Testing nucleation calculations for strong phase transitions

Oliver Gould - University of Nottingham
Anna Kormu and **David J. Weir [they/he]** - University of Helsinki

This talk: saoghal.net/slides/lattice2024

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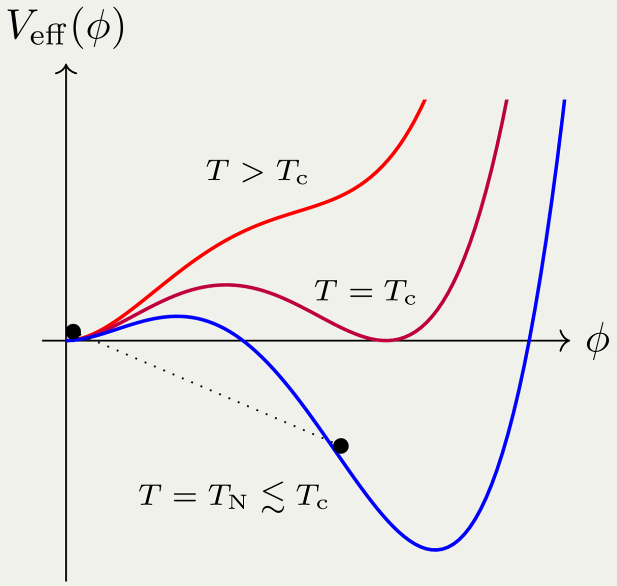
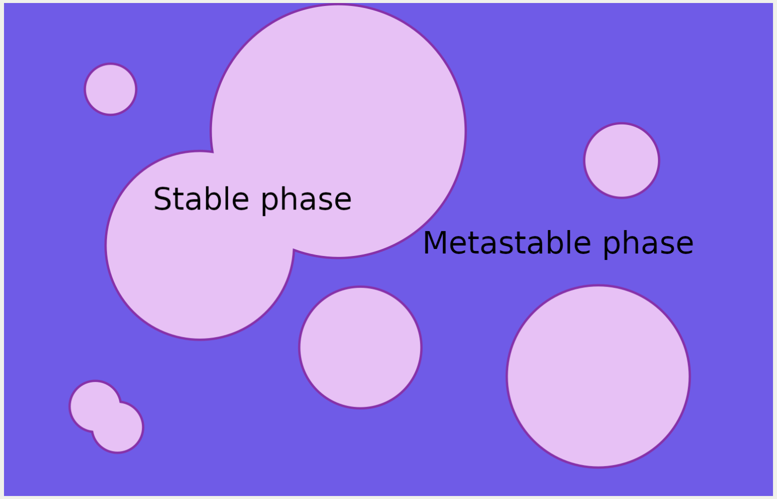
First-order phase transitions

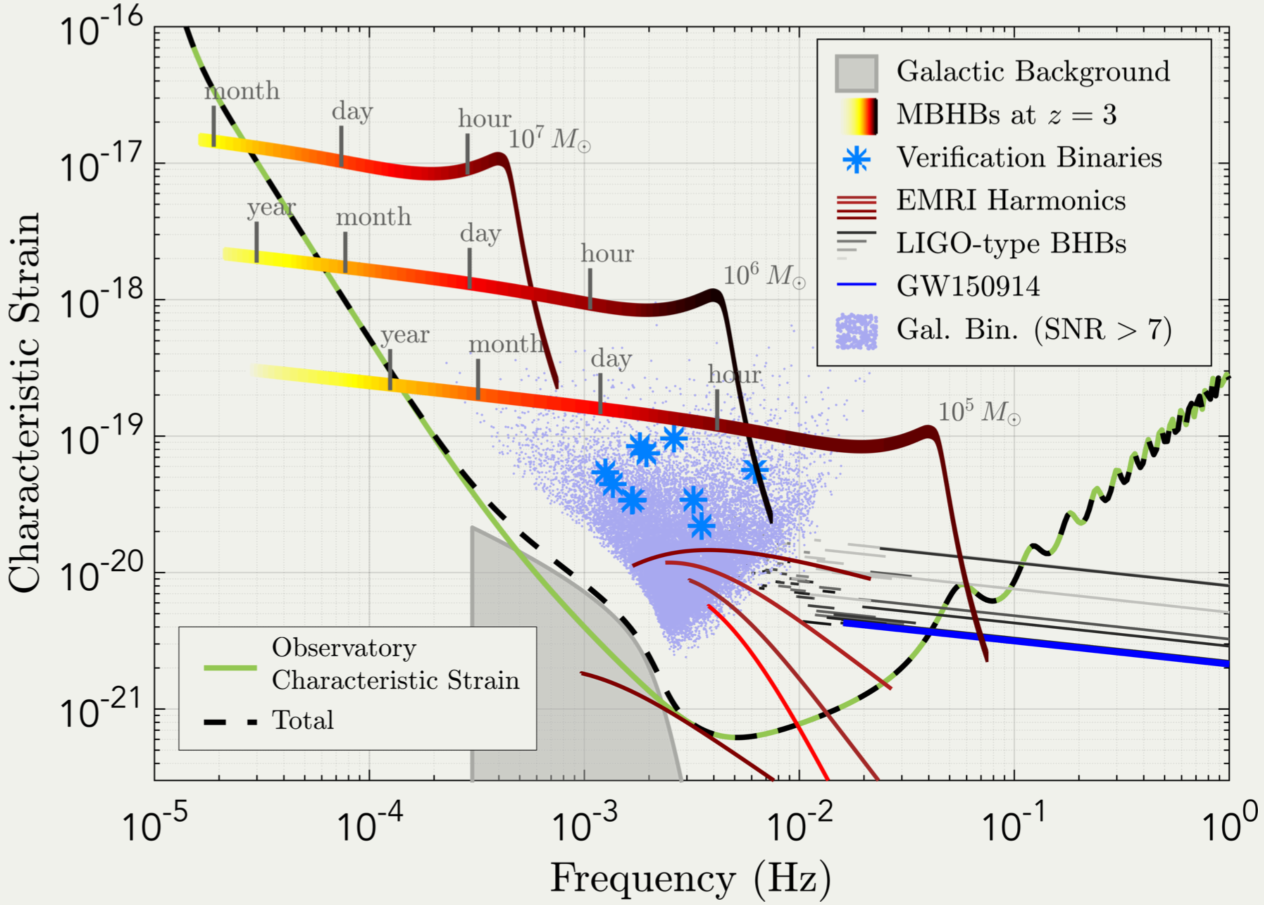
- Bubbles of stable phase nucleate in metastable phase
- Bubbles then expand and collide
  - Out-of-equilibrium: can facilitate baryogenesis
  - Collisions produce gravitational waves





