Non-equilibrium, quantum fluctuations of work

Armen Allahverdyan
(Yerevan Physics Institute)

-- Work fluctuations for non-equilibrium states

-- Why not to apply existing definitions

-- Another definition (PRE, '14)

-- Fluctuation theorem applicable to any initial state

Work

Unitary dynamics

$$U_\tau = \overleftarrow{\exp}\left[-\frac{i}{\hbar}\int_0^\tau \mathrm{d}t\, H(t)\right],$$

Initial and final Hamiltonians

$$H_\mathrm{I} \equiv H(0), \quad H_\mathrm{F} = U_\tau^\dagger H(\tau) U_\tau,$$

Average work is always well-defined energy conservation

$$W = \mathrm{tr}[\rho(H_\mathrm{F} - H_\mathrm{I})],$$

Non-equilibrium state (non-stationary)

$$[\rho, H_\mathrm{I}] \neq 0$$

Two energy measurements

eigenvalues of $H_{\mathrm{I}}, H_{\mathrm{F}}$ **eigenprojectors**

$$\varepsilon_l^{[\mathrm{F}]} - \varepsilon_k^{[\mathrm{I}]}$$

$$\tilde{p}_{kl} = \mathrm{tr}(\Pi_l^{[\mathrm{F}]} \Pi_k^{[\mathrm{I}]} \rho \Pi_k^{[\mathrm{I}]} \Pi_l^{[\mathrm{F}]})$$

probabilities

$$\tilde{W} = \sum_{kl} \tilde{p}_{kl} (\varepsilon_l^{[\mathrm{F}]} - \varepsilon_k^{[\mathrm{I}]}) = \mathrm{tr}(\tilde{\rho} (H_{\mathrm{F}} - H_{\mathrm{I}}))$$

$$\tilde{\rho} = \sum_k \Pi_k^{[\mathrm{I}]} \rho \Pi_k^{[\mathrm{I}]}$$

diagonal

$$\widetilde{W} \neq W,$$

Average is not the average work

Operator of work

Heisenberg operator of work = $H_{\mathrm{F}} - H_{\mathrm{I}}$

$$H(0) = H(t)$$

↓

$$(H_{\mathrm{F}} - H_{\mathrm{I}})|0\rangle = 0,$$

Does not fully relate to energy.
Non-equilibrium example:

$$[H_{\mathrm{F}}, H_{\mathrm{I}}] \neq 0$$

$$\langle 0|H_{\mathrm{F}}^{m}|0\rangle \neq \langle 0|H_{\mathrm{I}}^{m}|0\rangle \quad \text{for} \quad m > 2.$$

"Work" is strictly zero (together with fluctuations),
but energy does change

Two *necessary* conditions for any definition of fluctuating work

Zero work -->

Zero energy exchange

$$\mathrm{tr}(\rho H_{\mathrm{I}}^{m}) = \mathrm{tr}(\rho H_{\mathrm{F}}^{m}) \qquad m \geq 1$$

Average =

= Average work

Quasi-probability

$$\varepsilon_l^{[F]} - \varepsilon_k^{[I]}$$

$$p_{kl} = \mathrm{tr}\left(\rho \, \frac{\Pi_k^{[I]}\Pi_l^{[F]} + \Pi_k^{[F]}\Pi_l^{[I]}}{2}\right)$$

- $\sum_k p_{kl} = \sum_l p_{kl} = 1$ ⟶ $\text{average} = W$
- $p_{k \neq l} = 0$ ⟶ $\mathrm{tr}(\rho H_{\mathrm{I}}^m) = \mathrm{tr}(\rho H_{\mathrm{F}}^m)$

Kirkwood ('33), Terletsky ('37), Dirac ('45),
Barut ('57), Margenau & Hill ('61)
experiments: Bamber, PRL '14

$$p_{kl} = \mathrm{tr}\left(\rho\ \frac{\Pi_k^{[\mathrm{I}]}\Pi_l^{[\mathrm{F}]} + \Pi_l^{[\mathrm{F}]}\Pi_k^{[\mathrm{I}]}}{2}\right) \geq 0$$

applicability condition

$$[\Pi_k^{[\mathrm{I}]}, \Pi_l^{[\mathrm{F}]}] \neq 0$$

→

$$-\frac{1}{8} \leq \frac{\Pi_k^{[\mathrm{I}]}\Pi_l^{[\mathrm{F}]} + \Pi_k^{[\mathrm{F}]}\Pi_l^{[\mathrm{I}]}}{2}$$

negative eigenvalue(s)

