Energy Fluctuations in Driven, Thermalizing and Driven Dissipative Systems

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with

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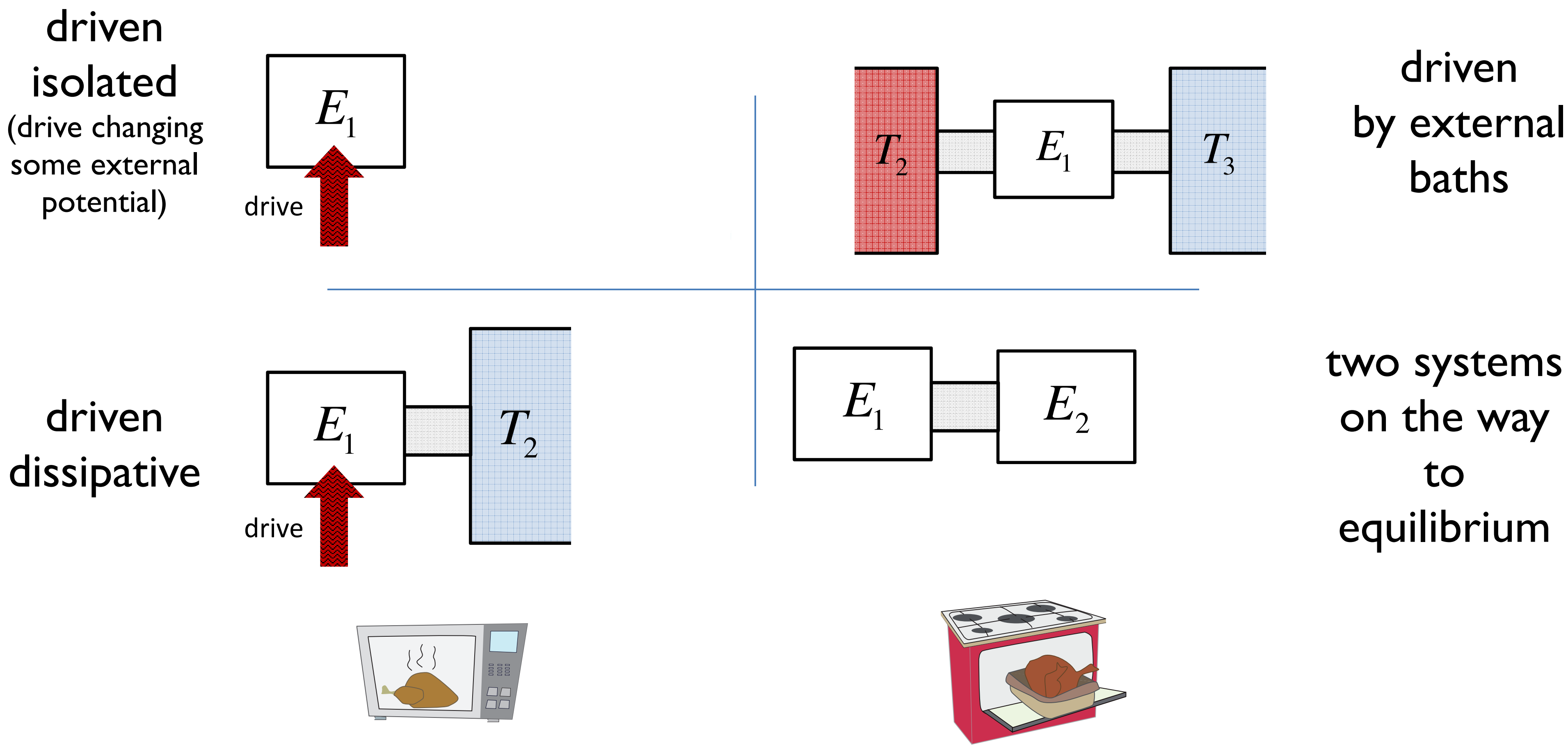
Discussed Energy Fluctuation in



Can say concrete statements when
relaxation time of subsystem << drive and coupling times
(note combined system may still be far from equilibrium)

Outline

- Discuss first in details the driven isolated case

- In particular observe *two broad classes of distributions*

- Illustrate the idea behind derivation in a trivial example

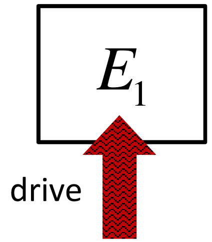
- Derivation and conditions for the relation to hold -
  derive using fluctuation relations (*quantum version see poster by Guy Bunin*)

- [Illustrate on another example (driven XY model in1d, driven quantum transverse field Ising model in 1d and particle in a chaotic cavity)]

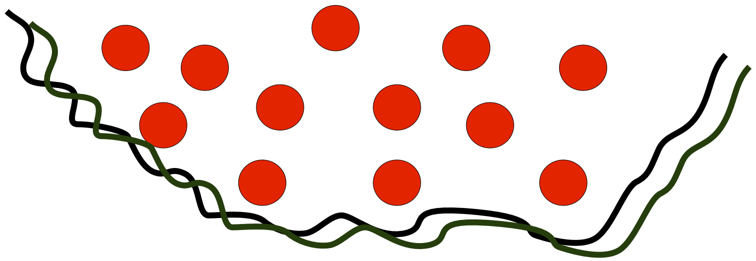
- Results for *driven dissipative, thermalizing and drive by external baths*

- Summarize

Driven Isolated - Setup



Many body ***isolated*** system in a potential

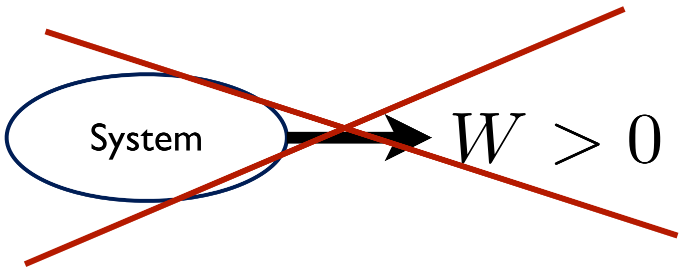


$$t + \delta t$$

Motivation:
cold atom systems, trapped ions...