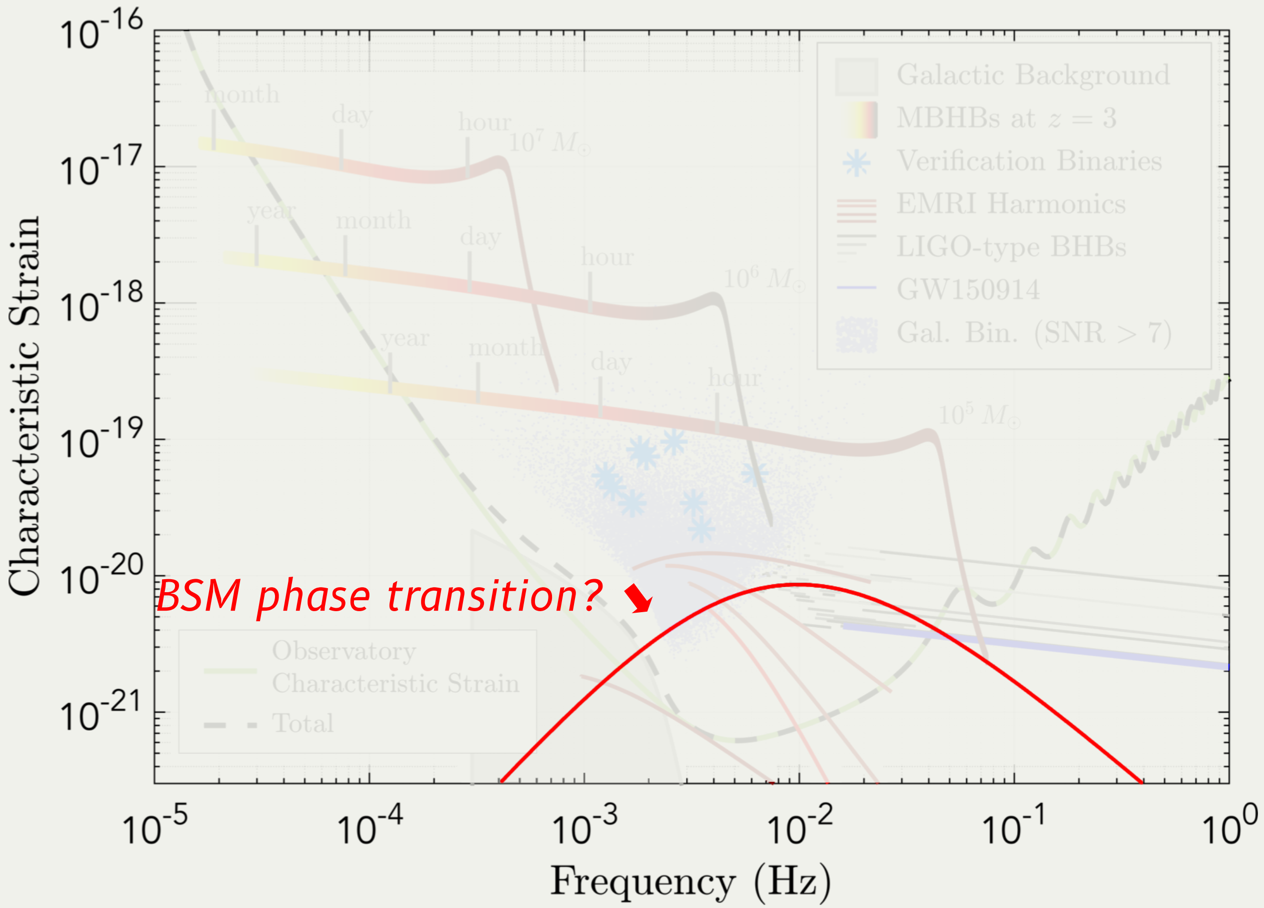
[Sketch: Anna Kormu]

