Dynamics of nucleation in first-order phase transitions

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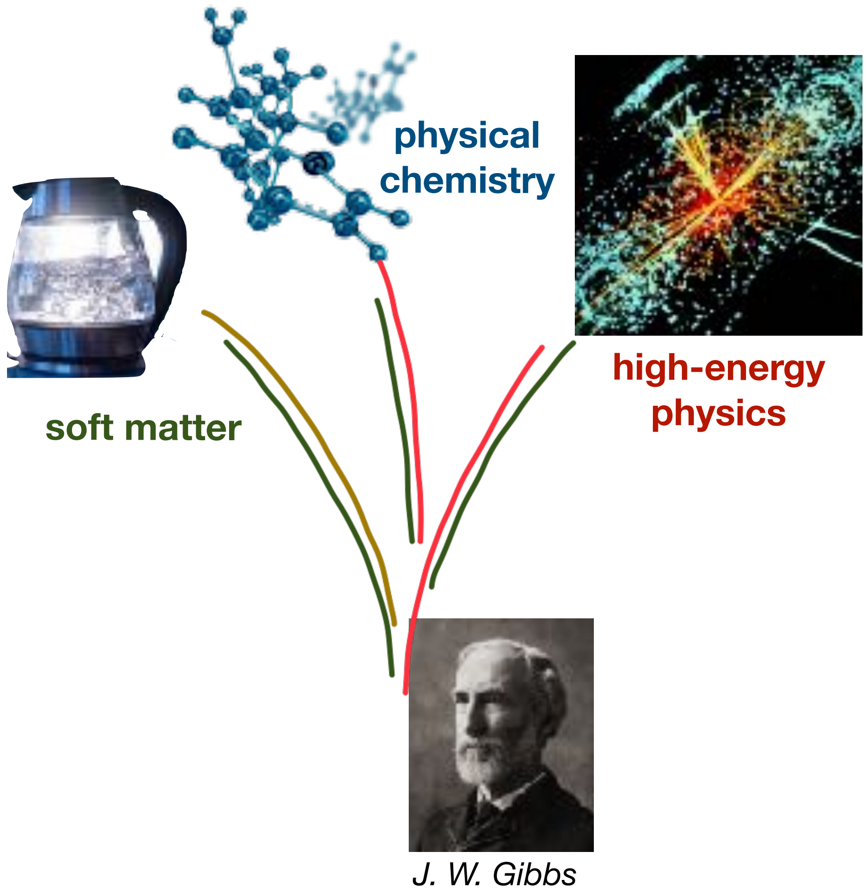
First-order phase transitions…

- play a fundamental role in various branches of physics

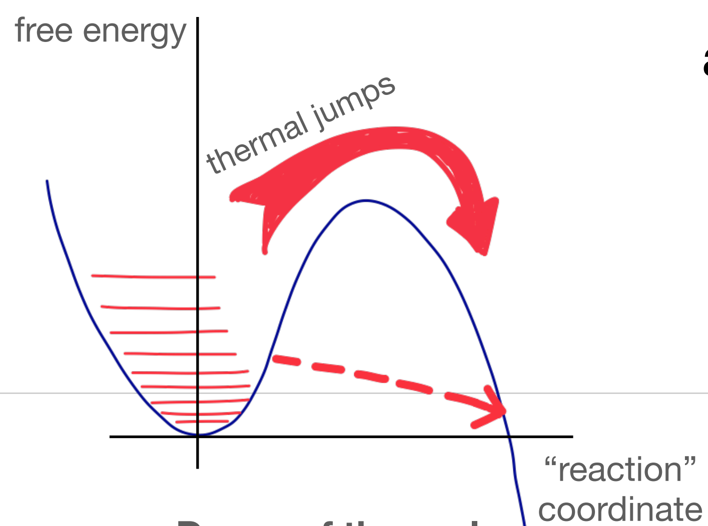
  from quantum cosmology to quantum matter

- have been studied for ~150 years

- many *dynamical* aspects are still poorly understood



Consider **thermal phase transitions** in the classical regime



Decay of thermal metastable state

and compute the **decay rate**:

$$\Gamma \propto e^{-E_{\rm ts}/T}$$

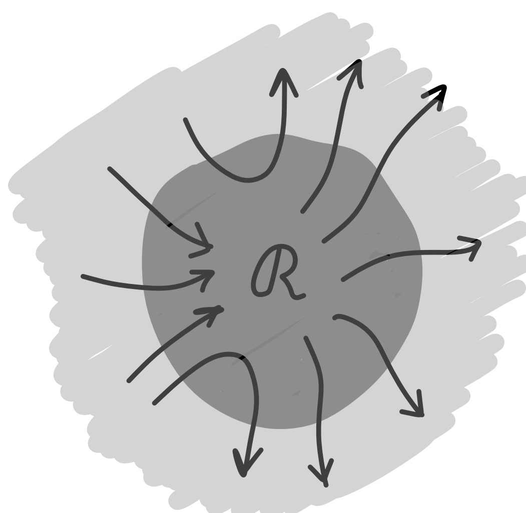
How to define decay rate

"Equilibrium" approach

$$\Gamma_{\rm TST} = \frac{1}{Z_{\mathcal{R}}} \int\limits_{\partial\mathcal{R}} \mathrm{d}S\, \mathbf{n}\cdot\dot{\mathbf{z}}\,\theta(\mathbf{n}\cdot\dot{\mathbf{z}})\,\mathrm{e}^{-H(\mathbf{z})/T}$$

