Nonequilibrium version of the Einstein relation

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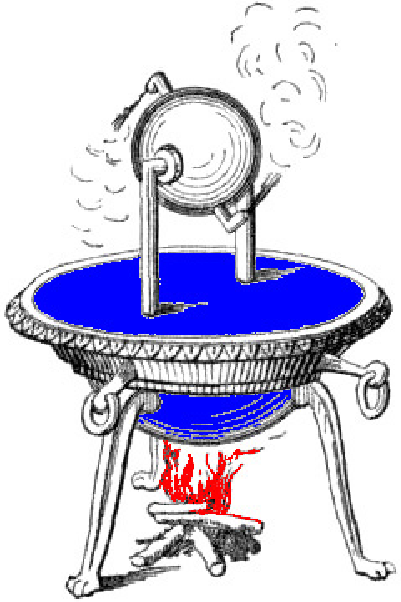
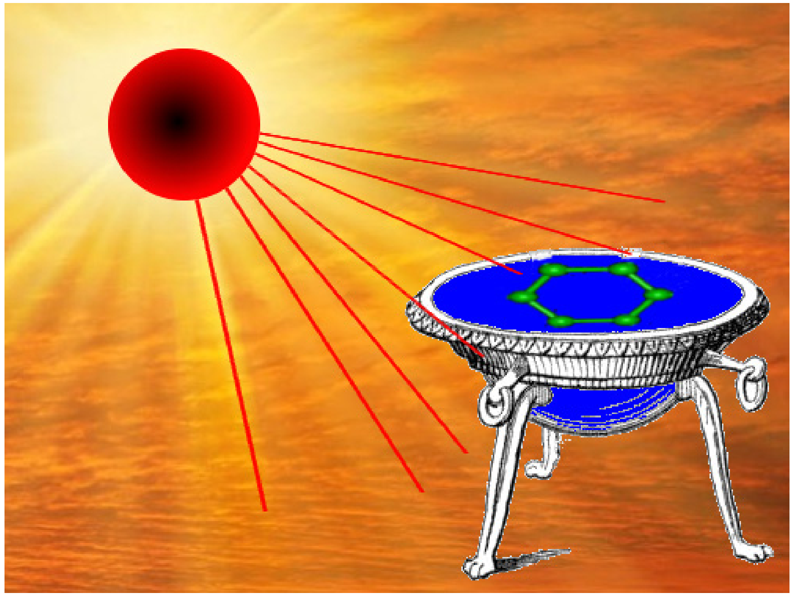


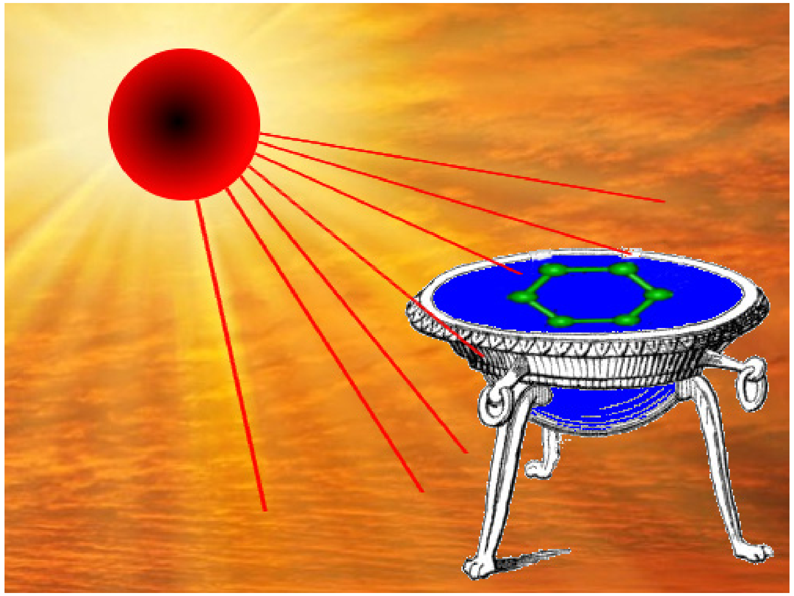


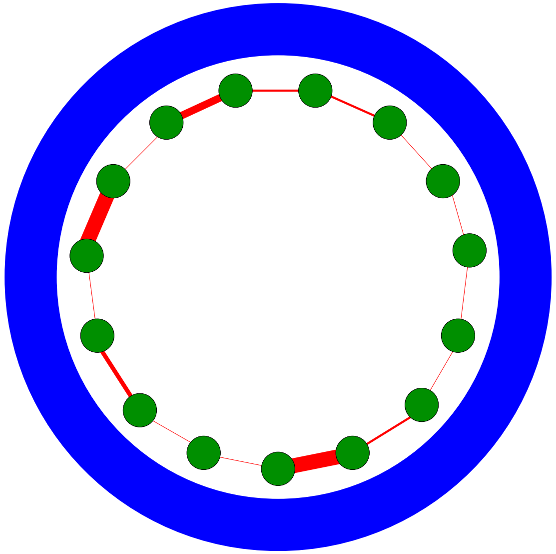
[1] Daniel Hurowitz, DC (PRE 2014)

