NONEQUILIBRIUM RESPONSE -II

RECAP

- Dynamical ensembles
- Action: decomposition according to time-reversal symmetry
- Entropy S and frenesy D
- Explicit form for S and D for jump processes
- Random walk
- Response ?

RESPONSE

- Consider a system in nonequilibrium (steady or transient)
- Add perturbation at t=0: Could be change in existing drive/addition of new drive
- For notational simplicity $\varepsilon \to \varepsilon + d\varepsilon$
- Linear change in observable $\langle O(\omega)\rangle_{\varepsilon+d\varepsilon} - \langle O(\omega)\rangle_{\varepsilon} = \chi \, d\varepsilon$
- Response $$\chi \equiv \frac{d}{d\varepsilon}\langle O(\omega)\rangle\Big|_{\varepsilon}$$

So far we have dealt with O(x_t) only

LINEAR RESPONSE

- Trajectory weight $P_\varepsilon(\omega) = e^{-A_\varepsilon(\omega)} P_0(\omega)$

Reference process independent of ε

- Expected value of observable

- $$\langle O(\omega) \rangle_\varepsilon = \sum_\omega P_\varepsilon(\omega) O(\omega) = \sum_\omega e^{-A_\varepsilon(\omega)} P_0(\omega) O(\omega)$$

- Differential response

$$\chi \equiv \frac{d}{d\varepsilon} \langle O \rangle \bigg|_\varepsilon = -\sum_\omega \frac{dA_\varepsilon(\omega)}{d\varepsilon} e^{-A_\varepsilon(\omega)} P_0(\omega) O(\omega)$$

$$= -\langle A'_\varepsilon(\omega) O(\omega) \rangle_\varepsilon$$

Expectation over unperturbed process

- Nonequilibrium linear response

$$\boxed{\frac{d}{d\varepsilon}\langle O(\omega)\rangle\Big|_{\varepsilon} = \frac{1}{2}\underbrace{\langle S_{\varepsilon}'(\omega)O(\omega)\rangle_{\varepsilon}}_{\text{Entropic component}} - \underbrace{\langle D_{\varepsilon}'(\omega)O(\omega)\rangle_{\varepsilon}}_{\text{Frenetic component}}}$$

- $S_{\varepsilon}' = \dfrac{dS_{\varepsilon}(\omega)}{d\varepsilon}$ and $D_{\varepsilon}' = \dfrac{dD_{\varepsilon}(\omega)}{d\varepsilon}$ are the excess entropy and frenesy generated due to the perturbation

- Fluctuation-dissipation theorem in nonequilibrium

- Take O=1

$$\frac{d}{d\varepsilon}\langle O\rangle = 0 \;\Rightarrow\; \frac{1}{2}\langle S'_\varepsilon(\omega)\rangle = \langle D'_\varepsilon(\omega)\rangle$$

Irrespective of the system details

- Linear response formula can be recast as

$$\boxed{\frac{d}{d\varepsilon}\langle O(\omega)\rangle\Big|_\varepsilon = \frac{1}{2}\langle S'_\varepsilon(\omega); O(\omega)\rangle_\varepsilon - \langle D'_\varepsilon(\omega); O(\omega)\rangle_\varepsilon}$$

Covariance <A;B>= <AB>-<A><B>

DISCUSSIONS

- Observable correlations, easily measurable in experiments and simulations
- Physical meaning in terms of excess entropy and frenesy
- Crucial for out of equilibrium situations
- Prescription for finding S and D
- No restriction on initial distribution
- Does not work if perturbation changes the trajectory space

BACK TO KUBO FORMULA

- Unperturbed state is equilibrium
- Take observable $Y(\omega) = O(x_t) - O(x_0)$ (time anti-symmetric)
- Susceptibility $\chi \equiv \left.\frac{d\langle Y\rangle}{d\varepsilon}\right|_0 = \frac{1}{2}\langle S_0' \, Y(\omega)\rangle_0 - \cancelto{0}{\langle D_0' \, Y(\omega)\rangle_0}$

Equilibrium is time-reversal invariant, average of anti-symmetric observable is zero

$$\chi = \frac{1}{2}\left[\langle S_0' \, O(x_t)\rangle_0 - \langle S_0' \, O(x_0)\rangle_0\right]$$

- Second term

$$\langle S_0' O(x_0)\rangle_0 = \sum_\omega S_0'(\omega)\, O(x_0)\, P_{eq}(\omega)$$

$$= -\sum S_0'(\omega)\, O(x_t)\, P_{eq}(\omega)$$

$$= -\langle S_0' O(x_t)\rangle_0$$

- Combining $\left.\dfrac{d\langle O(x_t)\rangle}{dh}\right|_0 = \langle S_0' O(x_t)\rangle_0$

- Only entropy, Kubo formula!

