Topological Defect Formation in a Phase Transition with Tunable Order: From Condensed Matter Physics to Quantum Computing

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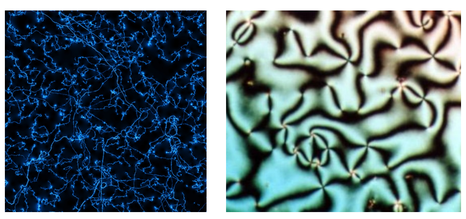
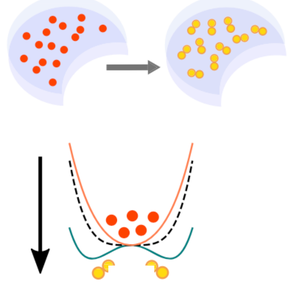
1 Introduction

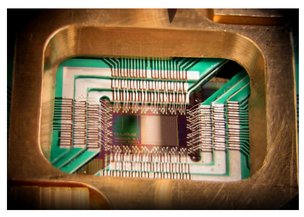
The Kibble-Zurek mechanism (KZM) describes the non-equilibrium dynamics and the formation of topological defects in a system that is driven through a second-order phase transition. It has applications in condensed matter physics, cosmology, ultracold chemistry, and quantum computing. KZM is generally applicable only to 2nd-order phase transitions. In this work, we extend the applicability of KZM to 1st-order phase transitions by integrating it with nucleation theory.



Defects formation in cosmology and condensed matter physics



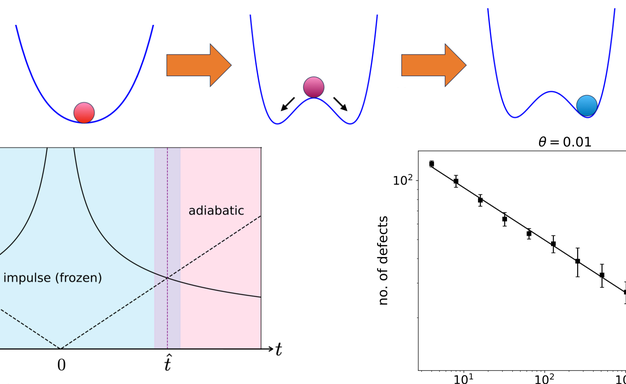
Ultracold reactions



Error rates in quantum computing

2 Kibble-Zurek Mechanism (KZM)

KZM predicts the density of defects in 2nd-order phase transitions. According to the theory, the number of defects follows a power-law scaling with respect to the quench time scale τ_Q of spontaneous symmetry breaking.

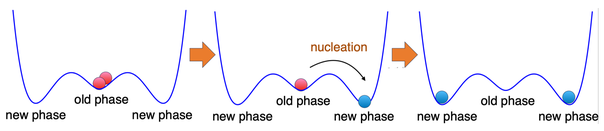


# of defects in 2nd-order phase transition

$$n_{KZM} = \tau_Q^{-a}$$

3 Nucleation Theory

In contrast, in a 1st-order phase transition, both the old and new phases can coexist, and the transition occurs through a nucleation process, where the order parameter overcomes a barrier separating the two phases.



# of defects in 1st-order phase transition

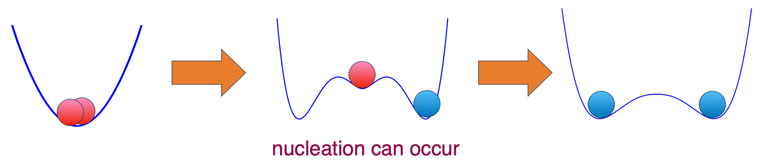
$$n_{nuc} \propto \Gamma / v$$

v: nucleus growth velocity
Γ: nucleation rate

4 Classical Weakly 1st-Order Phase Transition

Halperin, Lubensky, and Ma demonstrated that transitions associated with superconductors or superfluids can exhibit weakly 1st-order characteristics. This suggests that the order of the transition can be tuned between 2nd and 1st order, with weakly 1st-order characteristics in between. Given the critical properties shared between liquid crystals and superconductors, the transitions in liquid crystals can also exhibit a weakly 1st-order nature. In high-energy physics, an analogous model occurs in the Coleman–Weinberg potential.

A weakly 1st-order phase transition exhibits characteristics of both 1st-order and 2nd-order transitions. It evolves similarly to spontaneous symmetry breaking, but nucleation can occur during the intermediate time.



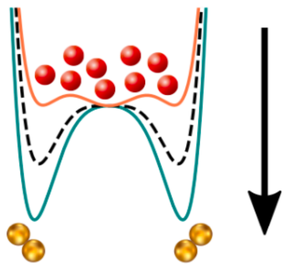
In this case, we need to combine the Kibble-Zurek mechanism and nucleation theory. This can be done by summing the contributions from the Kibble-Zurek mechanism and nucleation theory using the Avrami equation.