Due to noise in the system the potential is fluctuating in time

2nd law - Lord Kelvin: *No process is possible in which the sole result is the absorption of heat from a reservoir and its complete conversion into work*



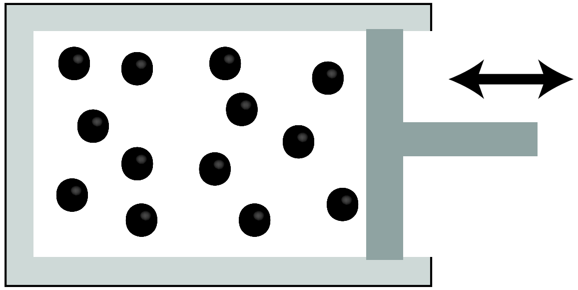
fluctuating potential can only increase (on average) the energy of the system

"X-rays will prove to be a hoax."
-- Lord Kelvin, president, Royal Society, 1895

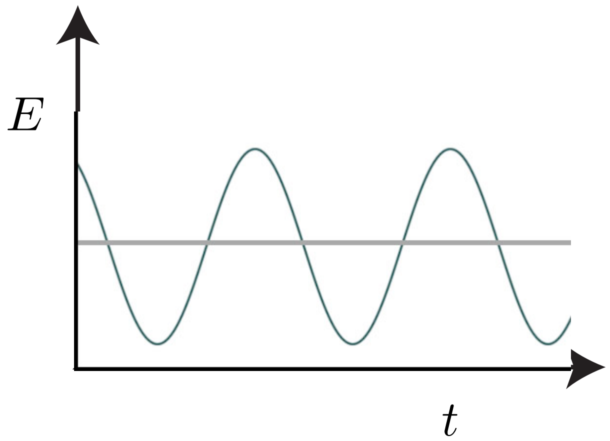
"Radio has no future."
-- Lord Kelvin

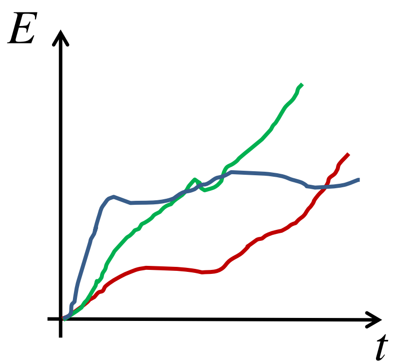
"Heavier than air flying machines are impossible."
-- Lord Kelvin

Essentially identical question: move piston with a given cyclic protocol



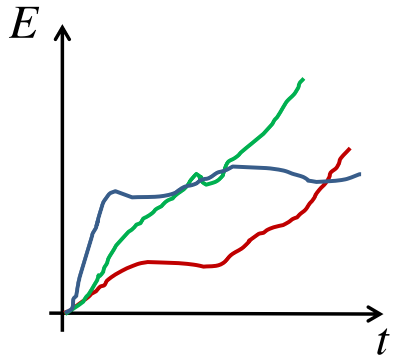
Thermodynamics - **adiabatic** process energy will remain constant every time cycle is completed



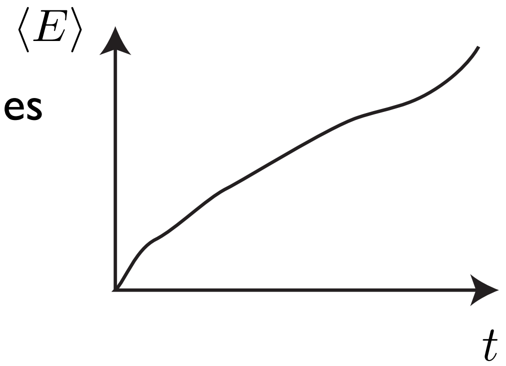


irreversible
process every experiment will give a different result (will be visible in small mesoscopic systems

irreversible
process every experiment will give a different result



Second law - repeat experiment many times and the average energy will always increase



Several questions (begin to address in this talk):

- Can we say something about the distribution of the final energies?

- How do they compare to changing the energy of the system by coupling the system to a *thermal bath*?