LISA: "Astrophysics" signals



Source: arXiv:1702.00786

LISA: Stochastic background?



[qualitative curve, sketched on]

[what BSM physics might there be?]

Particle physics model

$\Downarrow \mathcal{L}_{\mathrm{4d}}$

Dimensional reduction

$\Downarrow \mathcal{L}_{\mathrm{3d}}$

Phase transition parameters
from lattice simulations

$\Downarrow \alpha, \beta, T_N, v_w, \ldots$

Real time cosmological simulations

$\Downarrow \Omega_{\mathrm{gw}}(f)$

Cosmological GW background

[what would we see as a result?]

Particle physics model

$\Downarrow \mathcal{L}_{\rm 4d}$

Dimensional reduction

$\Downarrow \mathcal{L}_{\rm 3d}$

Phase transition parameters
from lattice simulations

$\Downarrow \alpha, \beta, T_N, v_{\rm w}, \ldots$

Real time cosmological simulations

$\Downarrow \Omega_{\rm gw}(f)$

Cosmological GW background

Phase transition parameters connect particle physics and cosmology

- α, the phase transition strength [$\sim$ latent heat]
- T_N, the temperature at which bubbles nucleate
- β, the inverse phase transition duration [$\sim$ peak nucleation rate]
- v_w, the speed at which bubbles expand

Our focus: nucleation rate

- We compute the bubble nucleation rate Γ
- Earlier work doing this on the lattice focussed on radiatively induced transitions

  hep-ph/0009132; hep-lat/0103036; arXiv:2205.07238

- Current BSM phenomenological interest is in stronger transitions with tree-level barriers, like ours:

$$\mathscr{L} = -\frac{1}{2}\partial_\mu \varphi \partial^\mu \varphi - V(\varphi) - J_1 \varphi - J_2 \varphi^2,$$

$$V(\varphi) = \sigma\varphi + \frac{1}{2}m^2\varphi^2 + \frac{1}{3!}g\varphi^3 + \frac{1}{4!}\lambda\varphi^4$$