GREEN-KUBO RELATIONS

- Prediction of transport coefficient near equilibrium
- Green-Kubo relation : $\langle j \rangle_\varepsilon = \varepsilon \int_0^\infty ds \ \langle j(0) j(s) \rangle_0$
- $\langle j \rangle$ conjugate flux (current/time) generated by the thermodynamic force ε
- Time integrated current $J(t) = \int_0^t ds \ j(s)$, anti-symmetric under time-reversal
- Entropy flux generated $S_0' = \beta J$

- Response for J around equilibrium $\left.\dfrac{d\langle J\rangle}{d\varepsilon}\right|_0 = \dfrac{1}{2}\langle S_0' J\rangle_0 = \dfrac{\beta}{2}\langle J^2\rangle_0$

- Current $\langle J(t)\rangle_\varepsilon = \dfrac{\varepsilon\beta}{2}\langle J^2(t)\rangle_0$ $= \dfrac{\varepsilon\beta}{2}\int_0^t ds \int_0^t ds' \; \langle j(s)\, j(s')\rangle_0$

$$= \varepsilon\beta \int_0^t ds \int_0^s ds' \langle j(s)\, j(s')\rangle_0$$

(Time-translation invariance) $$= \varepsilon\beta \int_0^t ds \int_0^s ds' \; \langle j(0)\, j(s')\rangle_0$$

- Derivative wrt t

$$\boxed{\langle j(t)\rangle_\varepsilon = \varepsilon\beta \int_0^t ds \; \langle j(0) j(s)\rangle_0}$$

→ Limit $t \to \infty$: conventional form of Green-Kubo relations

OTHER OBSERVABLES

- Time-symmetric observables $\theta O = O$
- Susceptibility $\left.\dfrac{d\langle O\rangle}{d\varepsilon}\right|_0 = -\,\langle D_0'(\omega)O(\omega)\rangle_0$
- Frenesy is important then even in equilibrium
- Example: momentum current generated by shear, total number of jumps (cf random walk) etc

EXAMPLE I- RANDOM WALK

- Random walk on a periodic 1d lattice,
- Bias : driving field ε, jump rates $p(\varepsilon), q(\varepsilon)$
- Local detailed balance : work done by the drive over one jump $W = \beta\varepsilon\Delta x$: released as entropy in the reservoir
- Condition $p/q = e^{\beta\varepsilon}$, does not specify the rates completely
- Parametrize $p(\varepsilon) = \psi(\varepsilon)e^{\beta\varepsilon/2}, q(\varepsilon) = \psi(\varepsilon)e^{-\beta\varepsilon/2}$
- Trajectory: sequence of left/right jumps - N_R, N_L

- Entropy flux

$$S(\omega) = \sum_i \log \frac{k(x_i, x_{i+1})}{k(x_{i+1}, x_i)} = (N_R - N_L)\log \frac{p}{q} = \beta\varepsilon\ J$$

- Frenesy

$$D(\omega) = -\frac{1}{2}\sum_i \log k(x_i, x_{i+1})k(x_{i+1}, x_i) + \int_0^t ds\ [\lambda(x_s) - \lambda_0(x_s)]$$

$$= -\frac{1}{2}(N_R + N_L)\log pq + (p + q - 2)t$$

- Observable $J = N_R - N_L$ (integrated current upto time t),

  $N = N_R + N_L$ (total number of jumps upto time t;
  time-symmetric current)