[2,3] Daniel Hurowitz, Saar Rahav, DC (EPL 2012, PRE 2013)

[4] Daniel Hurowitz, DC (EPL 2011)

Mesoscopic ring model





$$\frac{d}{dt}\boldsymbol{p} = \boldsymbol{W}\boldsymbol{p}$$

$$w_{n+1,n} \equiv w_{\overrightarrow{n}}$$

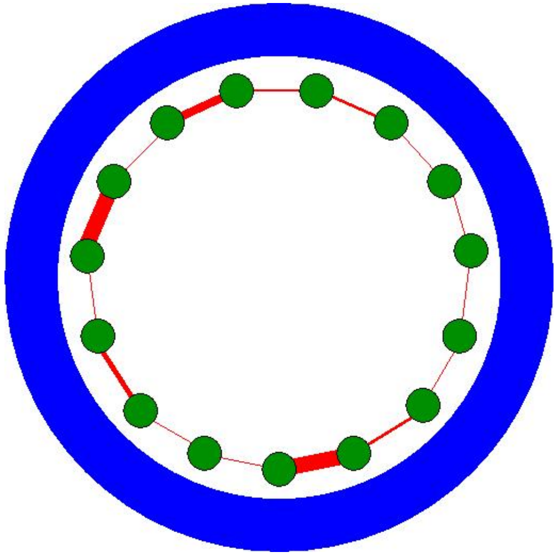
$$w_{n,n+1} \equiv w_{\overleftarrow{n}}$$

$$w_{\overrightarrow{n}} \quad = \quad w^{\beta}_{\overrightarrow{n}} + \nu g_n$$

In [2,3] we have considered systems that are "sparse" or "glassy", meaning that many time scales are involved.
Standard thermodynamics does not apply to such systems.

Minimal model of a "glassy" mesoscopic system

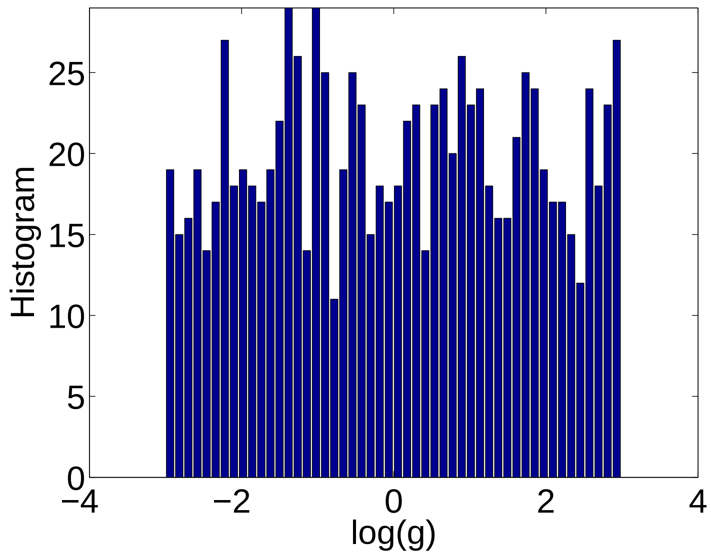
System + Bath + Driving



$$w_{\vec{n}} \;=\; w^{\beta}_{\vec{n}} + \nu g_n$$

$$g_n \;=\; \text{couplings}$$

Histogram of couplings



$\longleftarrow$ few decades $\longrightarrow$

"sparsity" = log wide distribution of couplings

$$w^{\nu}_{n} = \nu g_n$$ corresponds to $T_A = \infty$

$$\frac{w^{\beta}_{\vec{n}}}{w^{\beta}_{\overleftarrow{n}}} = \exp\left[-\frac{E_n - E_{n-1}}{T_B}\right]$$ corresponds to T_B = finite

The stochastic potential and the SMF

Rate equation:

$$\frac{d}{dt}\boldsymbol{p} \;=\; \boldsymbol{W}\boldsymbol{p} \qquad [=0 \text{ for NESS}]$$

$$I_n \;=\; w_{\overrightarrow{n}}\, p_n - w_{\overleftarrow{n}}\, p_{n+1} \qquad [\equiv I(\nu) \text{ for NESS}]$$

Stochastic field:

$$\mathcal{E}(x_n) \;\equiv\; \ln\left[\frac{w_{\overrightarrow{n}}}{w_{\overleftarrow{n}}}\right] \;\approx\; -\left[\frac{1}{1+g_n\nu}\right]\frac{E_n - E_{n-1}}{T_B}$$