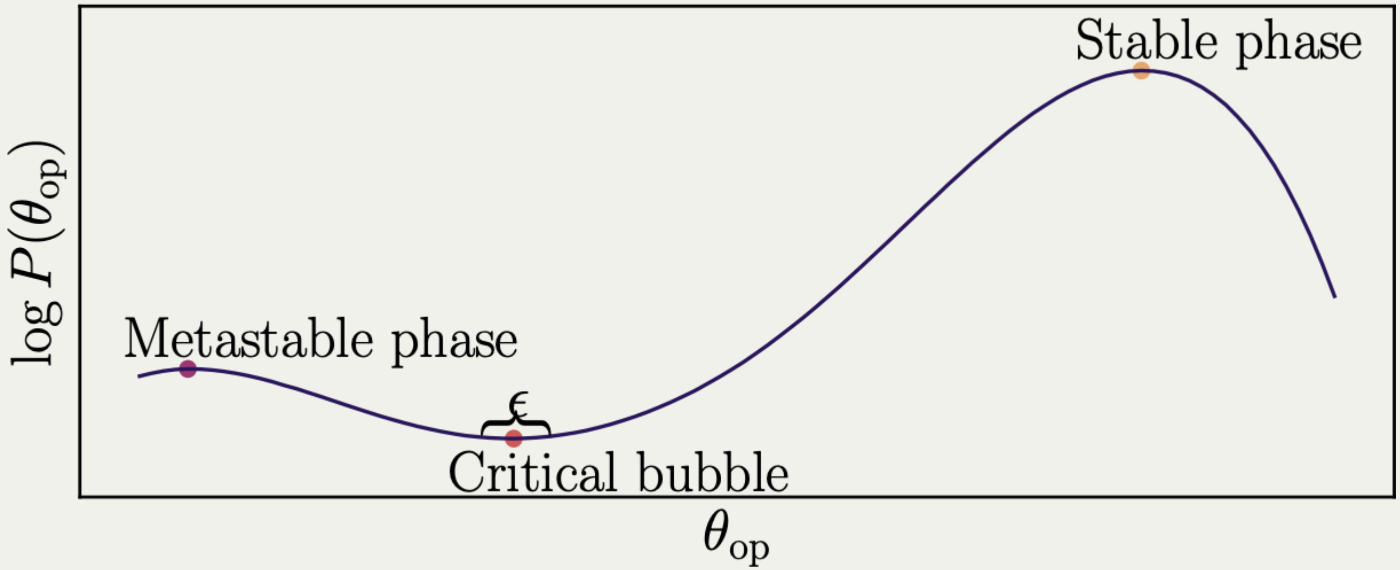
Bubbles in the lab

- Another motivation: test classical (non-relativistic) nucleation theory in the laboratory:
  - A-B transition in $^3\mathrm{He}$ arXiv:2401.07878
  - Ferromagnetic superfluids arXiv:2305.05225
  - Proposed: ultracold atomic gases

    arXiv:1408.1163; arXiv:2212.03621; arXiv:2307.02549
- Hints (e.g. from $^3\mathrm{He}$) that theory not totally consistent with experiment
- Lattice simulations provide a third path between nucleation theory and analogue experiments

How to compute the nucleation rate

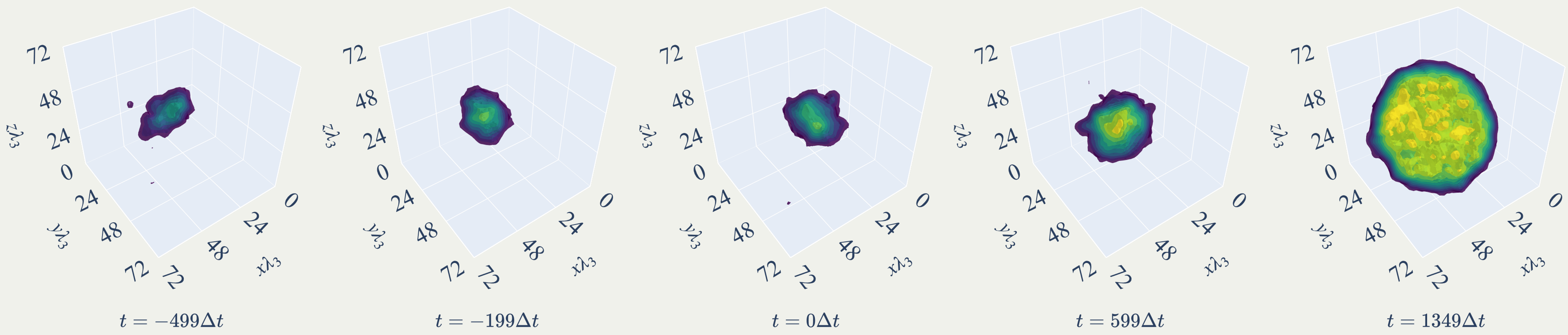
1. Use multicanonical simulations to generate order parameter histogram



2. Calculate probability of critical bubble $P_{\rm c}$ relative to metastable phase

How to compute the nucleation rate

3. Evolve critical bubble configurations forward and backward in a heat bath

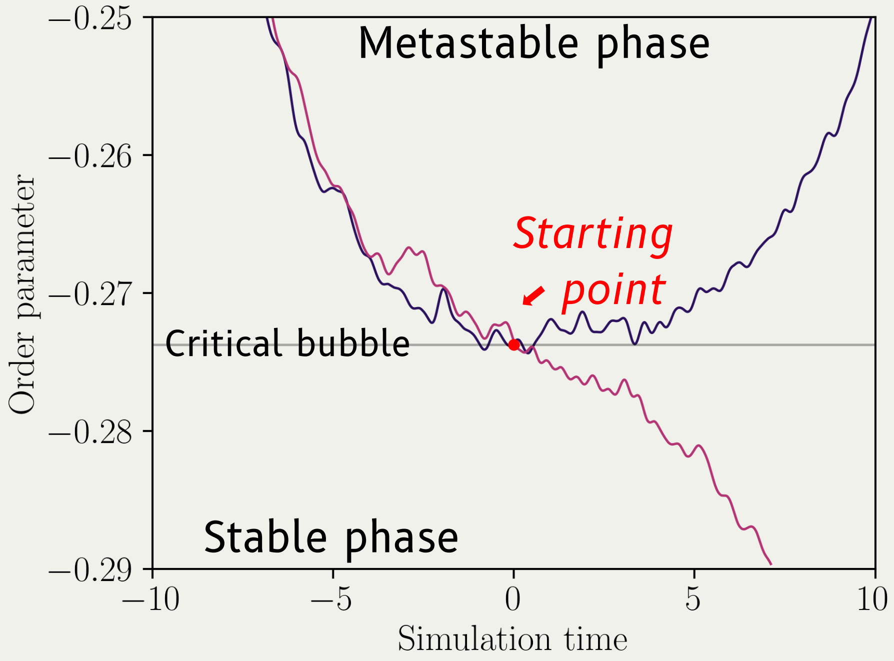


How to compute the nucleation rate

4. Compute fraction $\mathbf{d}$ of configurations that tunnel relative to crossings of $\theta_{\rm c}$

$$\mathbf{d} = \frac{\delta_{\rm tunnel}}{N_{\rm crossings}}$$

$\delta_{\rm tunnel} = 1$ if bubble tunnels, 0 otherwise



How to compute nucleation rate

5. Determine (analytically) rate of change of order parameter across *transition surface* (~ set of all critical bubbles in configuration space)