# of defects in weakly 1st-order phase transition

$$n = (1-f)n_{KZM} + f n_{nuc}$$

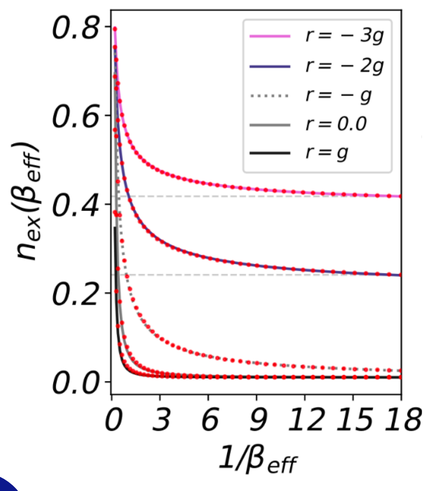
(Fraction of space f covered by new phase due to nucleation - Avrami equation)

5 Quantum Weakly 1st-Order Phase Transition



Analogous weakly 1st-order quantum phase transition can be observed in conversion between atomic and molecular Bose-Einstein condensate with molecular-molecular interactions, by detuning the magnetic field through the Feshbach resonance.

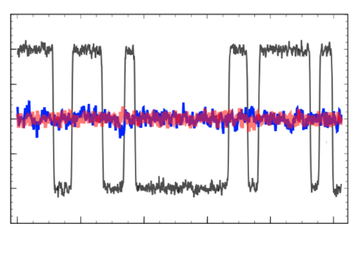
In this case as well, non-adiabatic excitations are sum of Kibble-Zurek scaling and contribution from 1st-order phase transitions.



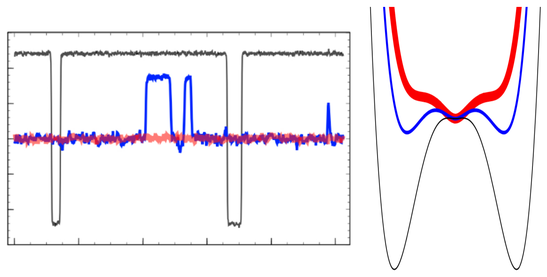
# of non-adiabatic excitations (efficiency of conversion)

$$n_{ex} \sim \tau_Q^{-a} + n_{ex}^{1st}$$

KZ-scaling; 1st-order correction



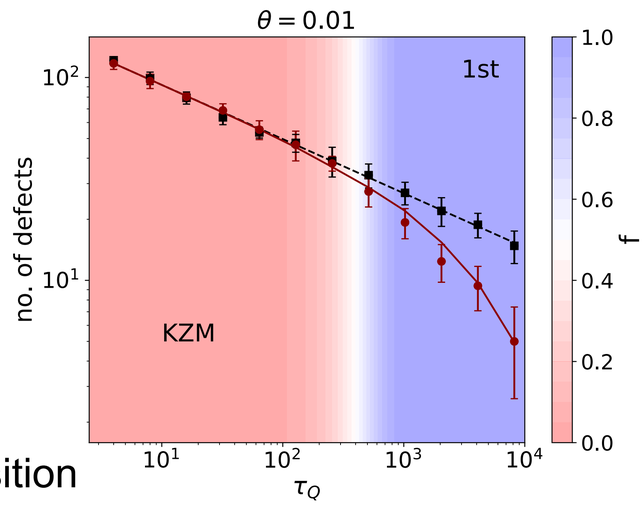
■ 2nd-order phase transition



● Weakly 1st-order phase transition

The numerical results ● agree with the analytical predictions — given by

$$n = (1-f)n_{KZM} + f n_{nuc}$$



6 Summary

The distinction between 1st-order and 2nd-order phase transitions has long been considered fundamental, with separate theoretical frameworks: nucleation theory for 1st-order transitions and KZM for 2nd-order transitions. However, it has become evident that many condensed matter systems, such as liquid crystals, exhibit a mixture of characteristics from both 1st- and 2nd-order phase transitions. Not only classical phase transitions, but also quantum phase transitions can exhibit weakly 1st-order behavior when complex systems with additional interactions are considered.
In our study, we extended the Kibble-Zurek mechanism and the theory of non-adiabatic excitations to weakly 1st-order phase transitions by incorporating corrections associated with 1st-order behavior. Our results open the door to exploring defect formation in exotic phase transitions in condensed matter systems, as well as extending studies of non-adiabatic excitations in quantum simulators and quantum annealers.

References & Acknowledgements

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