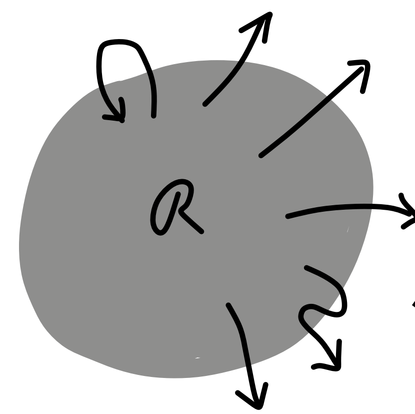
$\Big\downarrow$ SPA!

$$\Gamma_{\rm TST} \overset{\text{1-loop}}{=} \frac{|\omega_-|}{\pi T}\cdot \mathrm{Im}\,F$$



Dynamical picture

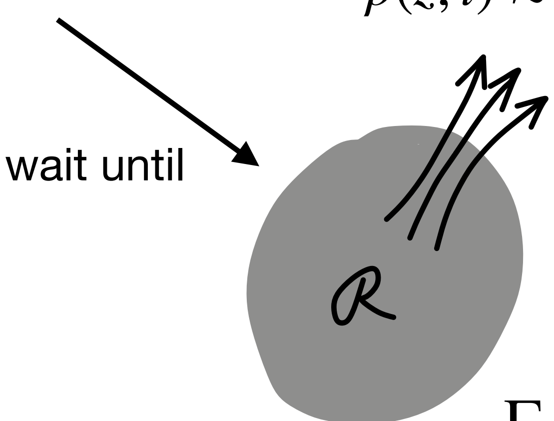
$$\rho(\mathbf{z};t=0) = \frac{1}{Z_{\mathcal{R}}}\mathrm{e}^{-H(\mathbf{z})/T}\theta(\mathbf{z}\in\mathcal{R})$$



wait until

stationary flux regime

$\rho(z;t) \approx \rho_*(z)$



$\Gamma = \mathscr{A}_{\rm dyn.}\Gamma_{\rm TST}$

Questions:

- Does $\rho_*(z)$ exist?
- How to compute $\mathscr{A}_{\rm dyn.}$?
- How is Γ independent of the choice of $\mathscr{R}$ and TS?
- What about **oscillons**?

Langer 69; Affleck 81; Arnold, McLerran 87; Hirvonen 25
Moore, Rummukainen, Tranberg 01

Dynamical decay rate

- In the *stationary flux* regime (more on its existence later)

$$\Gamma = \Gamma_{\mathrm{TST}} \cdot (1 - R)$$

This is similar to the reactive-flux method in chemistry

Chandler 77
P. Hanggi, P. Talkner and M. Borkovec 90

and to the MRT method

Moore, Rummukainen 00
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$$\Gamma = \Gamma_{\mathrm{TST}} \cdot (1 - R)$$

$$R = R^{(+)} + R^{(-)}$$

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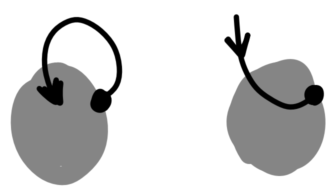
$$R = R^{(+)} + R^{(-)}$$ — re-crossing probability



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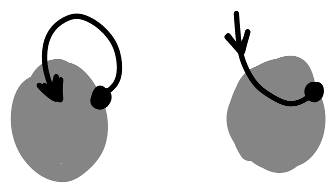

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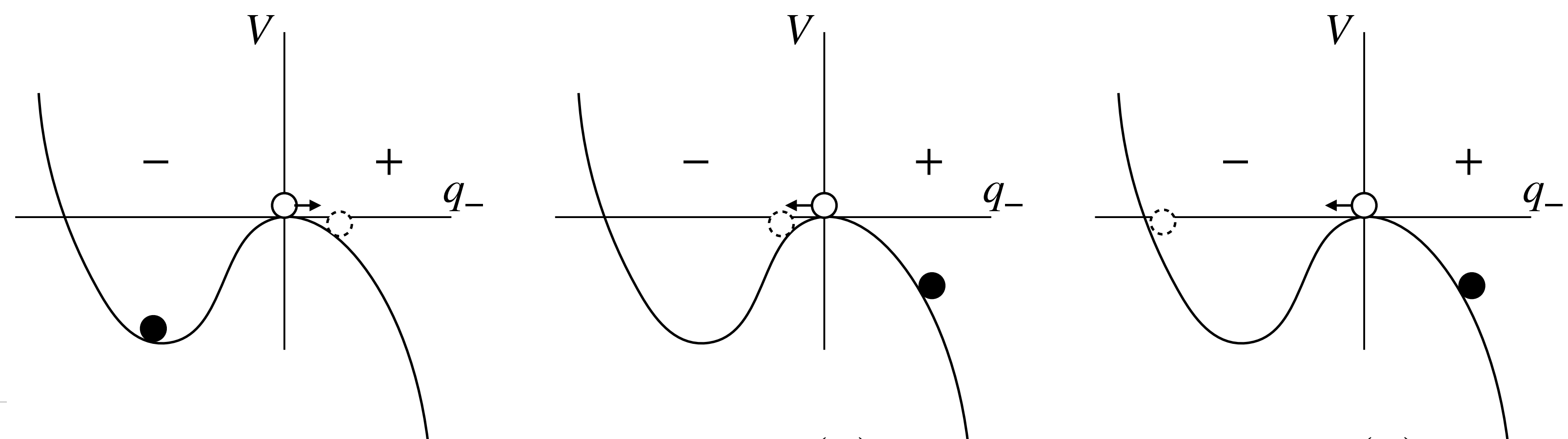
- It makes sense to split $R = R_{\mathrm{prompt}} + R_{\mathrm{slosh}}$.