$$\langle \text{flux} \rangle = \left\langle \left| \frac{\Delta\theta}{\Delta t} \right|_{\theta_c} \right\rangle = \sqrt{\frac{8}{\pi \mathcal{V}}(\theta_c + A^2)}$$

Then the nucleation rate is $\Gamma \mathcal{V} \approx P_c \langle \text{flux} \rangle \frac{\langle \mathbf{d} \rangle}{2}$

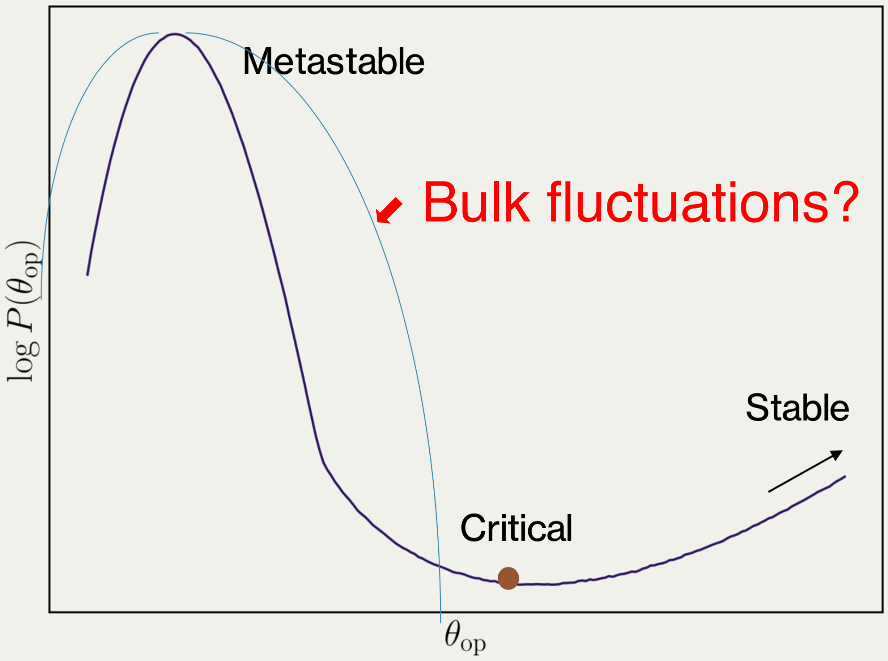
(assuming that $\langle \text{flux} \rangle$ consists of short-range fluctuations and $\mathbf{d}$ long-range fluctuations hep-lat/0103036)

Picking a good order parameter

- Tried two order parameters $\theta = \overline{\phi}$; $\theta' = \overline{\phi^2} - 2A\overline{\phi}$

- Metastable peak can be broadened by bulk (not bubble) fluctuations - hiding critical bubble

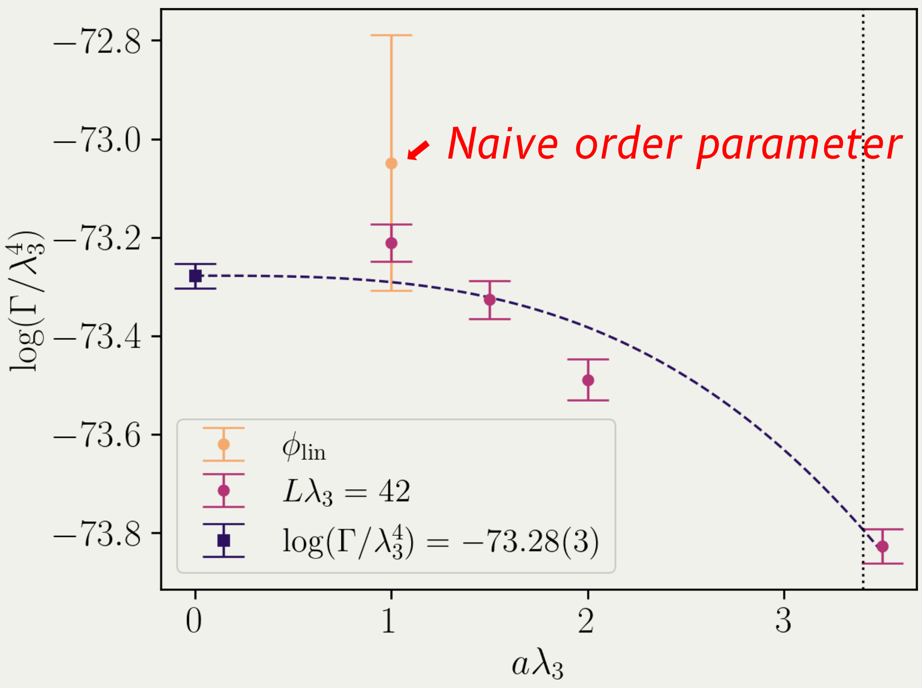
  [Sketch: Anna Kormu]

