; 1 ... N$

ESR $(s \to 0)$ $\quad \frac{v}{D} = s$

Given $(1, \; N, \; \sigma)$ $\qquad a_s = ?$

σ is the log-width of the stochastic field distribution

Nonequilibrium Fluctuation Theorem (NFT) derivation of the ESR

Define x as the winding number times the length of the ring.

$$\frac{P\left[\boldsymbol{r}(-t)\right]}{P\left[\boldsymbol{r}(t)\right]} = \exp\left[-\mathcal{S}[\boldsymbol{r}]\right] \quad \rightsquigarrow \quad \frac{p(-x;t)}{p(x;t)} = \mathrm{e}^{-sx}$$

Gaussian approximation (**Central Limit Theorem**)

$$p(x;t) \approx \overline{p}(x;t) = \frac{1}{\sqrt{4\pi Dt}}\exp\left[-\frac{(x-vt)^2}{4Dt}\right] \quad \rightsquigarrow \quad \frac{v}{D} = s$$

Does the ESR really hold?

NFT and coarse graining

Asymmetric random walk traversing a distance $x = X_1 + \ldots + X_{\mathcal{N}}$

$$\begin{aligned} P(X=+1) &= p \equiv \overrightarrow{w}\tau \\ P(X=-1) &= q \equiv \overleftarrow{w}\tau \\ P(X=0) &= 1-p-q \end{aligned}$$

Moment generating function $\quad Z(k) = \langle \mathrm{e}^{-ikx} \rangle = \left[p\mathrm{e}^{-ik} + q\mathrm{e}^{+ik} + (1-p-q)\right]^{\mathcal{N}}$

In the continuous time limit $p, q \ll 1$, $\quad \ln Z(k) = \mathcal{N}\left[p\mathrm{e}^{-ik} + q\mathrm{e}^{+ik} - (p+q)\right] + \mathcal{O}(\mathcal{N}\tau^2)$

Accordingly, one obtains:

$$p(x;t) = \int_{-\infty}^{\infty} dk\ \mathrm{e}^{ikx + \left(\overrightarrow{w}\mathrm{e}^{-ik} + \overleftarrow{w}\mathrm{e}^{ik} - (\overleftarrow{w} + \overrightarrow{w})\right)t}$$

satisfies NFT

Correct application of the CLT:

$$\overline{p}(x;t) = \int_{-\infty}^{\infty} dk\ \mathrm{e}^{ik(x-(\overrightarrow{w}-\overleftarrow{w})t) - \frac{k^2}{2}(\overrightarrow{w}+\overleftarrow{w})t + \cancel{\mathcal{O}(k^3 t)}} = \frac{1}{\sqrt{4\pi Dt}} \exp\left[-\frac{(x-vt)^2}{4Dt}\right]$$

$$v = \overrightarrow{w} - \overleftarrow{w}\ , \quad D = \frac{1}{2}(\overrightarrow{w} + \overleftarrow{w}) \qquad \rightsquigarrow \qquad \frac{v}{D} = \overline{s} = \frac{2}{a}\tanh\frac{as}{2}$$

The affinity is renormalized!

The naive reasoning, based on CLT, is wrong, If we smear $p(x)$ we get

$$\frac{\overline{p}(-x;t)}{\overline{p}(x;t)} = \mathrm{e}^{-\overline{s}x}$$

Recipe for computing v and D on a periodic array

Dynamics determined by rate equation: $(d/dt)\boldsymbol{p} = W\boldsymbol{p}$

W is not symmetric yet periodic, thus Bloch's theorem applies.

Reduced equation for the eigenmodes $\boldsymbol{W}(\varphi)\psi = -\lambda\psi$, where $\boldsymbol{W}(\varphi)$ is an $N \times N$ matrix.

Bloch's theorem: $\psi_{n+N} = \mathrm{e}^{i\varphi}\psi_n$, where n is the site index mod(N).

Bloch quasi-momentum $\varphi \equiv kN$.

Diagonalizing $\boldsymbol{W}(\varphi) \;\; \rightsquigarrow \;\; \{|k,\nu\rangle, -\lambda_\nu(k)\}$, where ν is the band index.