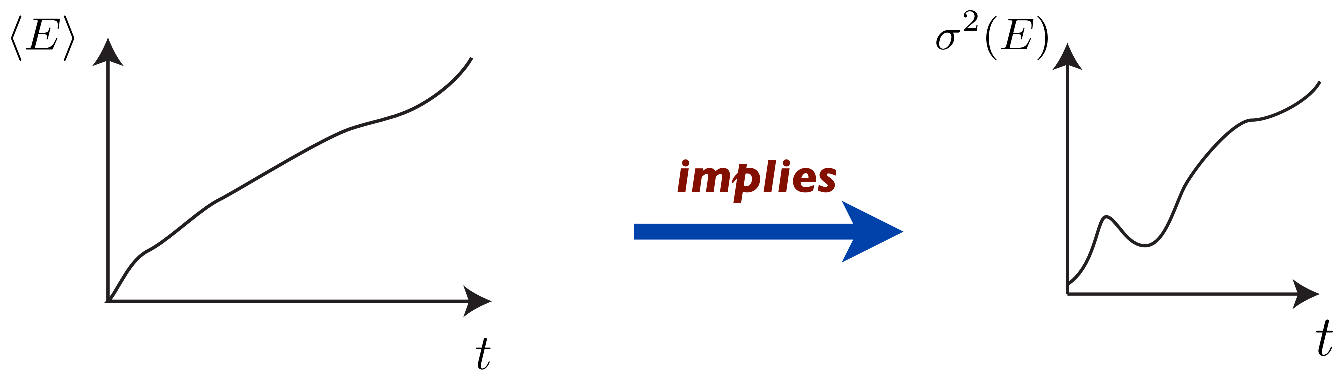
$$\sigma_{eq}^2(E) = T^2 C_v$$ independent of history, given energy know width

Can it be wider/narrower?

- Can one classify different systems with distinct behaviors?

Main Result for this setup

If the drive is slow enough (*still irreversible* + *exact conditions later*) the variance is governed by the rate of energy change in the system



Specifically, given $A(\langle E \rangle) = \partial_t \langle E \rangle$ (depends on how potential varies and for a given system can be controlled to a large extent) we can write:

$$\sigma^2(E) = \sigma_0^2 \frac{A^2(E)}{A^2(E_0)} + 2A^2(E) \int_{E_0}^{E} \frac{dE'}{A^2(E')\,\beta(E')}$$

at initial state

inverse temperature at energy E'

$\beta(E) = \partial \ln \Omega(E) / \partial E$

In essence a direct result of time-reversal symmetry

Implications of results I

thermal bath $\sigma_{eq}^2(E) = T^2 C_v$

Recall, given $A(\langle E \rangle) = \partial_t \langle E \rangle$ we can write:

$$\sigma^2(E) = \sigma_0^2 \frac{A^2(E)}{A^2(E_0)} + 2A^2(E) \int_{E_0}^{E} \frac{dE'}{A^2(E')\,\beta(E')}$$

at initial state

inverse temperature at energy E'

- Depending on the functional form of $A(E), \beta(E)$ the distribution can be larger and somewhat surprisingly *smaller* than the equilibrium distribution.

History Dependent

Implications of results - 2

thermal bath $\sigma_{eq}^2(E) = T^2 C_v$

Recall, given $A(\langle E\rangle) = \partial_t \langle E\rangle$ we can write:

$$\sigma^2(E) = \sigma_0^2 \frac{A^2(E)}{A^2(E_0)} + 2A^2(E) \int_{E_0}^{E} \frac{dE'}{A^2(E')\,\beta(E')}$$

at initial state

inverse temperature at energy E'

- **Two distinct behaviors** depending on integral controlled by upper or lower bound (of course doesn't have to be).

Namely, if integral diverges/converges asymptotically at large E

Illustrate last points for genetic $\beta(E) \propto E^{-\alpha}$ (Goldstone modes, Fermi liquid, Ideal gas ....)

from positivity of specific heat

$$0 < \alpha \leq 1$$

Take $A(\langle E \rangle) = \partial_t \langle E \rangle = c \langle E \rangle^s$, namely, rate of change power law in energy.

demanding finite energy at finite time

$$s \leq 1$$

Results normalized by equilibrium width:

$$\beta(E) \propto E^{-\alpha} \qquad\qquad A\left(E\right) = \partial_t E = E^s$$

$$\eta = 2s - 1 - \alpha$$

Regime	Condition	width
Gibbs-like	$\eta < 0$	$\frac{\sigma^2}{\sigma_{eq}^2} \sim \frac{2\alpha}{\lvert\eta\rvert}$
run-away	$\eta > 0$	$\frac{\sigma^2}{\sigma_{eq}^2} \sim \frac{2\alpha}{\eta}\left(\frac{E}{E_0}\right)^{\eta}$
critical	$\eta = 0$	$\frac{\sigma^2}{\sigma_{eq}^2} \sim 2\alpha \log\left(\frac{E}{E_0}\right)$

$\eta > 0$ integral converges

Broad classification remains valid as long as functions are monotonic, namely $A(E)$

- For large negative η the distribution becomes very narrow

- In terms of entropy the integral becomes

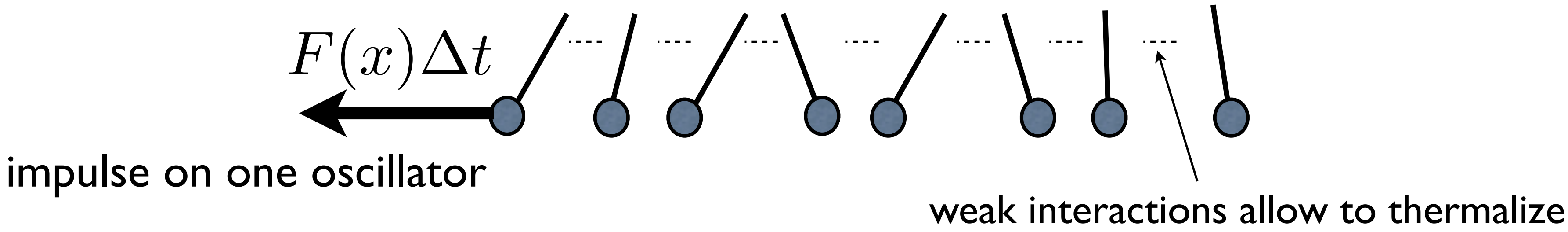
$$\int_{S_0}^{S} \frac{dS'}{\hat{A}^2(S')}$$

boarder line when $S \sim t^2$ (time measures number of cycles)