Stochastic potential:

$$V(x) = -\int^{x} \mathcal{E}(x')dx' \approx \sum_n \left[\frac{1}{1+g_n\nu}\right]\frac{E_n - E_{n-1}}{T_B}$$

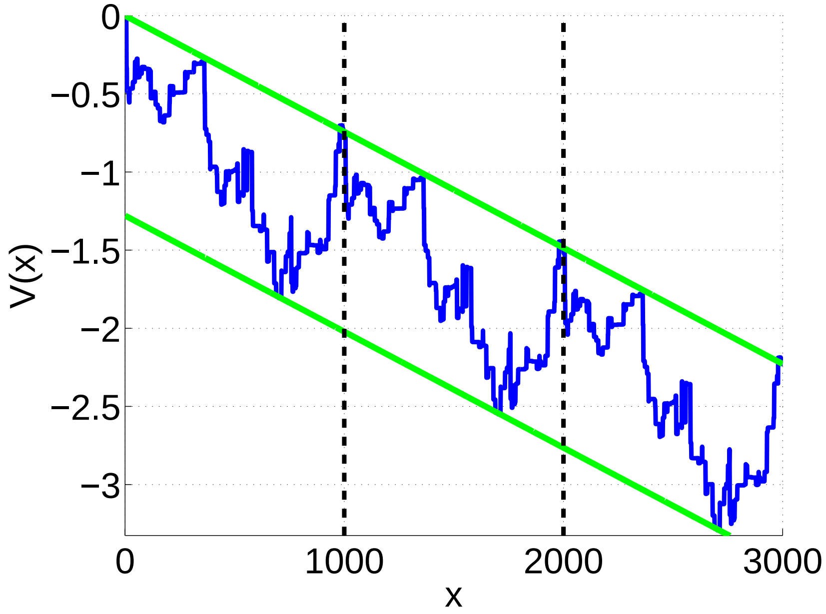
Stochastic Motive Force:

$$\mathcal{S}_{\circlearrowleft} \equiv \ln\left[\frac{\prod_n w_{\overrightarrow{n}}}{\prod_n w_{\overleftarrow{n}}}\right] = \oint \mathcal{E}(x)\,dx \qquad [0 \text{ if no driving}]$$

Telescopic correlations:

$$\mathcal{E}(x_n) \;\sim\; \Delta_n \;\equiv\; (E_n - E_{n+1})$$

Yet... we have sparsely distributed couplings



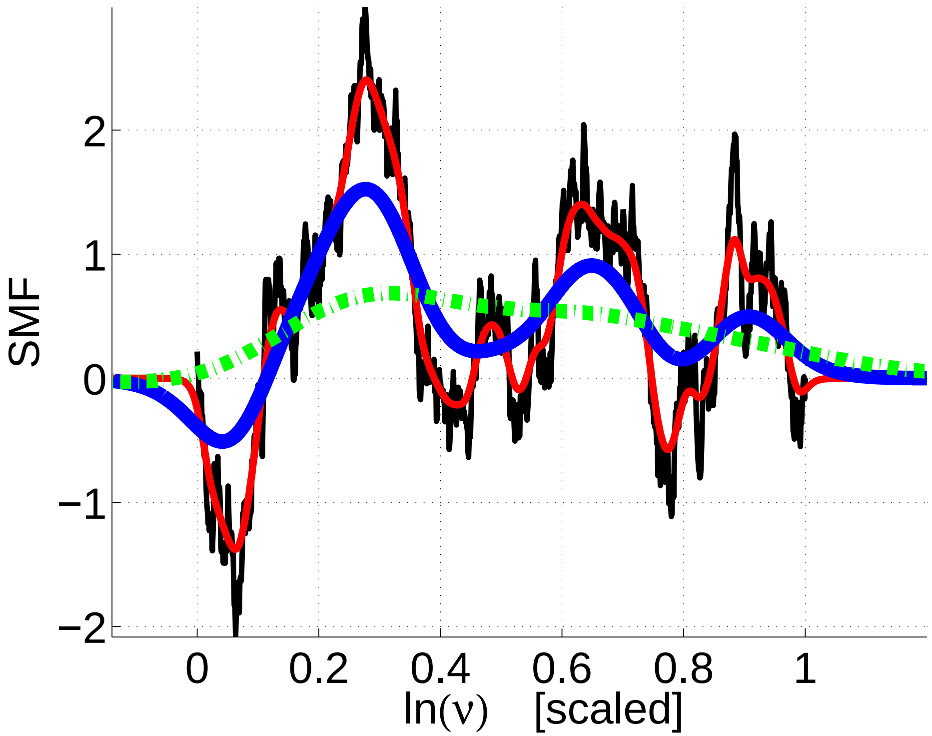
Sinai's Random-Walk [1982]:

Random, Uncorrelated & non symmetric transition rates

$\rightsquigarrow$ Buildup of activation barrier $B \sim \sqrt{N}$

$\rightsquigarrow$ Exponentially low current $I \sim e^{-\sqrt{N}}$

SMF and current vs Driving intensity



$$I(\nu) \quad \sim \quad \frac{1}{N}\, w_{\varepsilon}\, \mathrm{e}^{-B}\, 2\sinh\left(\frac{\mathcal{S}_{\circlearrowleft}}{2}\right)$$

$\mathcal{S}_{\circlearrowleft}$ - Stochastic Motive Force
B - Effective Activation Barrier

Valid for small SMF [see later]

The number of sign change ≈ $\sqrt{\mathbf{Var}(\log(g_n))}$ reflects the glassiness.

Summary of main results [2,3]

1. The current in the Sinai regime may be estimate by a single barrier approximation,
   $I(\nu) \sim \frac{1}{N}\, w_{\varepsilon}\, \mathrm{e}^{-B}\, 2\sinh\left(\frac{\mathcal{S}_{\circlearrowleft}}{2}\right)$ [small SMF assumed]

2. Number of current sign change is determined by the log-width of the coupling distribution,
   Expected number of sign change $\approx \sqrt{\mathrm{Var}(\log(\mathrm{couplings}))}$

3. Exact expression for (non-canonical) NESS occupation probability reflects crossover from Sinai spreading to resistor network picture.
   $p_n \;\propto\; \left(\frac{1}{w(x_n)}\right)_{\varepsilon} \mathrm{e}^{-(U(n)-U_{\varepsilon}(n))}$

4. Distribution of currents reflects Barrier statistics
   $\mathrm{Prob}\left\{\mathrm{barrier} < B\right\} \;\sim\; \exp\left[-\frac{1}{2}\left(\frac{\pi\sigma_{\mathrm{B}}}{2B}\right)^2\right]$

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.

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

$$s \equiv \text{entropy-production-per-distance} = \frac{\mathcal{S}_{\circlearrowleft}}{N} \quad \text{[for the ring/lattice geometry]}$$

FDT is valid close to equilibrium.

To what extent does the ESR hold?

Can it be derived from the NFT?

Non-equilibrium version?

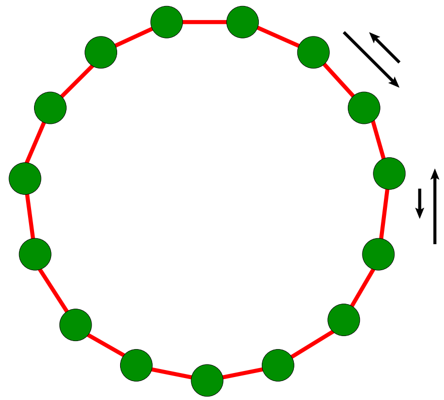
Sinai spreading

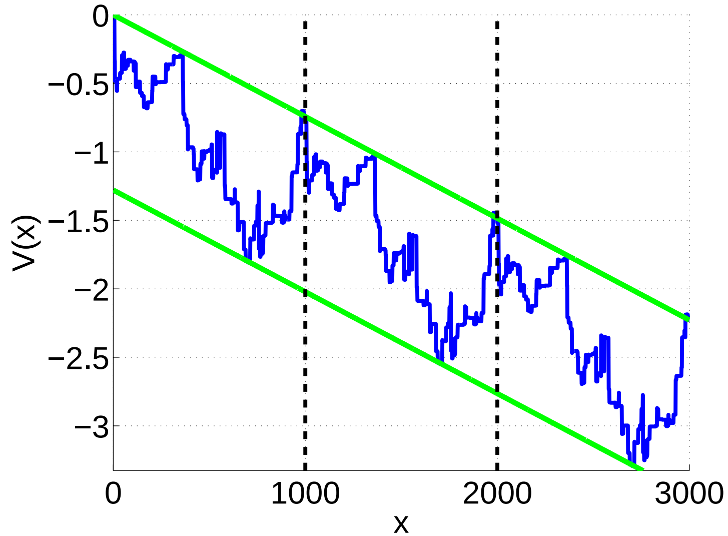
Stochastic field: $\mathcal{E}_n \equiv \ln\left[\frac{\overrightarrow{w}_n}{\overleftarrow{w}_n}\right]$, $\sigma = \sqrt{\mathrm{Var}(\mathcal{E}_n)}$

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

The generalized ESR - reasoning and outline

1 = the lattice constant (distance between sites)

N = the lattice periodicity (length of the ring)