CURRENT

- Of course, $\langle J \rangle_\varepsilon = (p - q)t$

- Differential response of current is $(p' - q')t$

- Use response formula:

$$\left.\frac{d\langle J \rangle}{d\varepsilon}\right|_\varepsilon = \frac{\beta}{2}\langle J; J \rangle_\varepsilon + \frac{1}{2}\frac{d}{d\varepsilon}\log(pq)\ \langle N; J \rangle_\varepsilon$$

$$= \frac{\beta}{2}\langle J; J \rangle_\varepsilon + \frac{1}{2}\frac{\psi'(\varepsilon)}{\psi(\varepsilon)}\ \langle N; J \rangle_\varepsilon$$

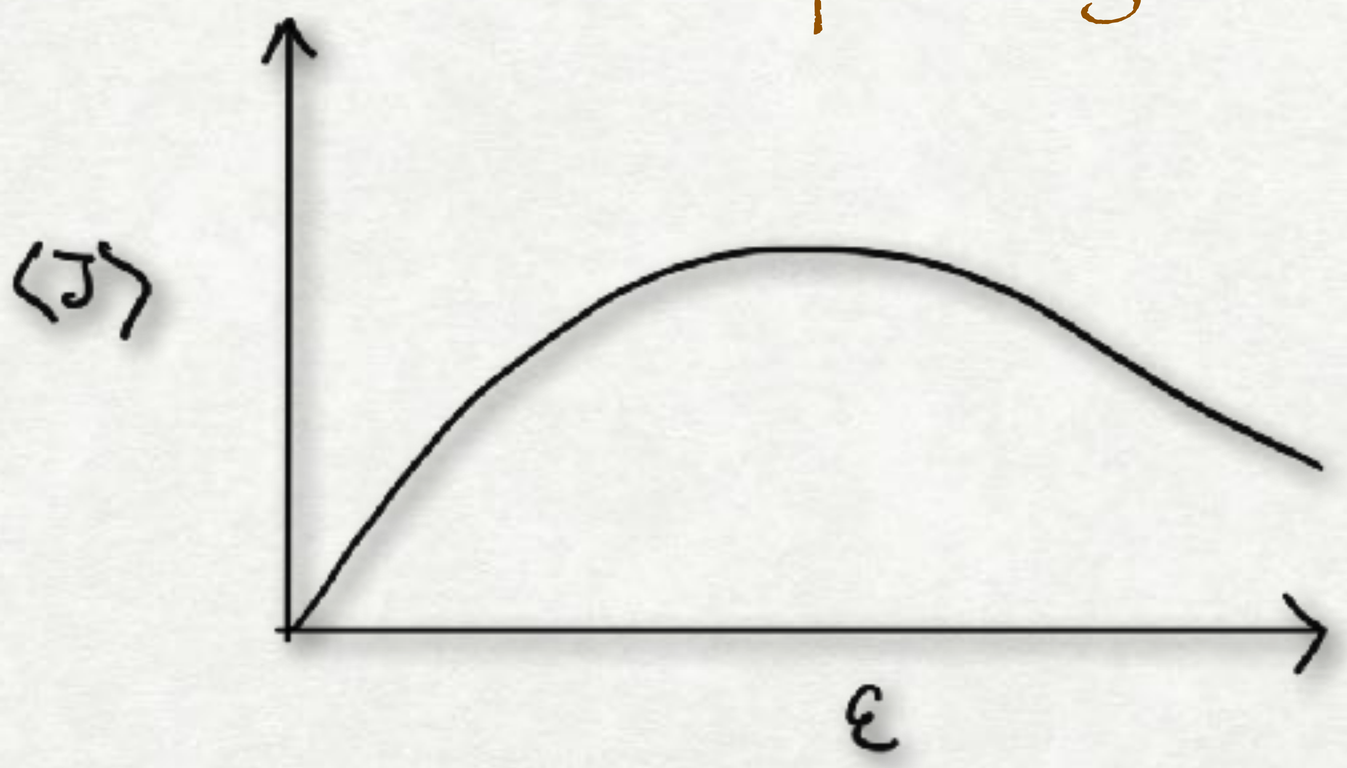
- N_R, N_L are independent Poisson processes with mean pt, qt : correlations can be explicitly calculated

- Physical meaning of different terms…
- Around equilibrium: second term vanishes, purely entropic