Derivation

Idea through a (really) simple example

Weakly interacting harmonic oscillators



$$p \to p + F(x)\Delta t$$

particle momentum

- Assume impulse short enough that position doesn't change (in general not needed)

- Let system equilibrate between pulses (quasi-static)

- Allow for general distribution of frequencies $g(\omega)$

Using fact that between impulses system equilibrates

$$\rho(x,v) \propto e^{-\beta(E)E} \qquad E = p^2 + \frac{kx^2}{2}$$

average over initial positions in eq. to obtain the first and second cumulants of the work

$$(p + F(x)\Delta t)^2 - p^2$$

$$\langle w \rangle \equiv A = \langle F(x)^2 \rangle \Delta t^2, \quad \langle w^2 \rangle_c \equiv B = \frac{2}{\beta} \langle F(x)^2 \rangle \Delta t^2$$

note that

$$\beta B = 2A$$

`Fluctuation - dissipation' relation

Comment - results will not change if act on several oscillators and will show completely general

Since we are essentially dealing with a quasi-static process we can describe the evolution of the energy by a Fokker-Planck equation

$$\partial_t P = -\partial_E (A(E)P) + \frac{1}{2}\partial_{EE}(B(E)P)$$

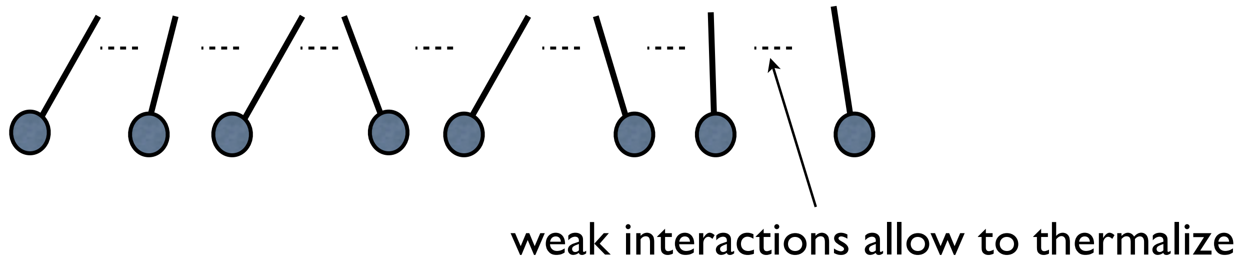
but with $\beta B = 2A$ and time the number of impulses

(Noted before in chaotic particles -C. Jarzynski 93, D. Cohen 99, Ott 79, Chirikov 70s)

↓

$$\sigma^2(E) = \sigma_0^2 \frac{A^2(E)}{A^2(E_0)} + 2A^2(E)\int_{E_0}^{E} \frac{dE'}{A^2(E')\,\beta(E')}$$

Weakly interacting harmonic oscillators



For impulse $F(x) = Cx^r$ can show

$$A(E) \propto E^{\alpha r}$$

Note, here easy to change $A(E)$

Where $\beta(E) \propto E^{-\alpha}$ depends on $g(\omega)$

For 1d harmonic chain $\alpha = 1/2$

$$r < \frac{3}{2} \quad \Rightarrow \quad \sigma^2(E) = \sigma^2_{\text{eq}}(E)\frac{1}{3/2 - r}$$

$$2 \geq r > \frac{3}{2} \quad \Rightarrow \quad \sigma^2(E) = C\sigma^2_{\text{eq}}(E)E^{r-3/2}$$

General derivation via Crooks equality (Evans, Galavoti, Cohen, Jarzynski.....) (will worry about 1/N corrections)

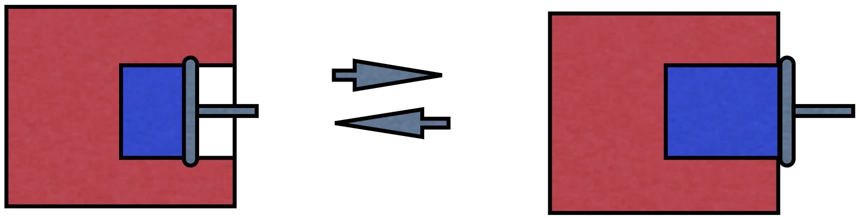
Recall - 1. Liouville's theorem   quantum mechanically - unitarity
(volumes in phase space are conserved under dynamics)