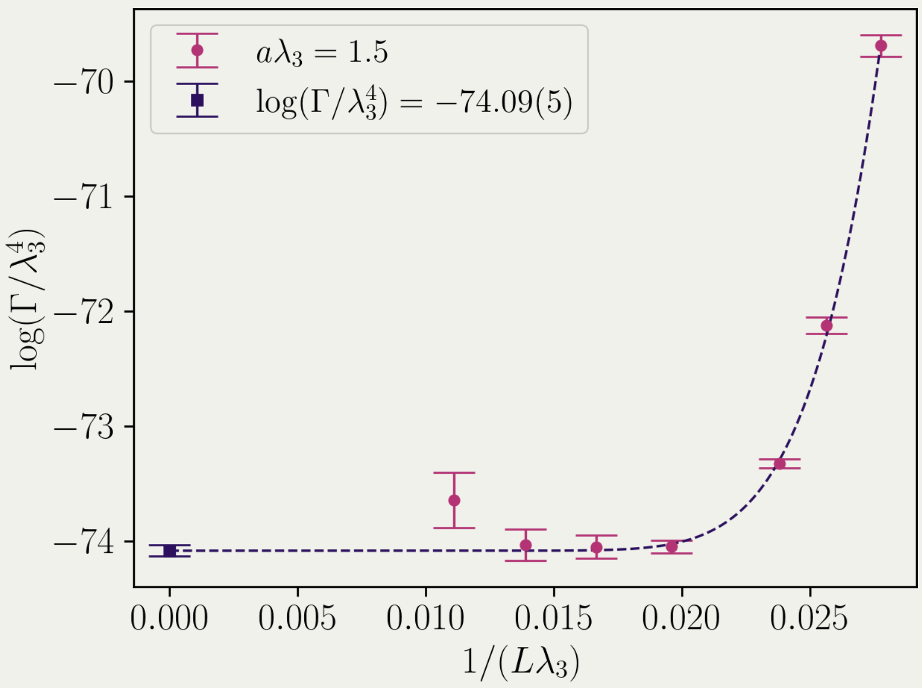


- We found θ' helped a lot (see arXiv:2205.07238)