$R^{(+)}$ $R^{(-)}_{\mathrm{prompt}}$ $R^{(-)}_{\mathrm{slosh}}$

Dynamical decay rate 2

- In the *stationary flux* regime (more on its existence later)

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- This formula is exact (up to corrections of order $\mathcal{O}(e^{-E_{\text{ts}}/T})$)
- R and Γ_{TST} depend on $\mathscr{R}$; Γ does not.
- R_{prompt} can be systematically evaluated (at weak coupling)

  R_{slosh} can give a big contribution! (due to oscillons)
- R can be found from simulations; no exponentially long simulation time required.
- Practically, choose $q_- = 0$ as a dividing surface,

sample $\rho^{(\pm)}(\mathbf{q}, \mathbf{p}; t = 0) = \mathcal{N}\delta(q_-)\theta(\pm\dot{q}_-)|\dot{q}_-|\mathrm{e}^{-H(\mathbf{q},\mathbf{p})/T}$

then $R^{(\pm)} = \lim_{t_{\text{plat.}} \ll t \ll t_{\text{dec.}}} \int \mathrm{d}\mathbf{q}\mathrm{d}\mathbf{p}\, \rho^{(\pm)}(\mathbf{q}, \mathbf{p}; t)\theta(\mp q_-)$ where $t_{\text{dyn.}} < t_{\text{plat.}} < t_{\text{therm.}}$

Two rates

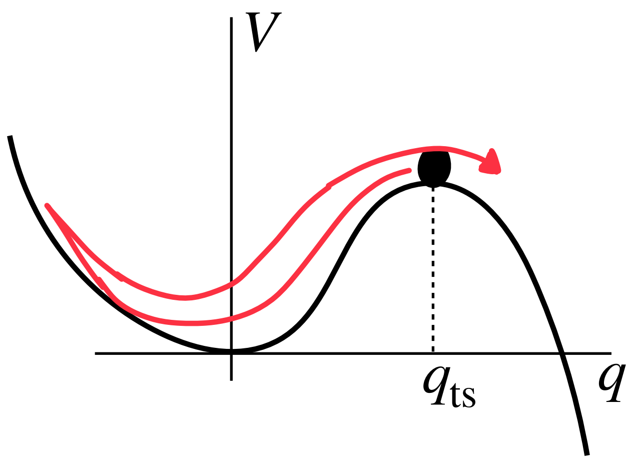
Consider classical-mechanical system coupled to thermal bath with the damping coefficient η.

Kramers

Mel’nikov, Meshkov 86

1 d.o.f.; weak damping

$$R = R_{\text{slosh}} + \ldots$$



$$R^{(-)} = 1 - \exp\left[\int_{-\infty}^{\infty} \frac{\mathrm{d}z}{\pi(z^2+1)} \ln\left(1 - \mathrm{e}^{-(z^2+1)\varepsilon/4T}\right)\right], \quad R^{(+)} = 0$$

where $\varepsilon = \eta \oint \dot{q}^2(t)\,\mathrm{d}t = \eta \oint p\,\mathrm{d}q$

oscillons?..

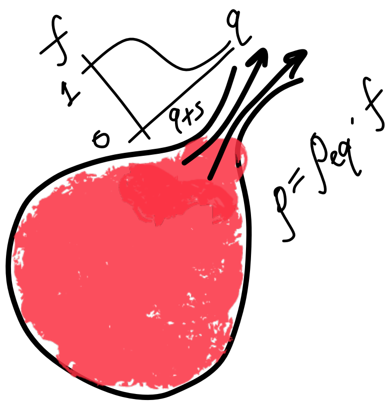
$$t_{\text{plat.}} \sim t_{slosh} \sim \frac{1}{\eta}\frac{T}{E_{\text{ts}}}$$

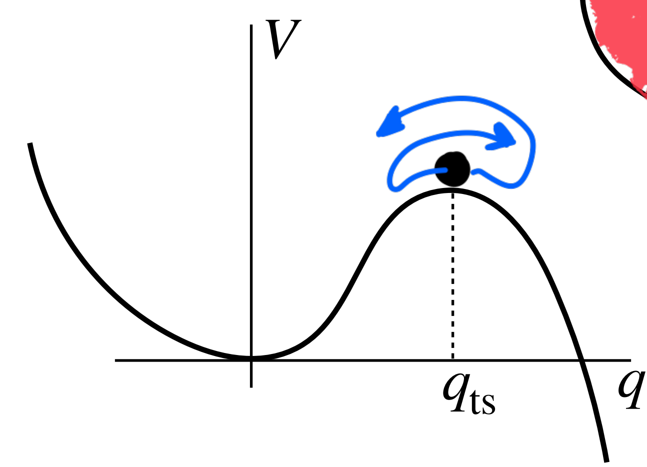
Langer

Langer 69

many d.o.f.; moderate to strong damping

$$R = R_{\text{prompt}} + \ldots$$
$$= R_{\text{pert}} + \ldots$$





To LO in T/E_{ts}:

$$R^{(-)} = R^{(+)} = \frac{1}{2}\left(1 - \sqrt{1 + \frac{\eta^2}{4\omega_-^2}} + \frac{\eta}{2\omega_-}\right)$$