2. Hamiltonian - $\mathcal{H}(\lambda(t))$
3. For a given λ dynamics have time reversal symmetry

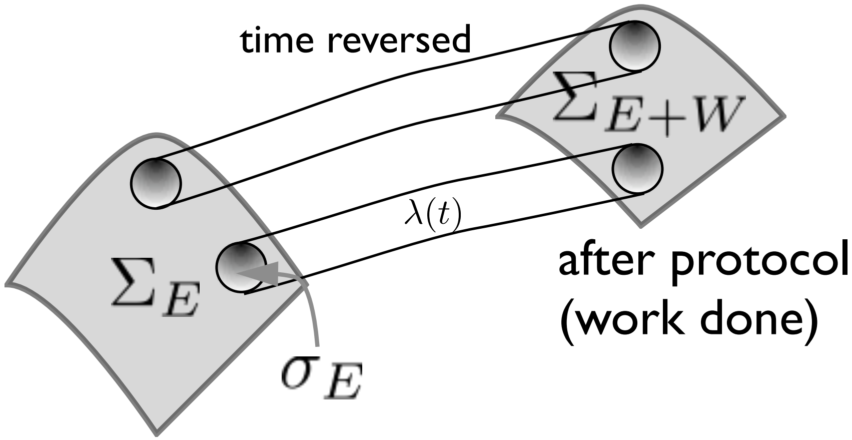
Consider changing $\lambda(t)$ on *isolated* system. $0 < t < \tau$

Forward direction - $\lambda(t)$

Backward direction - $\lambda(\tau - t)$



P. Pradhan, Y. Kafri, D. Levine,, PRE 77, 041129 (2008)



Isolated system - phase space
(microcanonical)

$$P_F(W,E) = \frac{\sigma_E}{\Sigma_E}$$

$$P_R(-W,E+W) = \frac{\sigma_E}{\Sigma_{E+W}}$$

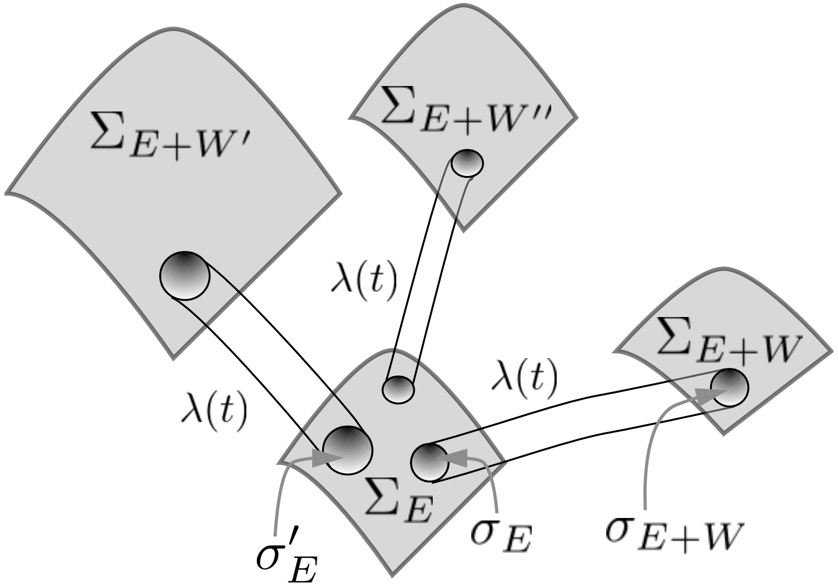
Then

$$\frac{P_F(W,E)}{P_R(-W,E+W)} = \frac{\Sigma_{E+W}}{\Sigma_E} = \exp(S_{\lambda_F}(E+W) - S_{\lambda_i}(E))$$

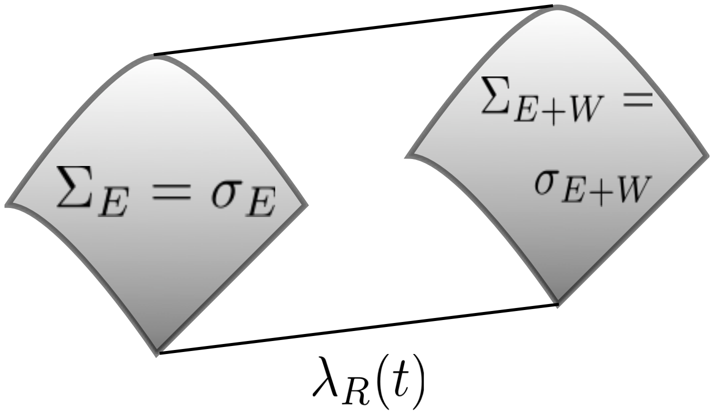
in our case $\lambda_F = \lambda_i$

Easy to obtain the same for quantum taking equilibrium density matrix and unitary evolution

Difference between reversible and irreversible



non-reversible



reversible (closed system đQ=0)

For **periodic** driving

$$\frac{P_F(W,E)}{P_R(-W,E+W)} = \frac{\Sigma_{E+W}}{\Sigma_E} = \exp(S(E+W)-S(E))$$

Using

$$S(E+W)-S(E) \simeq \beta W - \frac{1}{2\sigma_{eq}^2}W^2$$

need $\beta W \ll C_v$

$$P_R(-W,E+W) = P_R(-W,E) + W\partial_E P_R(-W,E)$$

Therefore, to leading order in 1/N the Crooks equality (G. E. Crooks PRE, 60, 2721,1999)

$$\frac{P_F(W,E)}{P_R(-W,E)} = \exp(\beta W)$$

$$\frac{P_F(W,E)}{P_R(-W,E)} = \exp(\beta W)$$

Not surprising that we get the Jarzynski relation to leading order

$$\langle e^{-\beta W} \rangle = 1 + \mathcal{O}(\frac{1}{N})$$

(C. Jarzynski, PRL, 78, 2690 (1997))