Time dependent solution of the rate equation

$$p_n(t) \quad \approx \quad \frac{1}{L}\sum_{k,\nu} C_{k,\nu}\; \mathrm{e}^{-\lambda_\nu(k)t}\; \mathrm{e}^{ikn} \qquad \text{where } \; C_{k,\nu} \; \text{ depend on initial conditions.}$$

In the long time limit only λ_0 survives

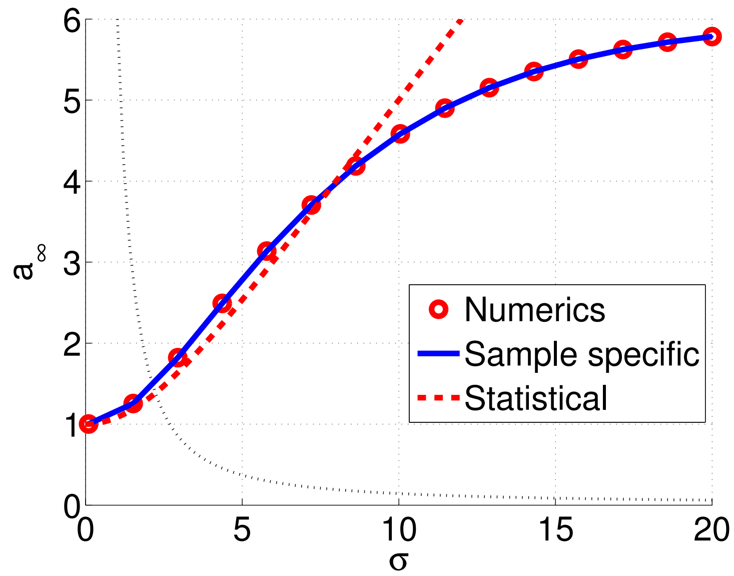
$$v \quad = \quad i\frac{\partial\lambda_0(k)}{\partial k}\bigg|_{k=0}$$

$$D \quad = \quad \frac{1}{2}\frac{\partial^2\lambda_0(k)}{\partial k^2}\bigg|_{k=0}$$

The Poisson Limit $(s \to \infty)$

The limit $s \to \infty$ corresponds to a uni-directional random walk traversing a distance $x = X_1 + ... + X_{\mathcal{N}}$

$$\begin{aligned} P(X_n = 1) &= w_n \tau \\ P(X_n = 0) &= 1 - w_n \tau \\ P(X_n = -1) &= 0 \end{aligned}$$



Effective lattice constant $(N = 6)$

Characteristic polynomial for eigenvalues of $\boldsymbol{W}(\varphi)$

$$\det(\lambda + \boldsymbol{W}(\varphi)) = \prod_{n=1}^{N} (\lambda - w_n) + e^{-i\varphi} \prod_{n=1}^{N} w_n = 0$$

Expanding to second order in λ and φ

$$\lambda = -i \left[\left(\sum_{n=1}^{N} \frac{1}{w_n} \right)^{-1} \right] \varphi + \frac{1}{2} \left[\left(\sum_{n=1}^{N} \frac{1}{w_n} \right)^{-3} \left(\sum_{n=1}^{N} \frac{1}{w_n^2} \right) \right] \varphi^2 + \mathcal{O}(\varphi^3)$$

From the recipe for v and D:

$$a_\infty = \left(\frac{2D}{v} \right)_{s \to \infty} = \left[\frac{\langle (1/\overrightarrow{w})^2 \rangle}{\langle (1/\overrightarrow{w}) \rangle^2} \right] = [\text{For log-box distribution}] = \frac{\sigma}{2} \coth\left(\frac{\sigma}{2} \right)$$

Spreading analysis and the "Sinai step"

$$\left\langle \left(\frac{\overleftarrow{w}}{\overrightarrow{w}} \right)^{\mu} \right\rangle \equiv \mathrm{e}^{-(s-s_\mu)\mu}$$ [defines s_μ]

The values $s_{1/2}$, s_1 and s_2 determine crossover points between transport regimes.

For $s = 0$, anomalous time dependent spreading [Sinai],

$$x \sim [\log(t)]^2 \quad \rightsquigarrow \quad v \sim e^{-\sqrt{N}}$$

For finite $s < s_1$ [Bouchaud, Comtet, Georges, Le Doussal, 1987],

$$x \sim t^{\mu}$$ [μ is the value for which $s_\mu = s$]

Time required to drift $x \sim N$ is $t \sim N^{1/\mu}$, hence we deduce

$$v \sim \frac{x}{t} \sim \left(\frac{1}{N} \right)^{\frac{1}{\mu}-1}$$

Crossover at $s = s_{1/2}$ from sub-Ohmic to super-Ohmic behaviour.