σ = the width of the stochastic-field distribution

ESR $(s \to 0)$

$$\frac{v}{D} = s$$

Poisson $(s \to \infty)$

$$\frac{v}{D} = \frac{2}{a_\infty}$$

$a_\infty(\sigma) : \; 1 \nearrow N$

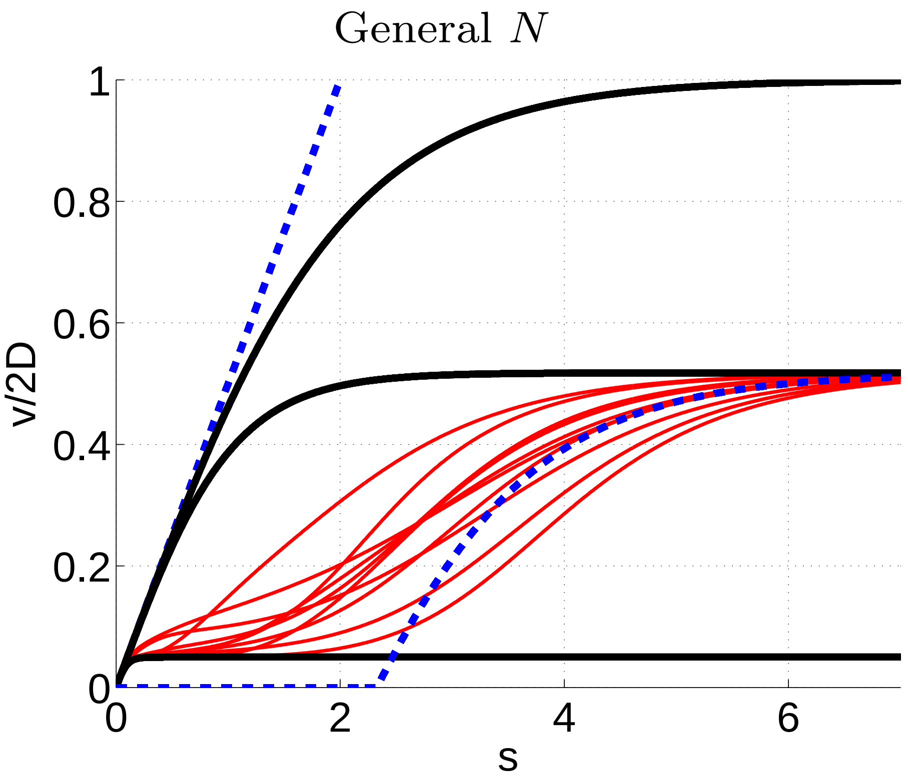
General s dependence

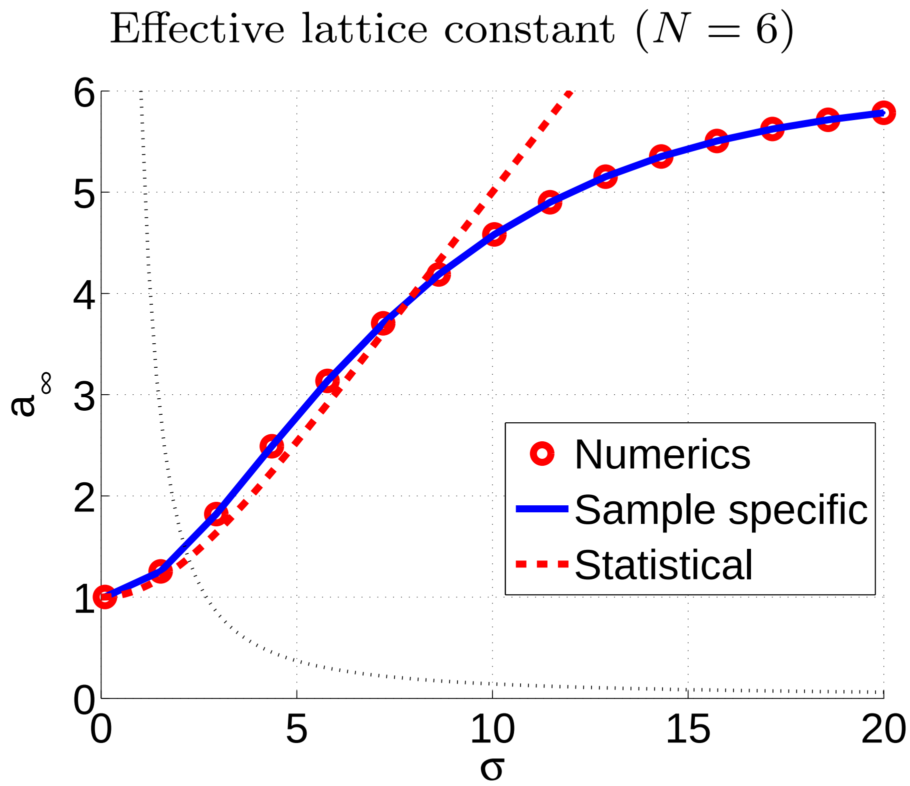
$$\frac{v}{D} = \frac{2}{a_s} \tanh \frac{a_s s}{2}$$

$a_s : \; N \searrow a_\infty$

Figure out how a_s depends on s. Then deduce D.