With the relation established for an *isolated* system to get the Fokker-Planck equation look at cumulant of the work from (everything up to 1/N)

$$\ln\langle e^{-\beta W}\rangle$$

$$\beta\langle W^2\rangle_c = 2\langle W\rangle + \mathcal{O}(1/N)$$

$$\beta B = 2A + \mathcal{O}(1/N)$$

$$\partial_t P = -\partial_E(A(E)P) + \frac{1}{2}\partial_{EE}(B(E)P)$$

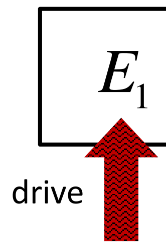
For Fokker-Planck to be valid need to demand third cumulant small

$$\beta^2\langle w^3(E)\rangle_c \ll \langle w(E)\rangle_c$$

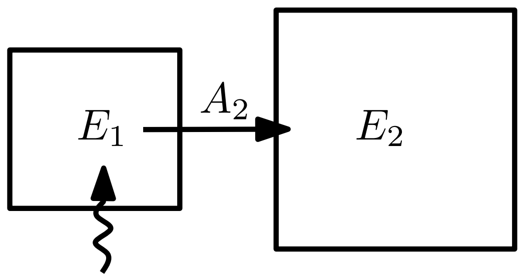
This is the quasi-static demand

Different derivation found in C. Jarzynski 93, D. Cohen 99, Ott 79

So far, Isolated system



The ideas can be generalized to account for a system that is driven and coupled to a bath



Two dimensional Fokker-Planck equation is reduced to one variable (E_1) the following fluctuation-dissipation relation holds

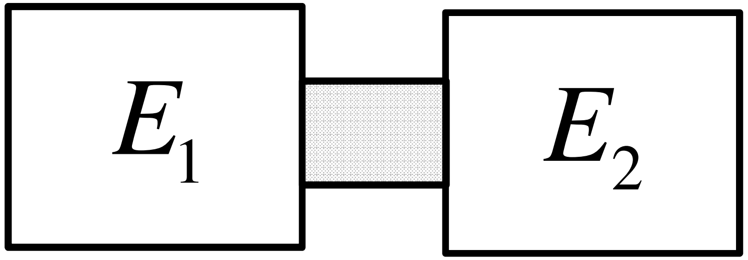
$$\partial_t P = -\partial_{E_1} (A_1 P) + \frac{1}{2}\partial^2_{E_1} (B_{11} P)$$

$$2A_1 - 2\beta_2/\beta_1 A_F = (\beta_1 - \beta_2) B_{11}$$

Drive in reduced equation

Diffusion coefficient of reduced equation

First Case:
No Driving - Just Dissipation (equilibrating)



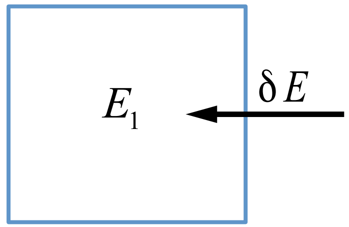
Assume $S = S_1(E_1) + S_2(E_2)$ - weak interactions between systems

$$\langle e^{\Delta S_1 + \Delta S_2} \rangle \simeq \langle e^{-(\beta_2 - \beta_1)\Delta E_B} \rangle = 1$$

Attaching two systems, equilibration

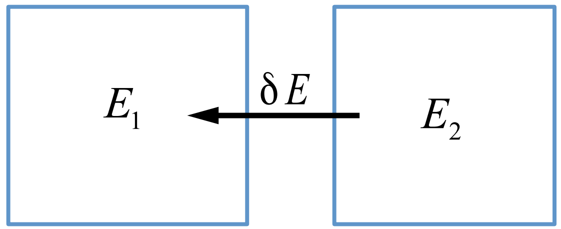
Isolated system, external drive

$$\sigma^2(E) = \sigma_0^2 \frac{A^2(E)}{A^2(E_0)} + 2A^2(E)\int_{E_0}^{E} \frac{dE'}{A^2(E')\beta_1(E')}$$



Two isolated systems, weak interaction (slightly modified fluctuation dissipation relation $2A = (\beta_1 - \beta_2)B$).

$$\sigma_1^2(E) = \sigma_{1_0}^2 \frac{A^2(E)}{A^2(E_0)} + 2A^2(E)\int_{E_0}^{E} \frac{dE'}{A^2(E')\left[\beta_1(E') - \beta_2(E_2)\right]}$$