(Always positive) $$\left.\frac{d\langle J\rangle}{d\varepsilon}\right|_0 = \frac{\beta}{2}\langle J; J\rangle_0$$ Green-Kubo

- Both terms contribute in general
- Differential response can even be negative if $\psi'(\varepsilon)$ is enough negative: crucial role of symmetric pre-factor $\psi(\varepsilon)$

"Getting more from pushing less"



- Many examples: Barma & Dhar 1984?
  Zia 2002
  Baerts et al 2013

TRAFFIC

- Time-symmetric current / traffic $N = N_R + N_L$
- Of course, $\langle N \rangle = (p+q)t$
- Response:

$$\left.\frac{d\langle N\rangle}{d\varepsilon}\right|_{\varepsilon} = \frac{\beta}{2}\langle J;N\rangle_{\varepsilon} + \frac{1}{2}\frac{d}{d\varepsilon}\log(pq)\ \langle N;N\rangle_{\varepsilon}$$

$$= \frac{\beta}{2}\langle J;N\rangle_{\varepsilon} + \frac{1}{2}\frac{\psi'(\varepsilon)}{\psi(\varepsilon)}\ \langle N;N\rangle_{\varepsilon}$$

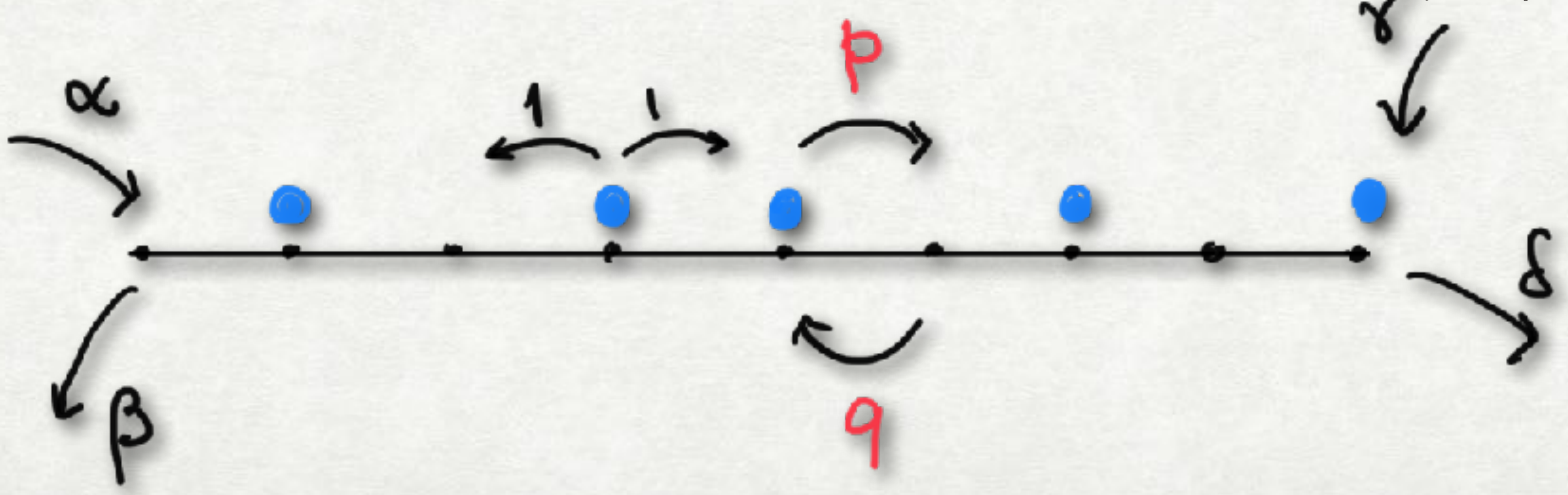
- Around equilibrium ($\varepsilon = 0$): first (entropic) term vanishes — response is purely frenetic

