Resonant Response in Nonequilibrium Stationary States

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and
3rd Lars Onsager Symposium
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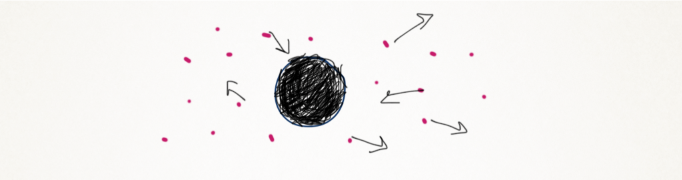
Outline

Markov Process



$$H = \frac{P^2}{2m} + V(x) + \text{interactions}, \rightarrow \frac{dx}{dt} = f(x) + \xi(t),$$

$$\langle \xi(t) \rangle = 0, \qquad \langle \xi(t)\xi(t') \rangle = 2\beta\delta(t - t')$$

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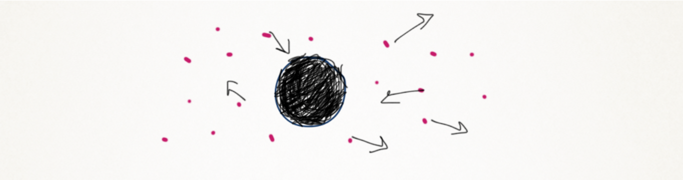

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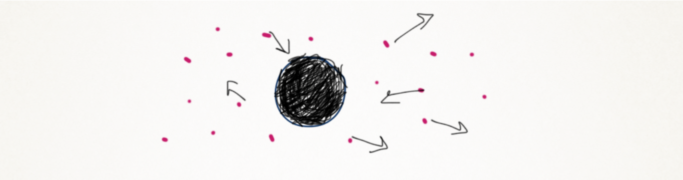

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Stationary States

- Statistical description : probability density $\rho(x,t)$

$$\mathcal{L}\rho = \partial_t \rho$$

- The observables: e. g. Particle current

$$j(t) = \langle v \rangle = \int v(x,t)\rho(x,t)dx$$

- Stationary state: $t \to \infty \Rightarrow \rho(x,t) \to P_{ss}$

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Equilibrium stationary states (ESS)

- Once the system has reached the stationary state, can we determine whether a system is in equilibrium or not?
- Detailed balance

$$P(x,t|x',t')\rho_{ss}(x') = P(x',t|x,t')\rho_{ss}(x)$$

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Linear response

$$\frac{\partial \rho_p}{\partial t} = \mathcal{L}\rho_p + \varepsilon e^{i\omega t}\mathcal{L}_p\rho_p$$

$$\rho_p \approx P_{ss} + \varepsilon e^{i\omega t} R, \qquad R = \text{Response function}$$

$$(\mathcal{L} - i\omega)R = \mathcal{L}_p P_{ss}$$

If we know R we can calculate the response for observables

$$j_p = j_{ss} + \varepsilon\mu(\omega)$$

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Einstein Relation and Kubo Formula

Is P_{ss} is a ESS,

- Einstein Relation: for $\omega = 0$

$$\mu = \beta D = \int_0^\infty \langle v(t_0) v(t_0 + \tau) \rangle d\tau, \quad D = \text{ Diffusion coefficient}$$

- Kubo's Formula

$$\mu(\omega) = \int_0^\infty \langle v(t_0) v(t_0 + \tau) \rangle e^{i\omega\tau} d\tau,$$

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Resonant Response

- $(\mathcal{L} - i\omega)R = \mathcal{L}_p P_{ss} \qquad \Rightarrow \qquad R = (i\omega - \mathcal{L})^{-1}\mathcal{L}_p P_{ss}.$
- For $Re[s] < 0$

$$(s - \mathcal{L})^{-1} = \int_0^\infty dt\, e^{st} e^{t\mathcal{L}}$$

- We obtain $(s = -\delta + i\omega)$

$$R = \lim_{\delta \to 0^+} \int_0^\infty dt\, e^{st} e^{t\mathcal{L}} \mathcal{L}_p P_{ss}.$$