where ω_-^2 is the negative e.v. of the critical bubble

$$t_{\text{plat.}} \sim t_{\text{dyn.}}$$

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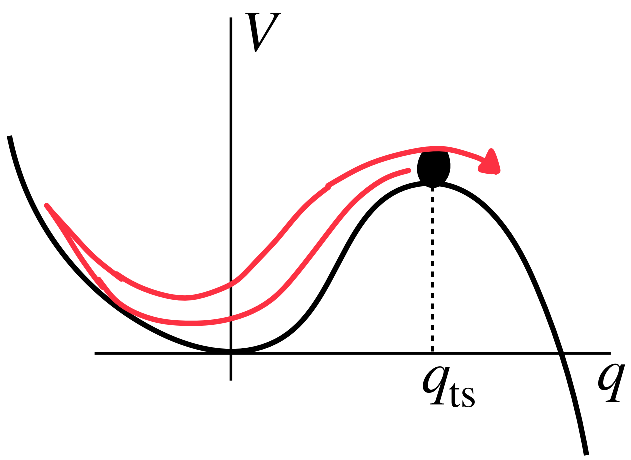
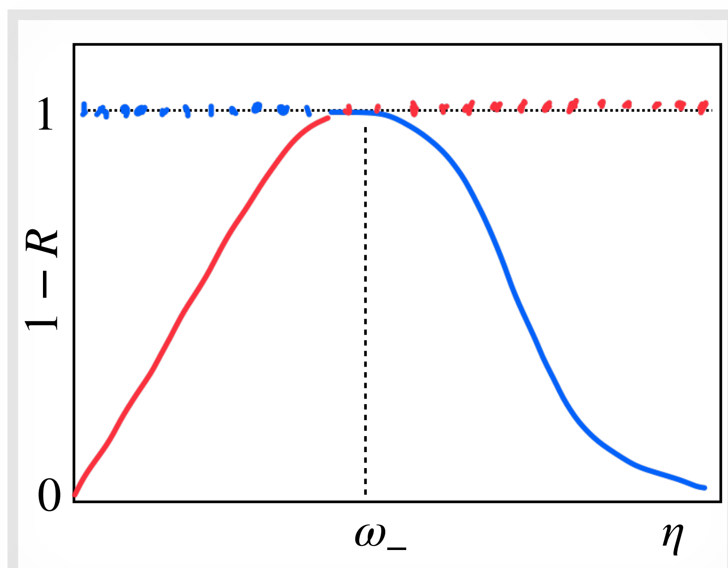


Dynamical factor R



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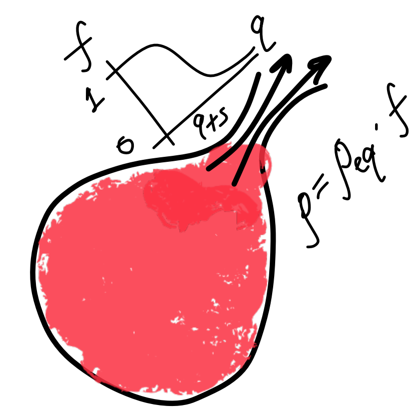

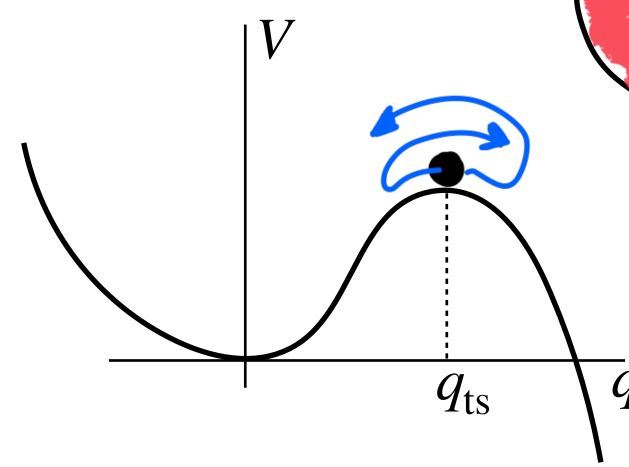

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oscillons?..

$$t_{\text{plat.}} \sim t_{slosh} \sim \frac{1}{\eta}\frac{T}{E_{\text{ts}}}$$

To LO in T/E_{ts}:

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where ω_-^2 is the negative e.v. of the critical bubble

$$t_{\text{plat.}} \sim t_{\text{dyn.}}$$

Structure of re-crossings

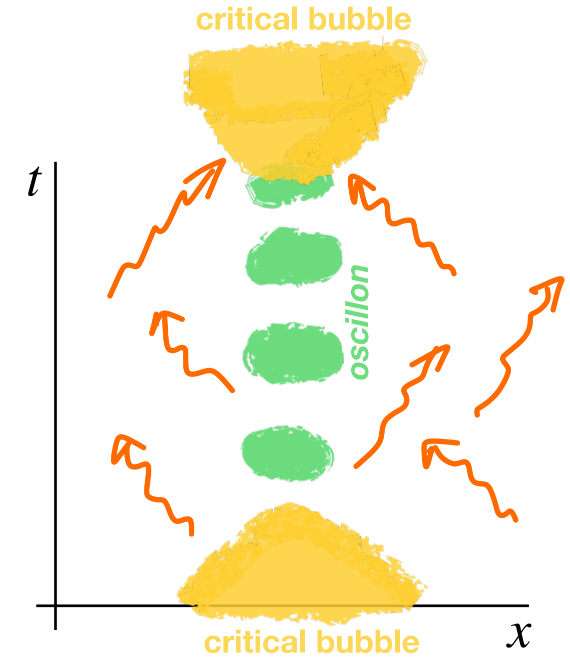
$$R = R_{\text{prompt}} + R_{\text{slosh}}$$