Numerical results for v/D





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".

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 $x = X_1 + ... + X_{\mathcal{N}}$

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

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:

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

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

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

The dynamics is determined by a rate equation: $\frac{d}{dt}\boldsymbol{p} = \boldsymbol{W}\boldsymbol{p}$

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

Time dependent solution of the rate equation:

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

In the long time limit only λ_0 survives

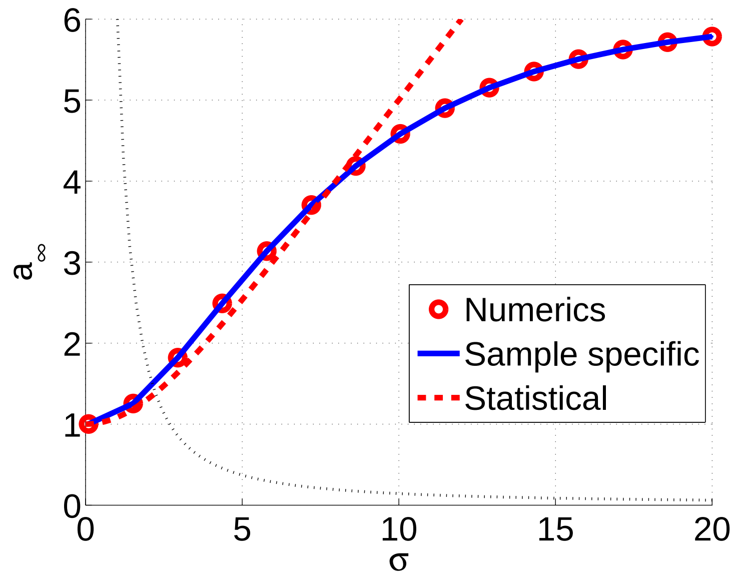
$$v \quad = \quad i\frac{\partial\lambda_0(k)}{\partial k}\bigg|_{k=0}$$