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Resonant Response

- By normalization we have that

$$e^{t\mathcal{L}}\mathcal{L}_p P_{ss} = \sum_{\lambda\neq 0} c_\lambda e^{\lambda t} P_\lambda$$

where $\{P_\lambda\}_\lambda$ is complete basis of eigenfunctions for $\mathcal{L}$, with $\mathcal{L}P_\lambda = \lambda P_\lambda,\ \lambda = 0 \ \Rightarrow\ P_0 = P_{ss}$

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- Proposition: If P_{ss} is an equilibrium state then the spectrum of $\mathcal{L}$ is real, i. e. $\lambda \in \mathbb{R}$

  The proof is based on a symmetry relation for the Fokker-Plank operator $\mathcal{L}$ due to J. Kurchan [*J. Phys. A: Math. and Gen.* **31**, 3719 (1998).]

- The amplitude of the response R has a maximum at $\omega = 0$.

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Relaxation–Response Relation

Relaxation and Linear Response

- J = flux operator $\Rightarrow j_{ss} = \langle J \rangle_{ss}$.
- $\varepsilon e^{i\omega t} J_p$ = perturbing flux operator

$$j_p(t) = \langle J + \varepsilon e^{i\omega t} J_p \rangle_p$$

- At first order in ε we have

$$\mu(\omega) := \frac{j_p - j_{ss}}{\varepsilon} = \langle J_p \rangle_{ss} + \int_0^\infty \langle J e^{t\mathcal{L}} \mathcal{L}_p \rangle_{ss} dt.$$

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- $e^{t\mathcal{L}}\mathcal{L}_p P_0$ has integral zero. Then,

$$P_{sp}(t) := P_{ss} + \gamma^{-1} e^{t\mathcal{L}}\mathcal{L}_p P_0$$

is properly normalized to 1 independently of the γ value.

- Then

$$\langle J e^{t\mathcal{L}}\mathcal{L}_p \rangle_{ss} = \langle J \rangle_{sp}(t) - \langle J \rangle_{ss}$$

- $$\langle J e^{t\mathcal{L}}\mathcal{L}_p \rangle_{ss} = j^*(t) - j_{ss}$$

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- The frequency-dependent mobility

$$\mu(\omega) = \langle J_p \rangle_{ss} + \gamma^{-1} \int_0^{\infty} (j^*(t) - j_{ss}) e^{i\omega t} dt$$

- $j^*(t)$ = time–dependent average flux which relaxes to a stationary value, $j^*(t) \to j_{ss}$ when $t \to \infty$, starting with a specific initial conditions

$$P_{initial} = P_{ss} + \gamma \mathcal{L}_p P_0$$

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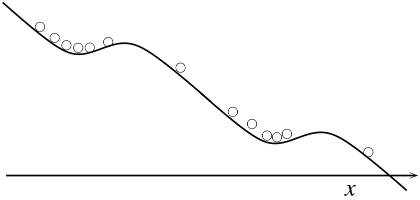
Numerical simulation



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- Langevin equation:

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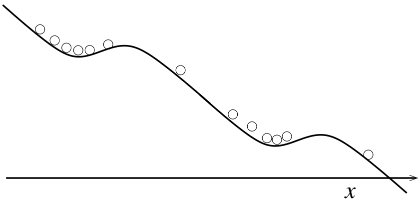

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- The curren operator is $J = f(x) + \beta^{-1}\partial_x$.
- The perturbing operator is $\mathcal{L}_p = -\partial_x$
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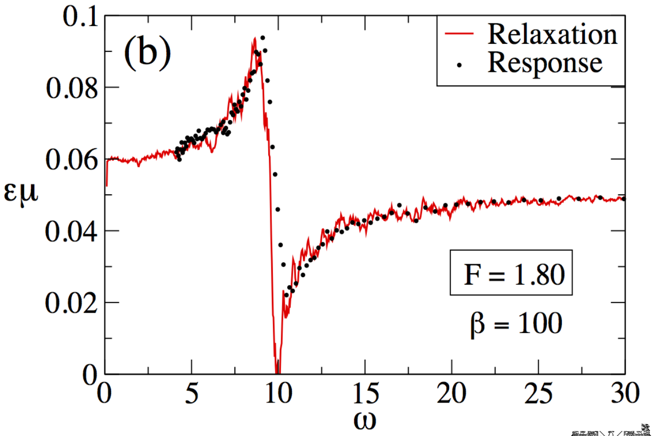