$$[\rho, \Pi_l^{[\mathrm{F}]}] = 0, \text{ or}$$

$$[\Pi_k^{[\mathrm{I}]}, \rho] = 0$$

→

previous definition

Fluctuation theorem

reference equilibrium states

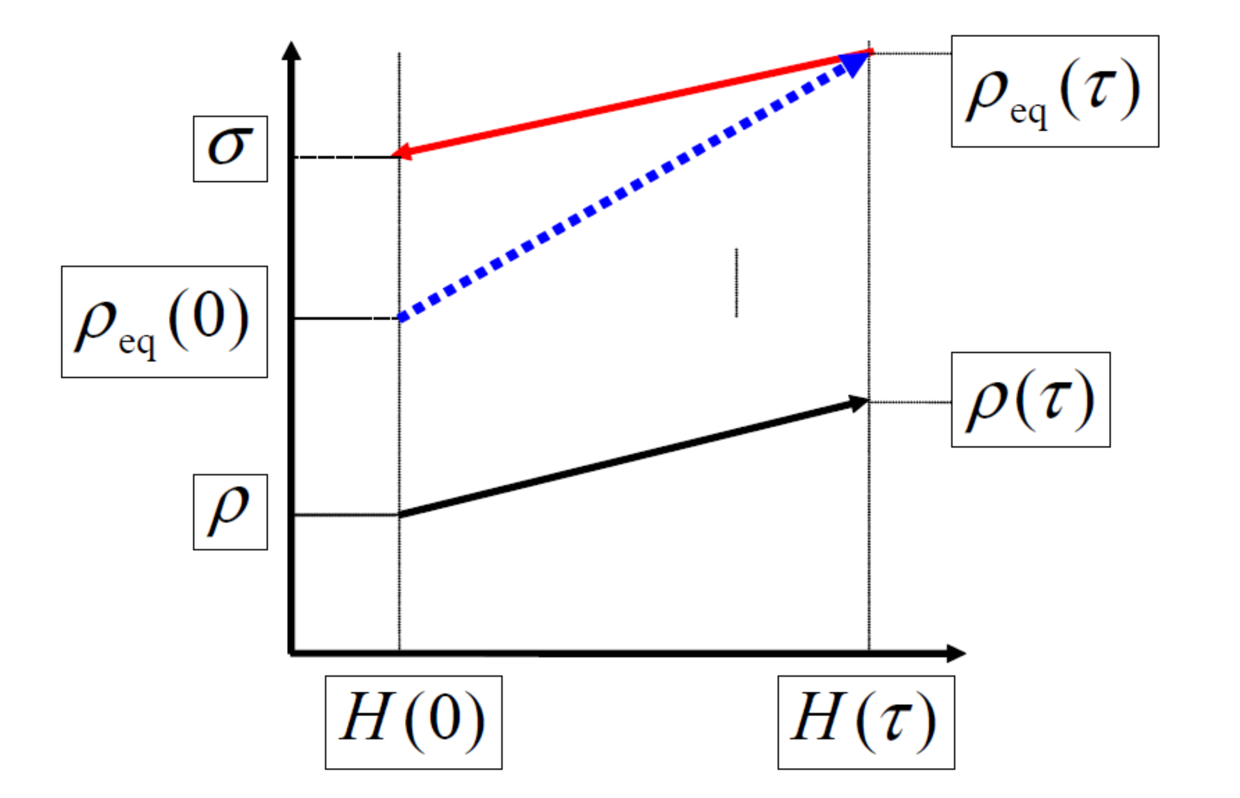
$H_{\mathrm{I}}, H_{\mathrm{F}}$ → $\sigma_{\mathrm{I}} \propto e^{-\beta H_{\mathrm{I}}}$ $\sigma_{\mathrm{F}} \propto e^{-\beta H_{\mathrm{F}}}$

$$\left\langle e^{-\beta(w-\Delta\Phi)} \right\rangle = \mathrm{Re}\ \mathrm{tr}(\sigma_{\mathrm{F}}\, \sigma_{\mathrm{I}}^{-1} \rho)$$

holds always

β **is free parameter**

Fluctuation theorem



$$\left\langle e^{-\beta(w-\Delta\mathcal{F})}\right\rangle = \mathrm{Re}\,\mathrm{tr}\left(\sigma\,\rho_{eq}^{-1}(0)\,\rho\right)$$

$$\rho_{eq}(t) \equiv e^{-\beta H(t)} \Big/ \mathrm{tr}(e^{-\beta H(t)})$$

$$\sigma \equiv U_\tau^\dagger \rho_{eq}(\tau) U_\tau$$

Summary

The existing definitions do not apply

Two necessary conditions for any definition

Fluctuation theorem for non-equilibrium states