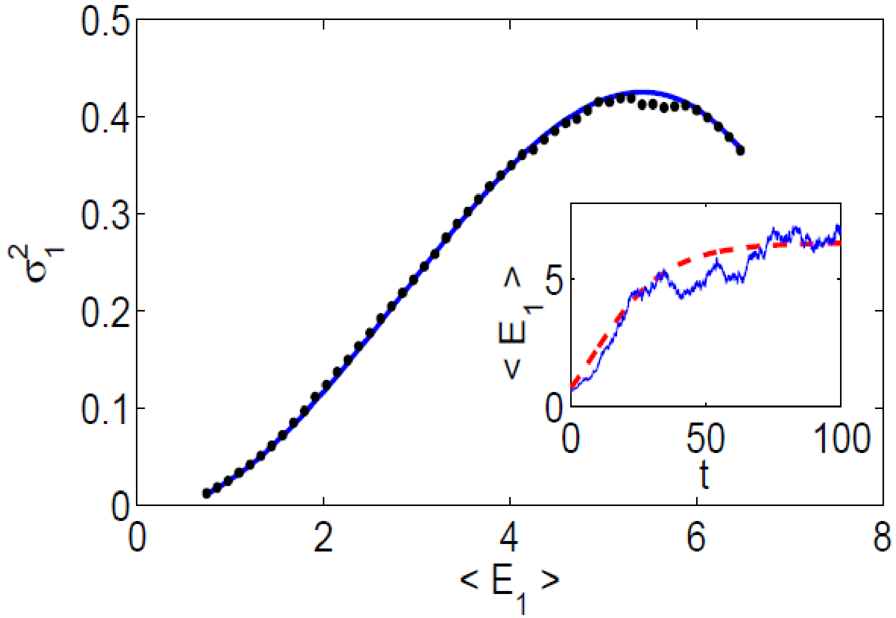


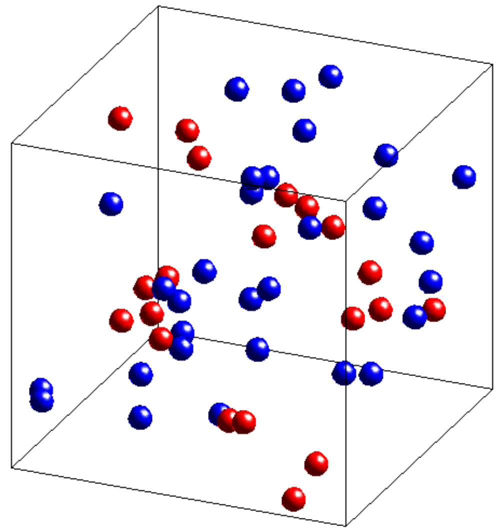
- Fluctuation dynamics of full equilibration process.
- External drive case is formally recovered by taking $T_2 \rightarrow \infty \quad (\beta_2 = 0)$.

Equilibrating systems: simulations

Hard spheres in a box,

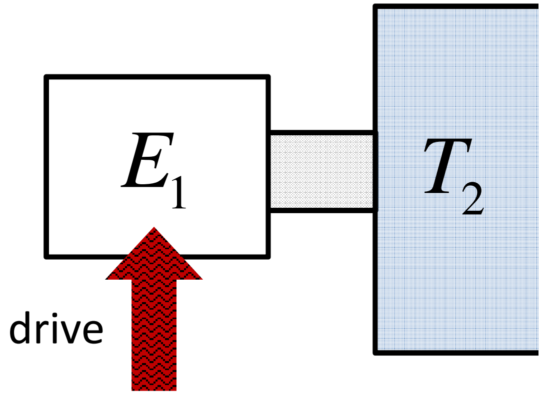
two different masses





$$N_{light} = 30$$
$$N_{heavy} = 20$$

Second Case:
Driven Dissipative

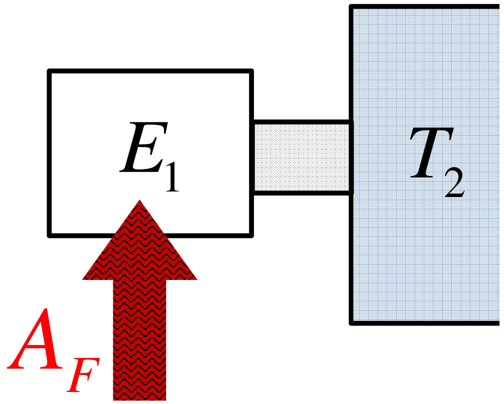


Can write expression for time evolutions of variance.
Present results only for steady-state

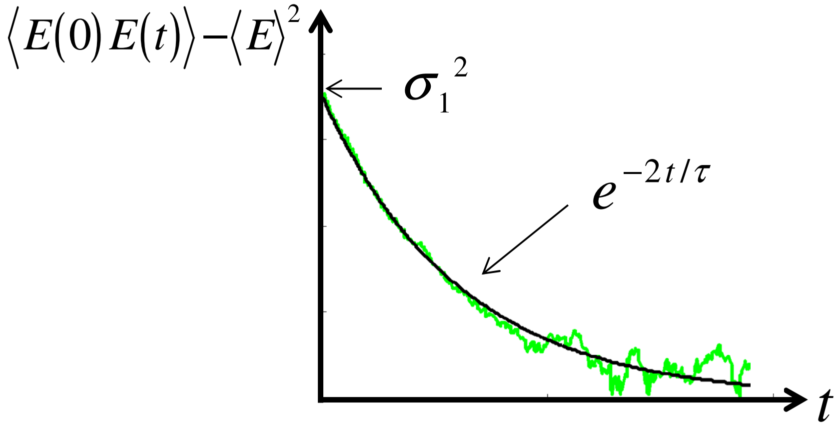
Driven-Dissipative setting: at steady-state