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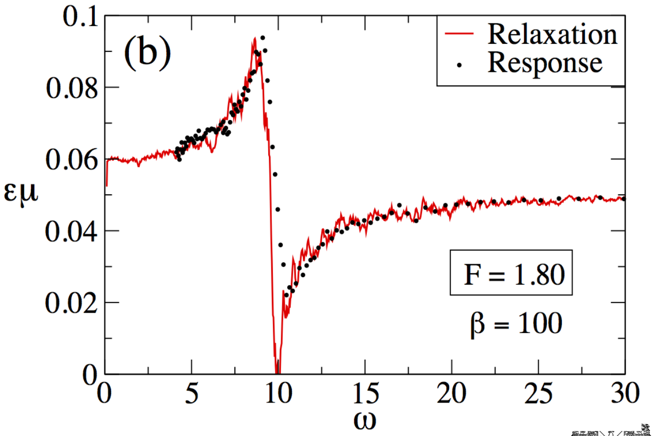

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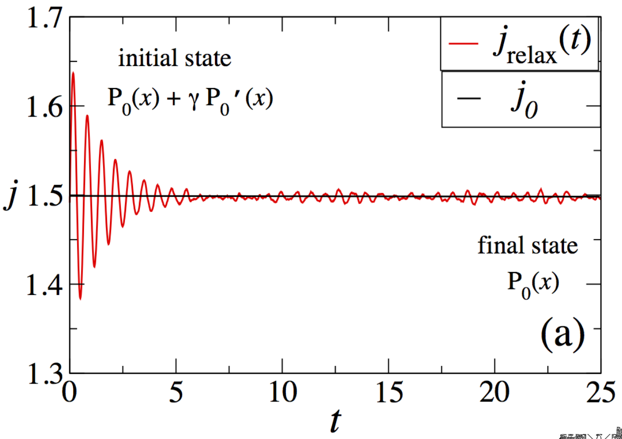

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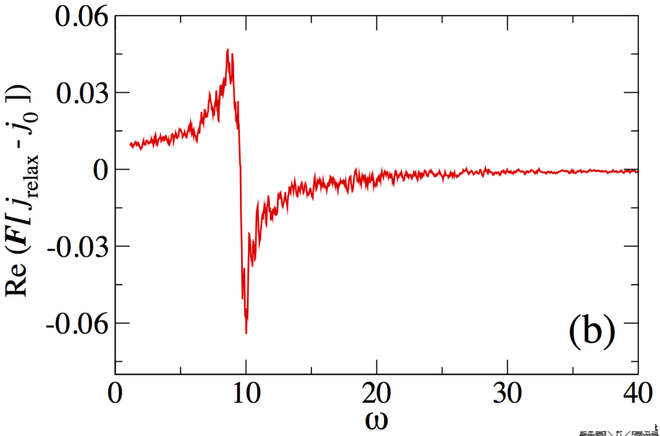

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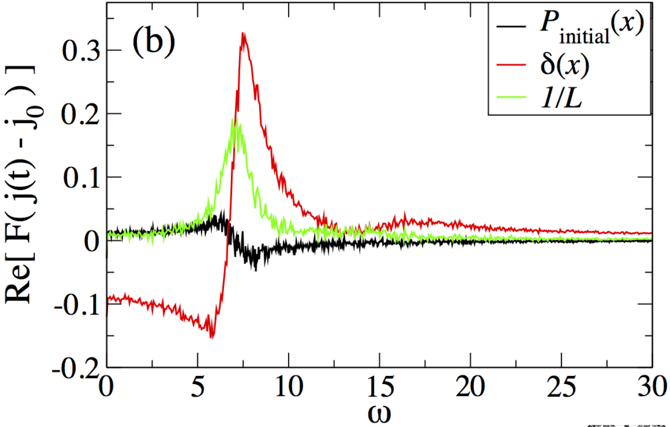

Conclusions

- If the system is in a NESS, it may show a resonant response at the frequencies given by the imaginary part of the complex eigenvalues.
- We have shown a relation between the *relaxation* of the system and its *response*.
- We tested these predictions by numerical simulations.

THANKS!