$$\overset{\text{weak coupling}}{=} R_{\text{pert}} + R_{\text{non-pert}}$$

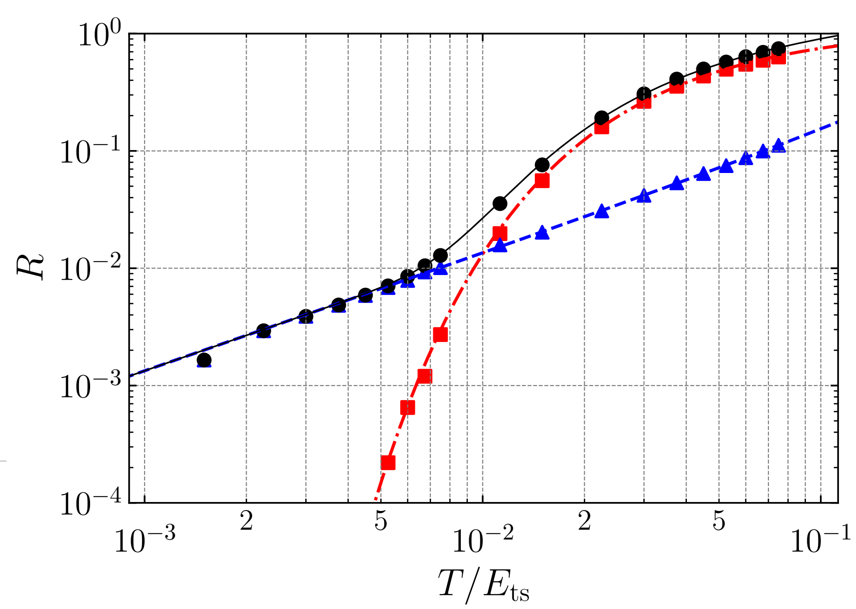
Sloshing re-crossings can be important in field theory!

They are amplified in theories with **oscillons**.

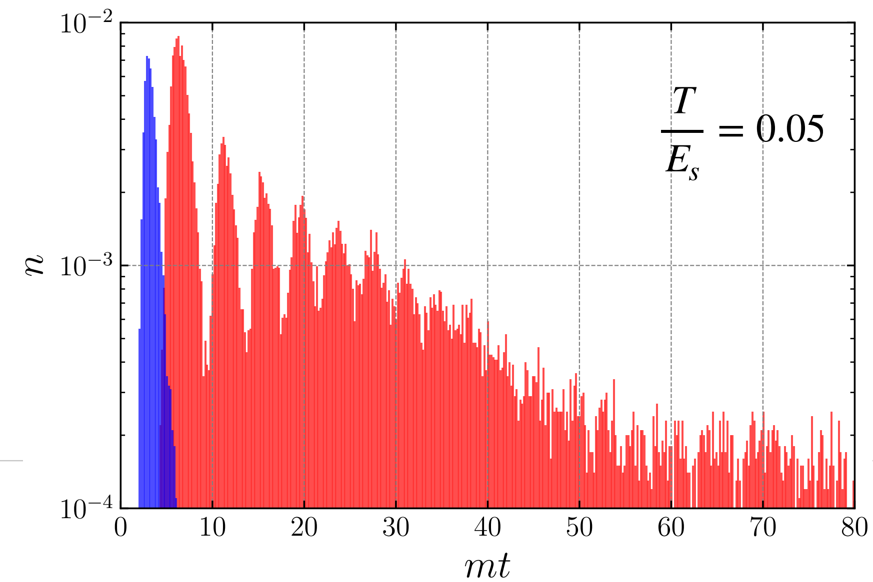
Example: scalar field with unstable quartic potential in (1+1)d, Hamiltonian dynamics



Dynamical factor R from simulations

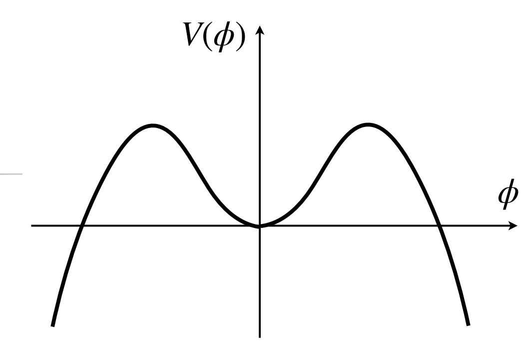


Re-crossings as a function of time



$$S = \int \mathrm{d}t\, \mathrm{d}x \left(\frac{(\partial_\mu \phi)^2}{2} - V(\phi) \right)$$