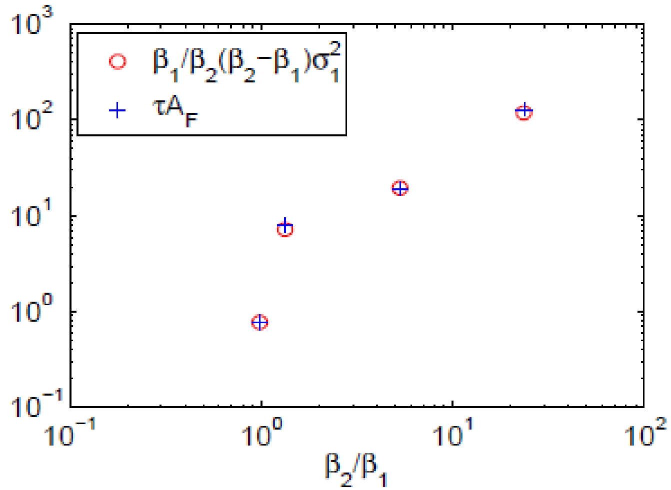
Relation between relaxation time, energy flow and fluctuations:

$$\tau A_F = \frac{\beta_1}{\beta_2}(\beta_2 - \beta_1)\sigma_1^{\ 2}$$



$$\beta_1 = \beta_1(E_1)$$
$$\beta_2 = 1/T_2$$





Derivation - essentially using Fokker-Planck at steady state

Near steady state

$$A_1 = -\frac{1}{\tau} e_1 \ , \quad B_{11} = B_s \qquad \text{with} \qquad e_1 \equiv E_1 - E_1^0$$

$$\partial_t e_1 = -e_1/\tau + \sqrt{B_s}\eta$$

Implies

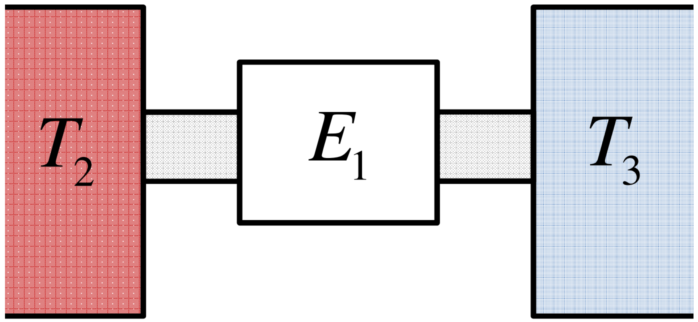
$$\langle e_1(t_1)\, e_1(t_2) \rangle = \frac{B_s \tau}{2} e^{-|t_2 - t_1|/\tau}$$

$$\sigma_1^2 = B_s \tau / 2$$

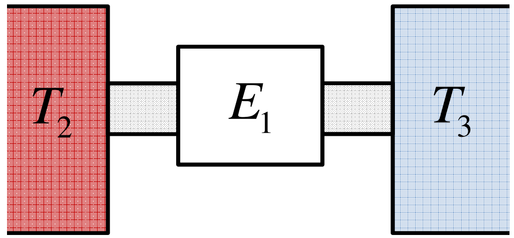
In addition the fluctuation dissipation relation implies at steady-state

$$-2\beta_2/\beta_1 A_F = (\beta_1 - \beta_2)\, B_{11}$$

Third Case:
Driven by two external baths



Can write expression for time evolutions of variance.
Present results only for steady-state

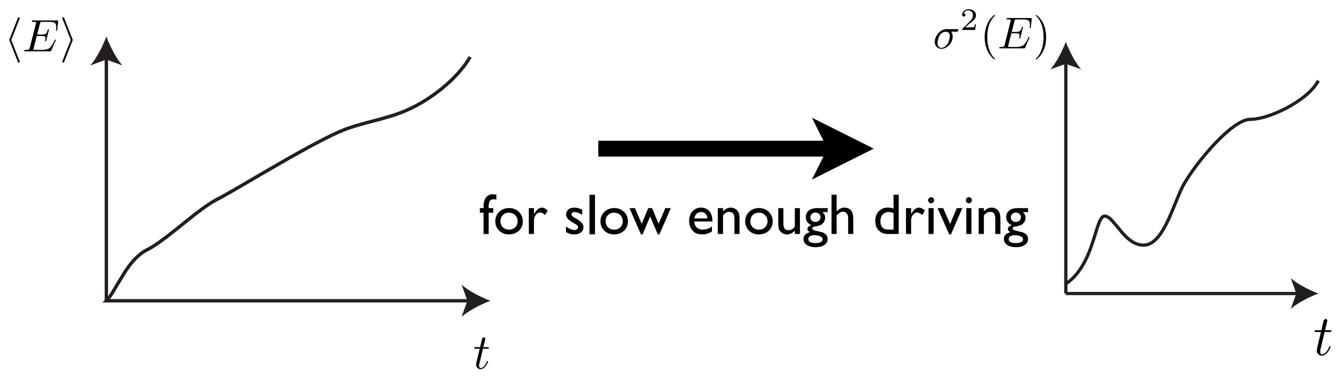


Again a relation between the relaxation time, energy fluctuations and rate of energy injection

$$A_F \tau = \frac{(\beta_1 - \beta_2)(\beta_3 - \beta_1)}{(\beta_3 - \beta_2)} \sigma^2$$

Summary

- For driven isolated systems (noisy potential, driving on purpose...)



- Simple expression - history dependent (in contrast to heating with thermal bath)
- Broadly two different regimes - equilibrium like and wide run away
- Can show hold for other examples (XY model in 1d, TF Ising model (quantum))
- Generalizing to thermalizing systems (teas cups)
- Generalizing to driven dissipative systems (fluctuation dissipation like relation)
- Generalize to drive by two external baths