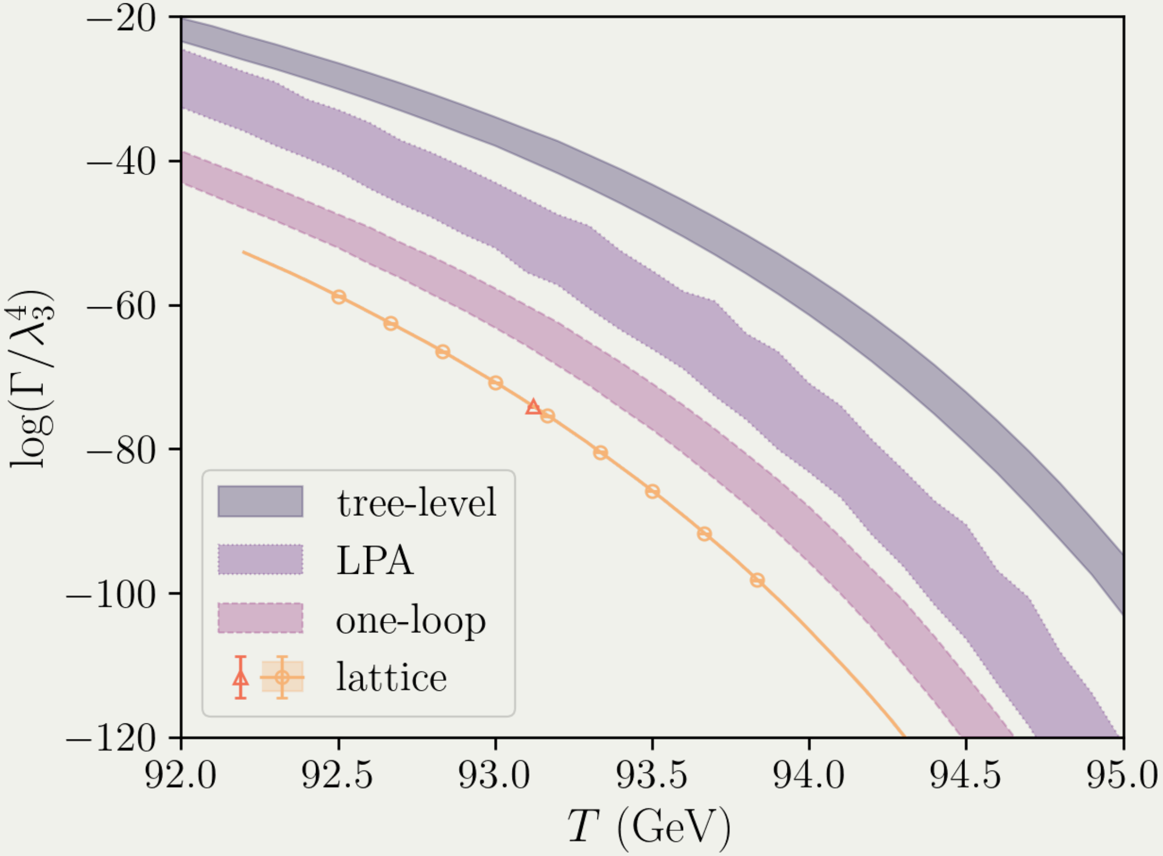
Main results: nucleation rate

- $a \to 0$ with $L\lambda_3 = 42$
- Up to 60^3 at $a\lambda_3 = 1.5$



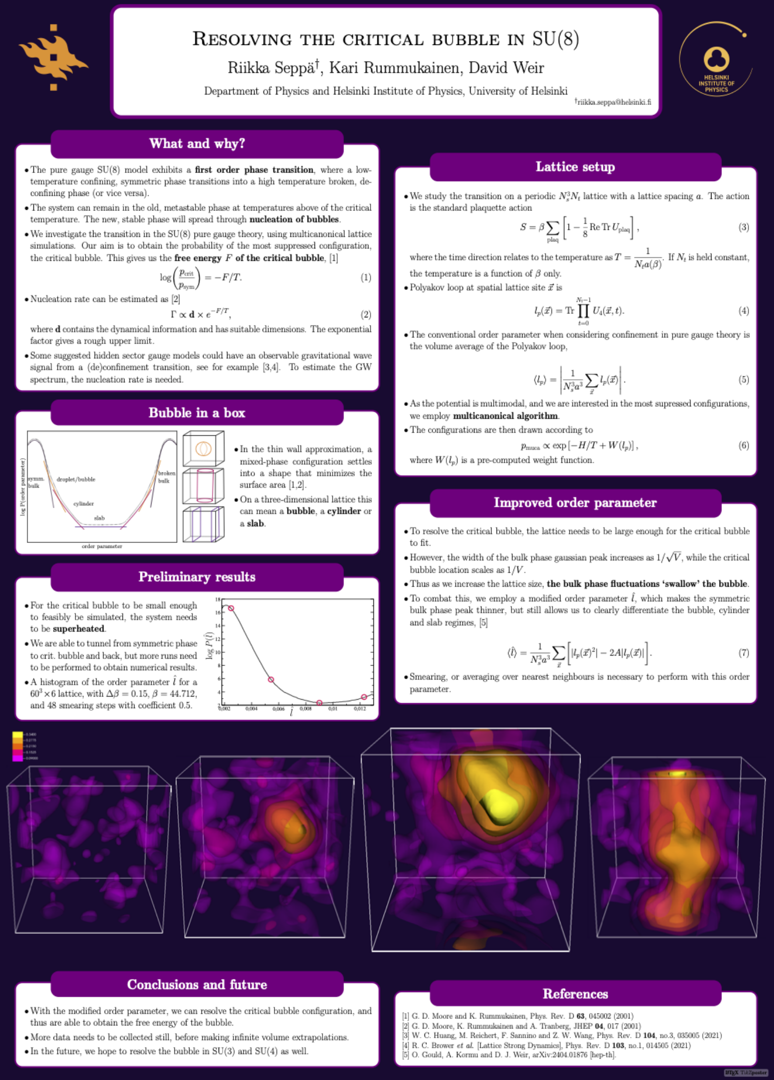


Reweighting; comparison with PT



20% discrepancy in $\log\ \Gamma \Rightarrow 10^{\text{several}}$ discrepancy in Γ

Check out Riikka Seppä's poster!



Resolving the critical bubble in SU(8)

Riikka Seppä†, Kari Rummukainen, David Weir
Department of Physics and Helsinki Institute of Physics, University of Helsinki
†riikka.seppa@helsinki.fi

What and why?