$$V(\phi) = \frac{m^2\phi^2}{2} - \frac{\lambda\phi^4}{4}$$

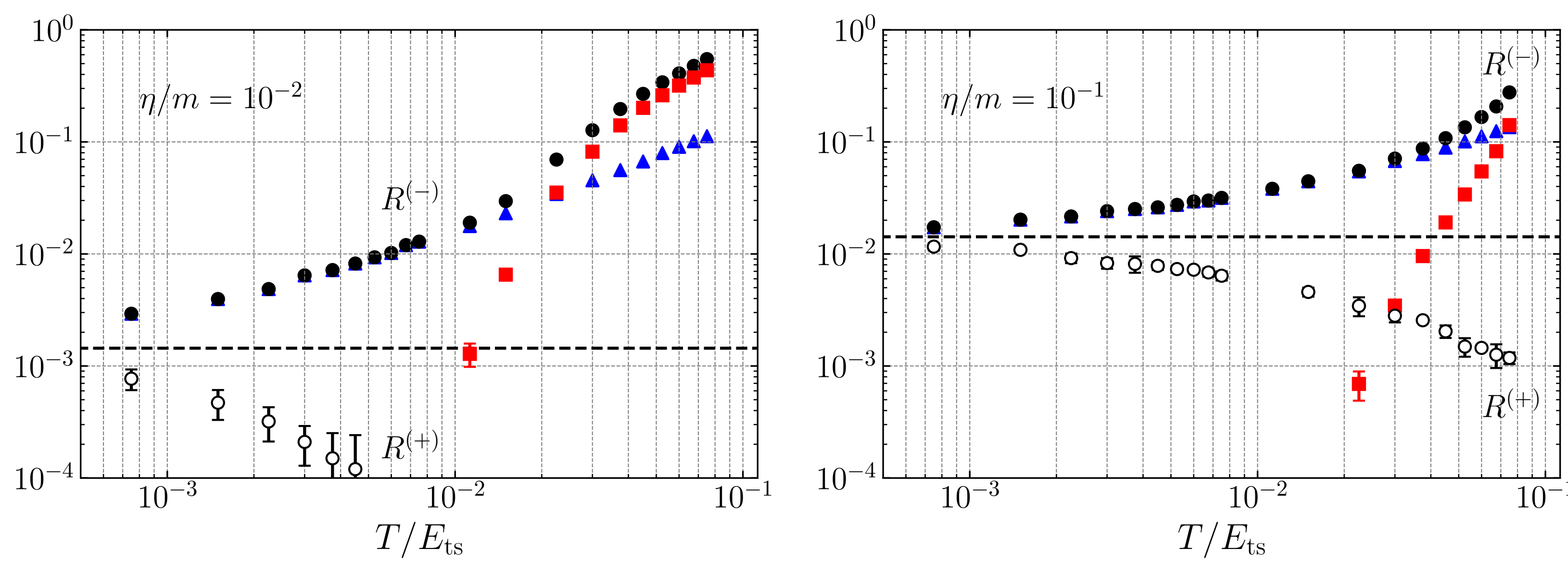


N.B.: $R \to 0$ at $T/E_{\text{ts}} \to 0$.

N.B.: No oscillons → sloshing re-crossings are suppressed, but still there.

Structure of re-crossings 2

Let's switch on dissipation and noise.



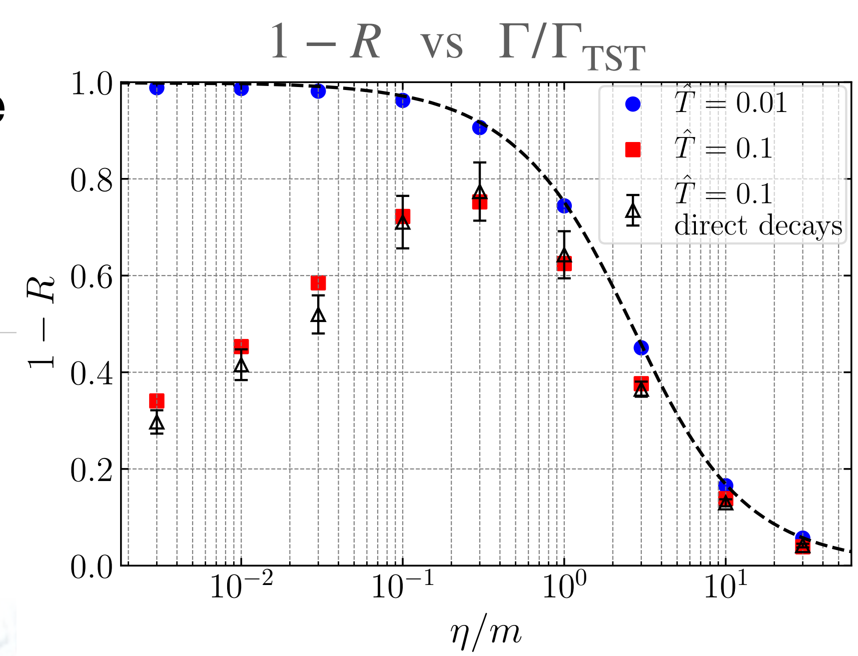
We observe:

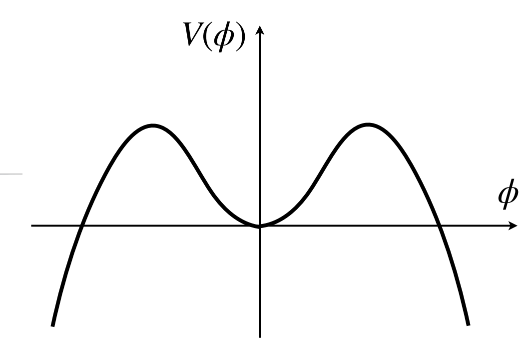
- $T/E_{\rm ts}$ correction to Langer
- sloshing re-crossings are damped by damping

$$S = \int \mathrm{d}t\,\mathrm{d}x \left(\frac{(\partial_\mu \phi)^2}{2} - V(\phi) \right)$$

$$V(\phi) = \frac{m^2\phi^2}{2} - \frac{\lambda\phi^4}{4}$$

➔ At $T/E_{\rm ts} \sim 10^{-1}$, we can compare with direct simulations of decays:





Small Systems

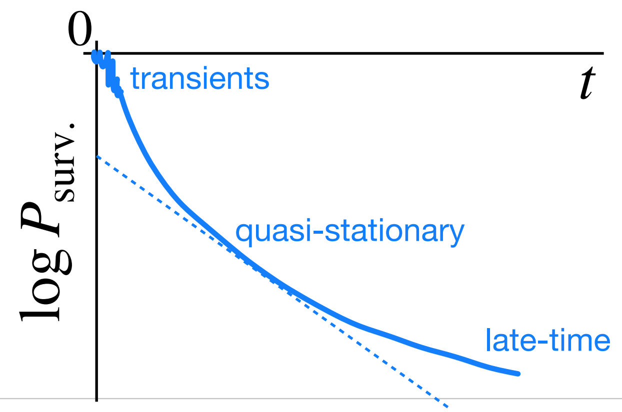
- System is **big** if $\mathscr{E} \gg E_{\rm ts}$ **and** $\delta\mathscr{E} \gg E_{\rm ts} \Leftrightarrow \sqrt{\mathscr{C}}T \gg E_{\rm ts}$.