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

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 $\boldsymbol{W}(\varphi)$

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

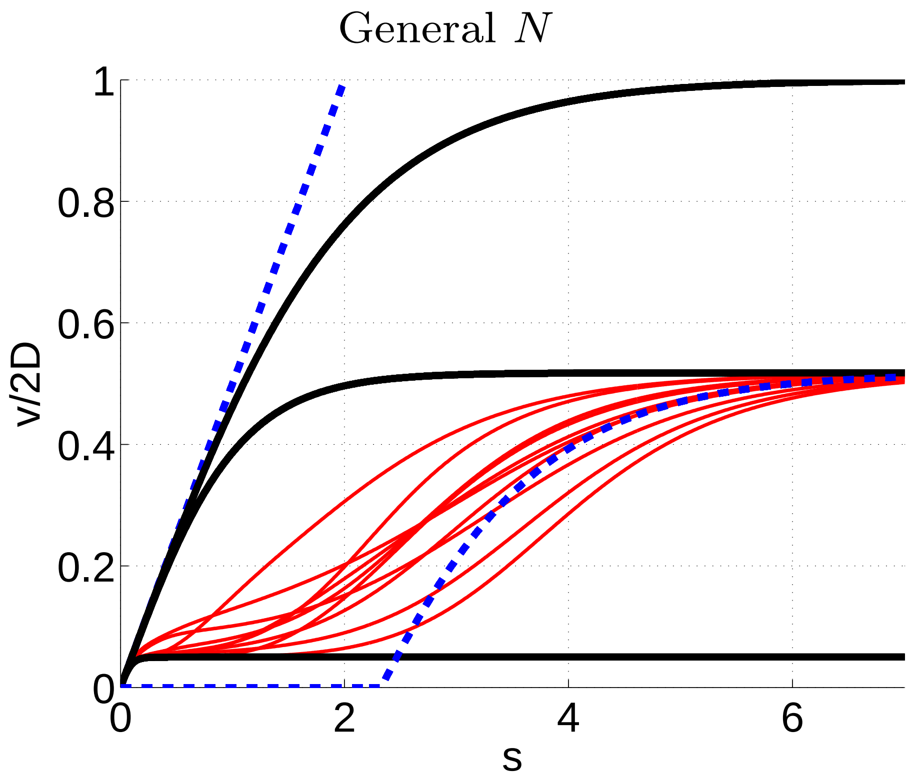
Expanding to second order in λ and φ

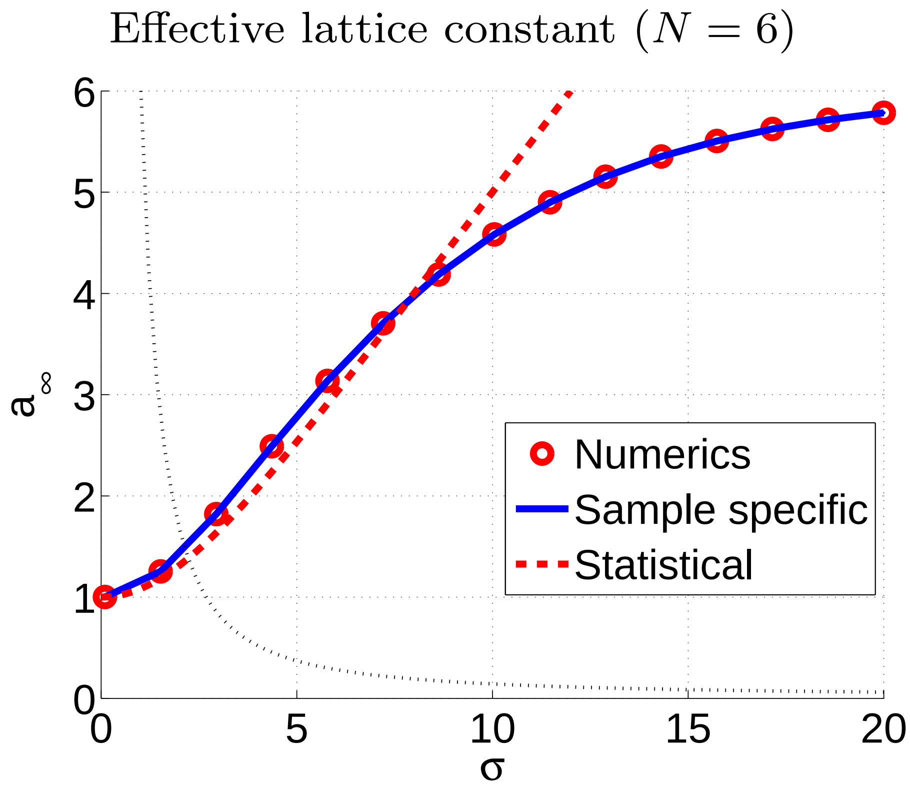
$$\lambda = -i \left[\left(\sum_{n=1}^{N} \frac{1}{w_n} \right)^{-1} \right] \varphi + \frac{1}{2} \left[\left(\sum_{n=1}^{N} \frac{1}{w_n} \right)^{-3} \left(\sum_{n=1}^{N} \frac{1}{w_n^2} \right) \right] \varphi^2 + \mathcal{O}(\varphi^3)$$

From the recipe for v and D:

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

Reminder: Numerical results for v/D





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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

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

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

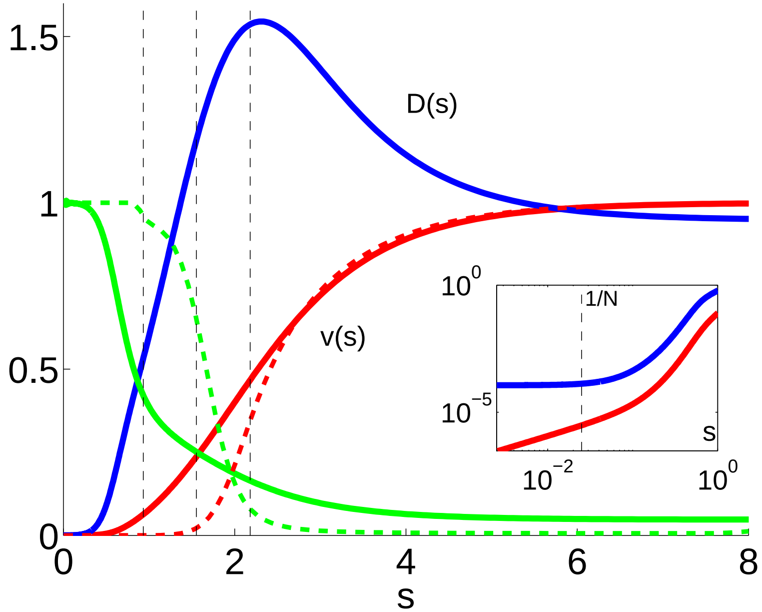
From "Derrida" we have an expression for v in the $N \to \infty$ limit.

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

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



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	$a_s \sim N$			$a_s \approx \left[1 - e^{-2(s-s_2)}\right]^{-1} a_\infty$
v_s	$v = 2D\, s$	$\sim \left(\frac{1}{N}\right)^{\frac{1}{\mu}-1}$		$v_s \approx \left[1 - e^{-(s-s_1)}\right] v_\infty$	
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 of the ESR topic [1]

To what extent does the ESR hold?

As long as $s < 1/N$.

Can it be derived from the NFT?

Yes, provided s is replaced by coarse grained $\bar{s}$.
coarse graining not related to "secondary loops" but to discreteness and/or disorder.