- The pure gauge SU(8) model exhibits a **first order phase transition**, where a low-temperature confining, symmetric phase transitions into a high temperature broken, deconfining phase (or vice versa).
- The system can remain in the old, metastable phase at temperatures above of the critical temperature. The new, stable phase will spread through **nucleation of bubbles**.
- We investigate the transition in the SU(8) pure gauge theory, using multicanonical lattice simulations. Our aim is to obtain the probability of the most suppressed configuration, the critical bubble. This gives us the **free energy F of the critical bubble**, [1]

$$\log\left(\frac{p_{\mathrm{crit}}}{p_{\mathrm{sym}}}\right) = -F/T. \quad (1)$$

- Nucleation rate can be estimated as [2]

$$\Gamma \propto \mathbf{d} \times e^{-F/T}, \quad (2)$$

where $\mathbf{d}$ contains the dynamical information and has suitable dimensions. The exponential factor gives a rough upper limit.
- Some suggested hidden sector gauge models could have an observable gravitational wave signal from a (de)confinement transition, see for example [3,4]. To estimate the GW spectrum, the nucleation rate is needed.

Bubble in a box

- In the thin wall approximation, a mixed-phase configuration settles into a shape that minimizes the surface area [1,2].
- On a three-dimensional lattice this can mean a **bubble**, a **cylinder** or a **slab**.

Preliminary results

- For the critical bubble to be small enough to feasibly be simulated, the system needs to be **superheated**.
- We are able to tunnel from symmetric phase to crit. bubble and back, but more runs need to be performed to obtain numerical results.
- A histogram of the order parameter $\hat{l}$ for a $60^3 \times 6$ lattice, with $\Delta\beta = 0.15$, $\beta = 44.712$, and 48 smearing steps with coefficient 0.5.

Lattice setup

- We study the transition on a periodic $N_s^3 N_t$ lattice with a lattice spacing a. The action is the standard plaquette action

$$S = \beta \sum_{\mathrm{plaq}} \left[1 - \frac{1}{8}\mathrm{Re}\,\mathrm{Tr}\, U_{\mathrm{plaq}}\right], \quad (3)$$

where the time direction relates to the temperature as $T = \frac{1}{N_t a(\beta)}$. If N_t is held constant, the temperature is a function of β only.
- Polyakov loop at spatial lattice site $\vec{x}$ is

$$l_p(\vec{x}) = \mathrm{Tr} \prod_{t=0}^{N_t-1} U_4(\vec{x}, t). \quad (4)$$

- The conventional order parameter when considering confinement in pure gauge theory is the volume average of the Polyakov loop,

$$\langle l_p \rangle = \left| \frac{1}{N_s^3 a^3} \sum_{\vec{x}} l_p(\vec{x}) \right|. \quad (5)$$

- As the potential is multimodal, and we are interested in the most supressed configurations, we employ **multicanonical algorithm**.
- The configurations are then drawn according to

$$p_{\mathrm{muca}} \propto \exp\left[-H/T + W(l_p)\right], \quad (6)$$

where $W(l_p)$ is a pre-computed weight function.

Improved order parameter

- To resolve the critical bubble, the lattice needs to be large enough for the critical bubble to fit.
- However, the width of the bulk phase gaussian peak increases as $1/\sqrt{V}$, while the critical bubble location scales as $1/V$.
- Thus as we increase the lattice size, **the bulk phase fluctuations 'swallow' the bubble**.
- To combat this, we employ a modified order parameter $\hat{l}$, which makes the symmetric bulk phase peak thinner, but still allows us to clearly differentiate the bubble, cylinder and slab regimes, [5]

$$\langle \hat{l} \rangle = \frac{1}{N_s^3 a^3} \sum_{\vec{x}} \left[|l_p(\vec{x})^2| - 2A|l_p(\vec{x})| \right]. \quad (7)$$

- Smearing, or averaging over nearest neighbours is necessary to perform with this order parameter.

Conclusions and future

- With the modified order parameter, we can resolve the critical bubble configuration, and thus are able to obtain the free energy of the bubble.
- More data needs to be collected still, before making infinite volume extrapolations.
- In the future, we hope to resolve the bubble in SU(3) and SU(4) as well.

References

[1] G. D. Moore and K. Rummukainen, Phys. Rev. D **63**, 045002 (2001)
[2] G. D. Moore, K. Rummukainen and A. Tranberg, JHEP **04**, 017 (2001)
[3] W. C. Huang, M. Reichert, F. Sannino and Z. W. Wang, Phys. Rev. D **104**, no.3, 035005 (2021)
[4] R. C. Brower *et al.* [Lattice Strong Dynamics], Phys. Rev. D **103**, no.1, 014505 (2021)
[5] O. Gould, A. Kormu and D. J. Weir, arXiv:2404.01876 [hep-th].

LaTeX TikZposter

Key points

- Testing nucleation theory is important for particle physics, cosmology (and lab experiments).
- Our potential (with tree level barrier) shows a significant discrepancy with analytical nucleation theory.
- Need a good [quasi]order parameter to suppress bulk fluctuations in multicanonical simulations.