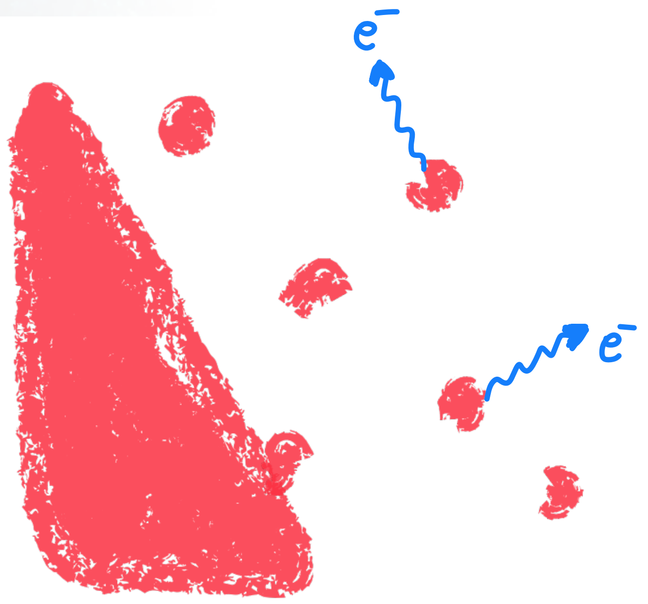
  In small systems, there can be no steady-state decay

  — the decay rate *drifts*.

  $$t_{\rm drift} \sim t_{\rm dec.}\, \mathrm{e}^{-\beta}, \qquad \beta = \frac{E_{\rm ts}^2}{\mathscr{C}T^2}$$

  Moreover, $\Gamma_{\rm canonical} = e^{\beta/2} \cdot \Gamma_{\rm microcanonical}$





Thermionic decay in molecular clusters

Klots '85
Hansen, Andersen et al '01

- Big systems with poor thermalization ($t_{\rm therm.} > t_{\rm dec.}$) are small.

  We see this in numerical simulations of direct decays.

  Can be important in quantum simulators. Not in cosmology, perhaps.

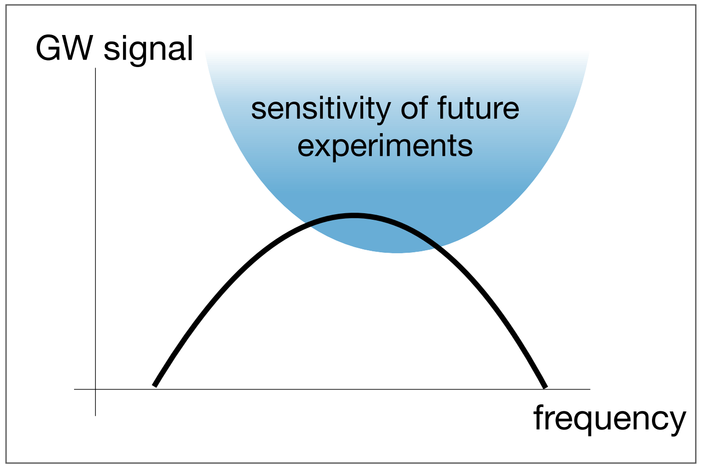
Discussion

- Application to cosmological phase transitions
- Application to *quantum simulators*
- Revisiting Coleman's tunnelling
- Other N^3 effects

Motivation

First order phase transitions in the early universe

Nucleating, propagating and colliding bubbles generate gravitational waves (GWs). This is a motivation to improve the existing and build new GW detectors.



Generation of baryon asymmetry of the universe

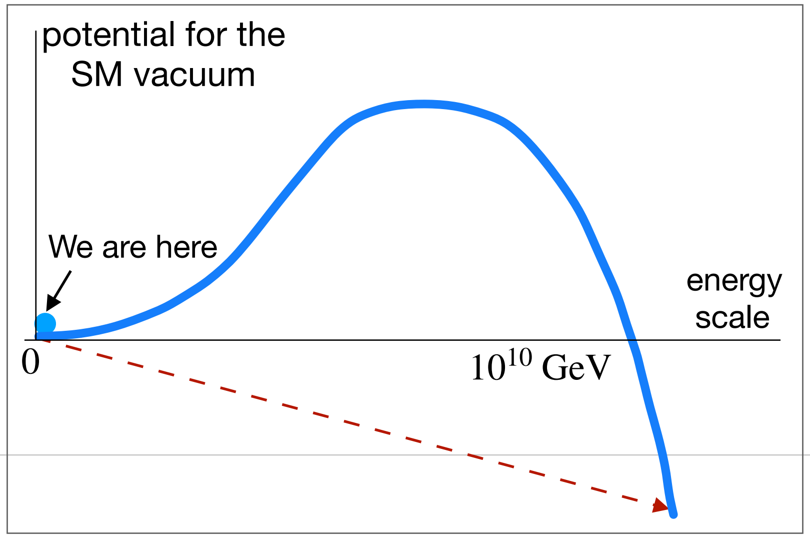
Expanding bubbles moving through cosmic plasma can generate asymmetry between particles and anti-particles.

Metastability of the Standard Model vacuum

According to the measured values of the parameters of the Standard Model (SM), our "fundamental" vacuum may itself be metastable.

In habitable parts of the present-day universe the decay probability is very small.

This may not be so in extreme environments (e.g. black holes) or earlier epochs (e.g. inflation).



Experimental tests of nucleation theory

Zenesini et al, Nature Physics 20, 558–563 (2024) — first experimental result using a cold atom system