EXAMPLE II - BOUNDARY DRIVEN SEP

- Symmetric exclusion process on a 1D lattice: $s_i = 0,1; i = 1,2,\ldots L$
- Symmetric hopping at the bulk 10 <—> 01 with rate 1
- Attached to particle reservoirs at the boundaries, different chemical potentials μ_L, μ_R
- Particles enter and exit at the boundaries
- Perturbation: bias ε across one bond; rates p,q

$$p/q = e^{\beta\varepsilon}$$

$$\frac{\alpha}{\beta} = e^{\beta\mu_L}$$



$$\frac{\gamma}{\delta} = e^{\beta\mu_R}$$

- Example of perturbing with a different drive
- Configuration $x := \{s_i; i = 1,2,\ldots L\}$
- Escape rate:

$$\lambda(x) = \sum_{i \neq k} [s_i(1 - s_{i+1}) + (1 - s_i)s_{i+1}] + ps_k(1 - s_{k+1}) + q(1 - s_k)s_{k+1} + \alpha(1 - s_1) + \beta s_1 + \gamma(1 - s_L) + \delta s_L$$

driven bond: (k—k+1)

- p=q=1: still Nonequilibrium (boundary drive) for $\alpha/\beta \neq \gamma/\delta$
- Observable: current across the central bond $J = N_{\rightarrow} - N_{\leftarrow}$

  nonzero even for $\varepsilon = 0$

- Response around $\varepsilon = 0$

- Only p,q dependent terms are relevant

- Entopy flux

$$\boxed{S(\omega) = (N_{\rightarrow} - N_{\leftarrow}) \log \frac{p}{q} = \varepsilon \beta J} \quad + \varepsilon \text{ independent terms}$$

- Frenesy

$$\boxed{D(\omega) = -\frac{1}{2} (N_{\rightarrow} + N_{\leftarrow}) \log pq + p\, t_{10} + q\, t_{01}} \quad + \varepsilon \text{ independent terms}$$

- t_{10}, t_{01} : total time (in t) during which local configuration is 10(01) at the k-bond (symmetric under time-reversal)

- Conductivity: change in current due to added drive

$$\left.\frac{d\langle J\rangle}{d\varepsilon}\right|_{\varepsilon} = \frac{\beta}{2}\langle J;J\rangle_{\varepsilon} + \frac{1}{2}\frac{d}{d\varepsilon}\log(pq)\ \langle N;J\rangle_{\varepsilon} - p'\langle t_{10};J\rangle_{\varepsilon} - q'\langle t_{01};J\rangle_{\varepsilon}$$

- More complicated form: effect of interaction
- Modified Green-Kubo even for $\varepsilon = 0$: frenetic contribution
- Different perturbation: change in chemical potential of one of the reservoirs —> form changes

- Change in boundary drive: $\mu_L \to \mu_L + d\mu_L$
- Different terms become relevant: involving jumps at the left boundary
- Entropy $S(\omega) = N_L^{\rightarrow} \log \frac{\alpha}{\beta} + N_L^{\leftarrow} \log \frac{\beta}{\alpha} = J_L^{in} \log \frac{\alpha}{\beta} = J_L^{in} \beta \mu_L$

  $+\mu_L$ independent terms
- Net influx at the left boundary $J_L^{in} = N_L^{\rightarrow} - N_L^{\leftarrow}$
- Frenesy $D(\omega) = -\frac{1}{2}(N_L^{\rightarrow} + N_L^{\leftarrow}) \log \alpha\beta + \alpha t_0 + \beta t_1$ $+\mu_L$ independent terms
- t_0, t_1 time during which $s_1 = 0{,}1$ respectively

- Response of k-bond current (still)

$$\left.\frac{d\langle J\rangle}{d\mu_L}\right|_{\mu,\varepsilon} = \frac{\beta}{2}\langle J_L^{in}; J\rangle_{\mu,\varepsilon} + \frac{1}{2}\frac{d}{d\mu_L}\log(\alpha\beta)\ \langle N_L; J\rangle_{\mu,\varepsilon} - (\alpha' - \beta')\langle t_0; J\rangle_{\mu,\varepsilon}$$

- Kubo-term is a correlation of different currents - perturbation and observable are not conjugate

- Frenetic term depends explicitly on how α, β depend on the chemical potential

SUMMARY

- General prescription for Nonequilibrium linear response
- Reduction to equilibrium limit
- Explicit examples: random walk, boundary driven SEP
- Time-symmetric (kinematical) aspects become crucial