For large $s > s_1$ and $N \to \infty$ [Derrida],

$$v_s = \frac{1 - \langle (\overleftarrow{w}/\overrightarrow{w}) \rangle}{\langle (1/\overrightarrow{w}) \rangle} = \left[1 - \mathrm{e}^{-(s-s_1)} \right] v_\infty$$

The affinity dependent length scale a_s

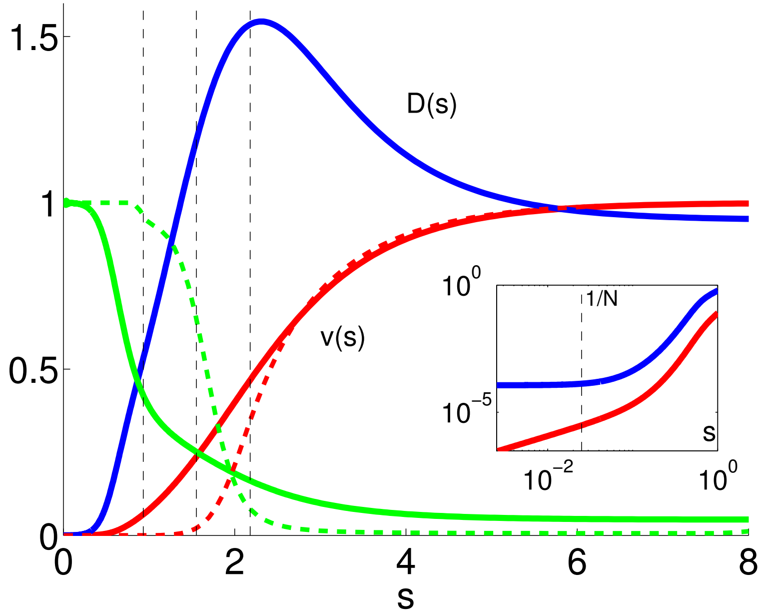
From "Derrida" we have an expression for v in the $N \to \infty$ limit.

From our reasoning we have in general

$$\frac{v}{D} = \frac{2}{a_s} \tanh \frac{a_s s}{2} \quad \text{with some } a_s.$$

By "reverse engineering" we deduce

$$\begin{cases} a_s \sim N, & s < s_2 \\ a_s \approx \dfrac{a_\infty}{1-\langle(\overleftarrow{w}/\overrightarrow{w})^2\rangle} = \dfrac{a_\infty}{1-\mathrm{e}^{-2(s-s_2)}}, & s > s_2 \end{cases}$$



s regime	$[0, 1/N]$	$[1/N, s_{1/2}]$	$[s_{1/2}, s_1]$	$[s_1, s_2]$	$[s_2, \infty]$
a_s	irrelevant	$a_s \sim N$			$a_s \approx \left[1-\mathrm{e}^{-2(s-s_2)}\right]^{-1} a_\infty$
v_s	$v = 2D\, s$	$\sim \left(\frac{1}{N}\right)^{\frac{1}{\mu}-1}$		$v_s \approx \left[1-\mathrm{e}^{-(s-s_1)}\right] v_\infty$	
D	$\sim \exp\left(-\sqrt{N}\right)$	$\sim \left(\frac{1}{N}\right)^{\frac{1}{\mu}-2}$	$\sim (N)^{2-\frac{1}{\mu}}$	$\sim N$	$D = \frac{1}{2} a_s v_s$

Summary

To what extent does the ESR hold?

As long as $s < 1/N$, for a disordered lattice.

Can it be derived from the NFT?

Yes, provided s is replaced by coarse grained $\bar{s}$.

Non-equilibrium version?

$$\frac{v}{D} = \frac{2}{a_s} \tanh \frac{a_s s}{2}$$

$$\begin{cases} v \sim \left(\frac{1}{N}\right)^{\frac{1}{\mu}-1}, & s < s_1 \\ v \approx \left[1 - \mathrm{e}^{-(s-s_1)}\right] v_\infty, & s > s_1 \end{cases}$$

$$\begin{cases} a_s \sim N, & s < s_2 \\ a_s \approx \frac{a_\infty}{1-\left\langle(\overleftarrow{w}/\overrightarrow{w})^2\right\rangle} = \frac{a_\infty}{1-\mathrm{e}^{-2(s-s_2)}}, & s > s_2 \end{cases}$$

Epilog: Experiments

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- Giorgio Volpe, Giovanni Volpe, Sylvain Gigan, **Brownian Motion in a Speckle Light Field: Tunable Anomalous Diffusion and Selective Optical Manipulation**, Scientific Reports 2014
- S. Nakamura, Y. Yamauchi, M. Hashisaka, K. Chida, K. Kobayashi, T. Ono, R. Leturcq, K. Ensslin, K. Saito, Y. Utsumi, A.C. Gossard, **Nonequilibrium fluctuation relations in a quantum coherent conductor** , PRL 2010
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