Example from simulations

Pirvu, Johnson, Sibiryakov 23; Pirvu, AS, Sibiryakov 24

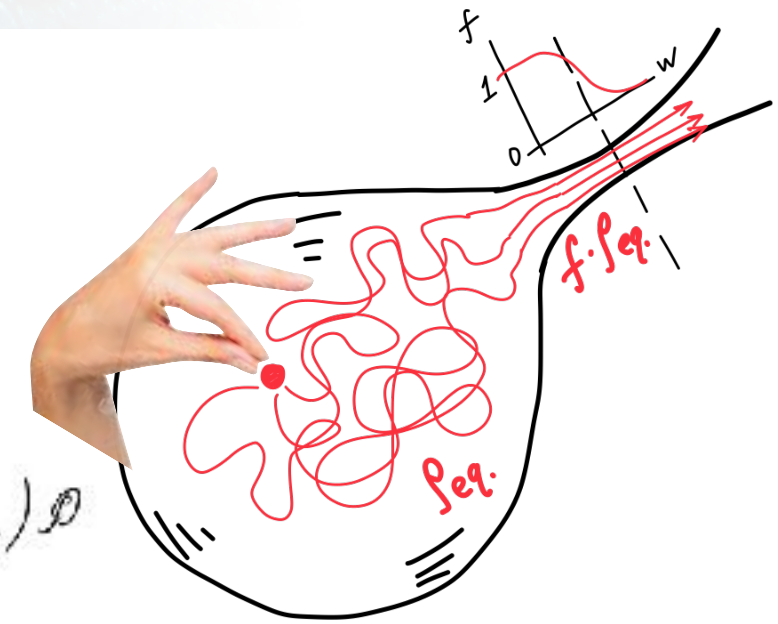
- Take scalar field theory in (1+1) dimensions, with unstable potential, evolve it on a classical lattice, *measure* the survival probability.

$$\ln P_{surv}(t) = \text{const} - \underbrace{\Gamma}_{\text{thermal decay rate}} L \cdot t$$

$$\frac{\partial \mathcal{P}}{\partial t} = -\frac{\partial \mathcal{J}_I}{\partial x_I}$$

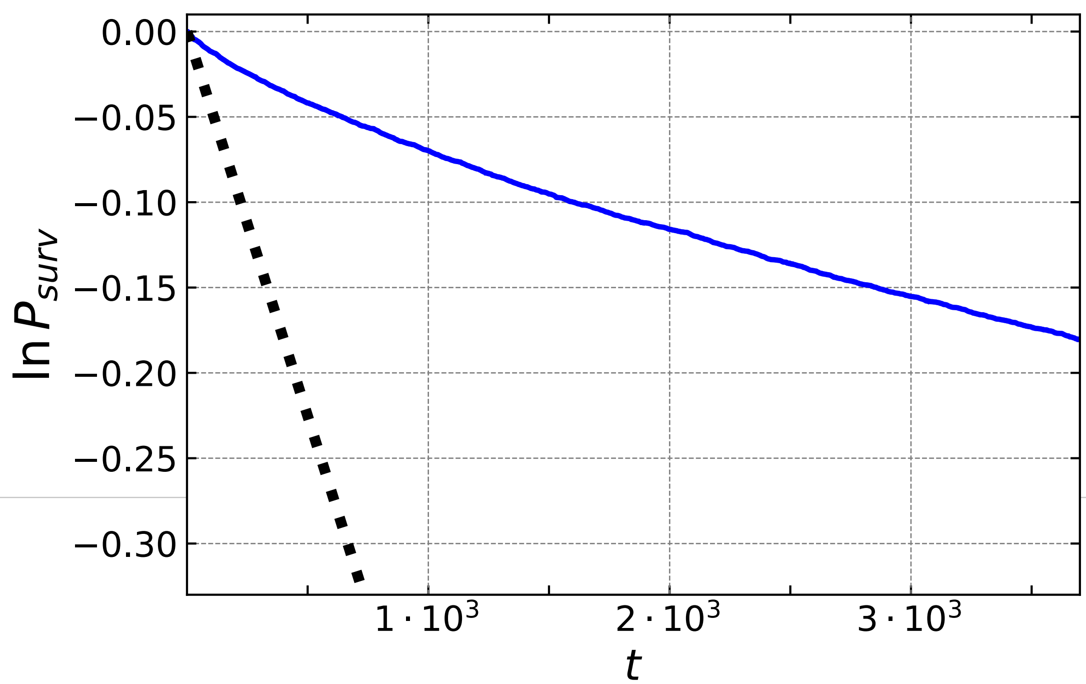
$$\mathcal{J}_I = -\mathcal{M}_{IJ}\left(\frac{\partial \mathcal{H}}{\partial x_J} + T\frac{\partial}{\partial x_J}\right)\mathcal{P}$$

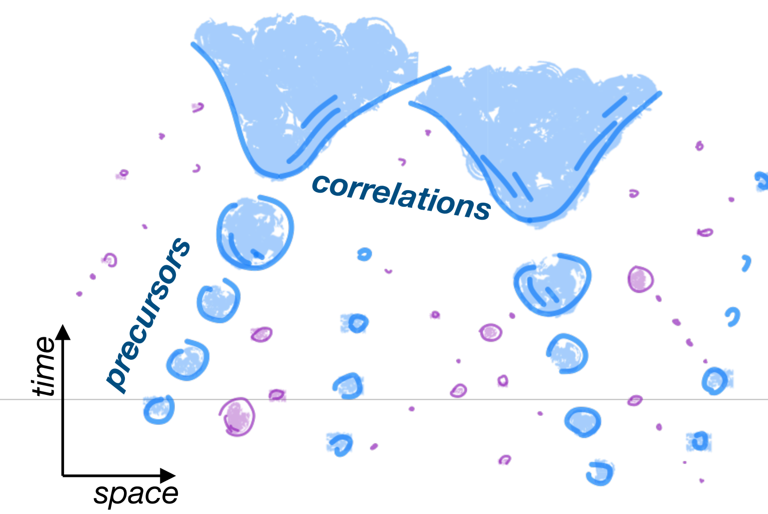
$$\Gamma = \int_{w=0} dx\, \mathcal{J}_\perp$$



Stationary flux regime

Simulation vs TST prediction





Real-time dynamics of critical bubble nucleation

Here we evolve massive scalar field with negative quartic coupling:

$$\begin{cases} \dot{\phi} = \pi \\ \dot{\pi} = \Delta\phi - m^2\phi + \lambda\phi^3 \end{cases}$$