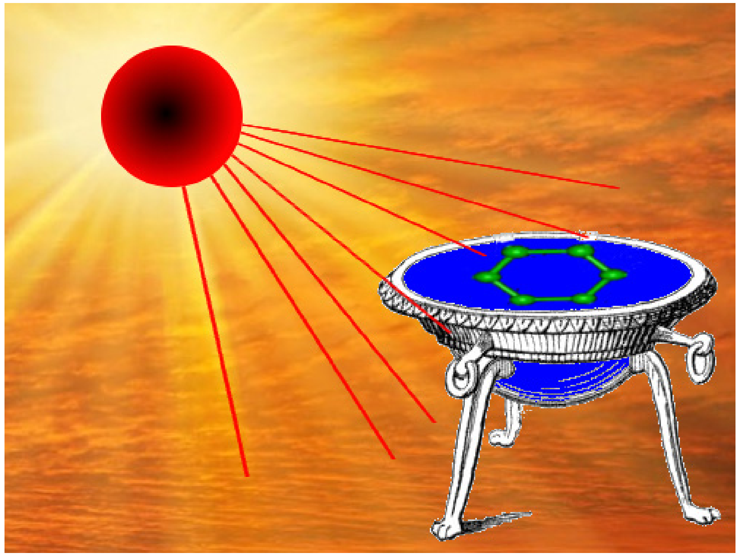
Non-equilibrium version?

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

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

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

Thermodynamics of a “glassy” system [4]



$$w_{nm} = w^{\beta}_{nm} + w^{\nu}_{nm} = w^{\beta}_{nm} + \nu g_{nm}$$

Cold bath: $$\frac{w^{\beta}_{nm}}{w^{\beta}_{mn}} = \exp\left[-\frac{E_n - E_m}{T_B}\right]$$

Hot source: $$g_{nm} = g_{mn}$$

w^{ν} by themselves - induces diffusion / ergodization

w^{β} by themselves - leads to equilibrium

Combined - leads to **NESS**

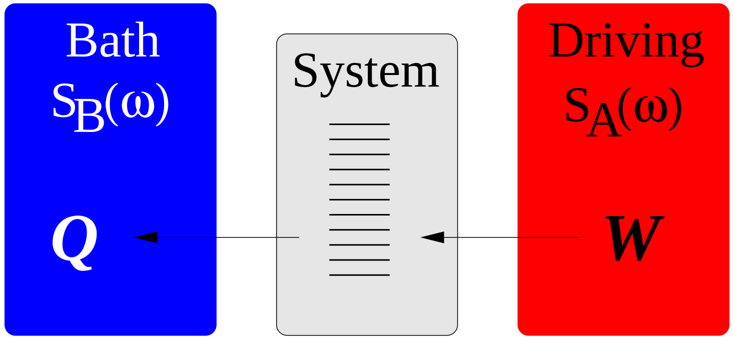
Linear response and traditional FD: $\nu \times \{g\} \ll \{w^{\beta}\}$

Glassy response and Sinai physics: [within a wide crossover regime]

Semi-linear response and Saturation: $\nu \times \{g\} \gg \{w^{\beta}\}$

Generalized FD relation for the rate of energy flow

$$w_{nm} \quad = \quad w^{\beta}_{nm} + w^{\nu}_{nm} \quad = \quad w^{\beta}_{nm} + \nu g_{nm}$$



$$\dot{\mathsf{W}} \quad = \quad \text{rate of heating} \; = \; \frac{D_A(\nu)}{T_{\text{system}}}$$

$$\dot{\mathsf{Q}} \quad = \quad \text{rate of cooling} \; = \; \frac{D_B}{T_B} - \frac{D_B}{T_{\text{system}}}$$

Hence at the NESS:

$$T_{\text{system}} \quad = \quad \left(1 + \frac{D_A(\nu)}{D_B}\right) T_B$$

$$\dot{Q} \; = \; \dot{W} \quad = \quad \frac{1/T_B}{D_B^{-1} + D_A(\nu)^{-1}}$$

Experimental way to extract response:

$$D_A(\nu) \; = \; \frac{\dot{Q}(\nu)}{\dot{Q}(\infty) - \dot{Q}(\nu)} \, D_B$$

$D_A(\nu)$ exhibits LRT to SLRT crossover

$$D_A(\nu) \quad = \quad \left[\overline{\left(\frac{w_n}{w_\beta + w_n}\right)}\right] \left[\overline{\left(\frac{1}{w_\beta + w_n}\right)}\right]^{-1}$$

$$D_{A\,[\text{LRT}]} \quad = \quad \overline{g_n}\;\nu \qquad \text{[weak driving]}$$

$$D_{A\,[\text{SLRT}]} \quad = \quad [\overline{1/g_n}]^{-1}\nu \qquad \text{[strong driving]}$$

Expressions above assume n.n. transitions only.