Seminar 1: Kibble - Zurek Mechanism

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January 5, 2020
1 Introduction

Phase transitions are intriguing phenomena of nature occurring with important transformations in the properties of physical systems [1]. For a lot of systems the phase diagrams are known. For example: the phase diagram of water is well known. But what is the response of a system, if one dependent parameter or more does not change quasi-statically but with a finite rate? Especially interesting is a system response during a phase transition in non-equilibrium dynamics. This is where the so called Kibble–Zurek mechanism steps in. The Kibble-Zurek mechanism (KZM) describes the dynamics of a system, that is driven through a continuous phase transition at a finite rate. In the process, topological defects can be formed, such as vortexes, strings, domain walls, etc. Their numbers are estimated by the KZM model.

In the seminar, the basic idea of KZM will be explained, following a quick revision of phase transitions. Next, a heuristic example of a paramagnetic to ferromagnetic phase transition will be introduced followed by the KZM theory. At the end, some experiments will be mentioned and explained.

2 Kibble - Zurek Mechanism

2.1 Basic Idea

It is believed, that the universe as we know, was created from a very high density and high temperature state, which soon after the “Big Bang” rapidly expanded and cooled. This cosmological model is called The Big Bang theory. The fields that mediate fundamental forces (believed to be unified at a very high temperature - there would be only one type of force) underwent a sequence of spontaneous symmetry breaking phase transformations while cooling. Because phase transformations were driven by a fast temperature quench, the phase properties (order parameter) cannot necessarily be the same in regions which are not connected by causality. Regions are not connected by causality if they are separated far enough (at the given age of the universe) that they cannot “communicate” even with the speed of light (same cause can have a different effect in two distant enough regions). This implies that the symmetry cannot be broken globally (in the whole spacetime). The phase properties will be different (order parameter will take different values) in causally disconnected regions and the domains will be separated by domain walls after further evolution of the universe [2, 3]. Depending of the symmetry properties of the system and the nature of the phase transition, different topological defects can be formed such as domain walls, cosmic strings, monopoles and textures [4]. This theory was proposed and argued by Tom W. B. Kibble around 1974-1976 and is called Kibble Mechanism.

In 1985, the idea of Kibble was subsequently extended by Wojciech H. Zurek to second order phase transitions in condensed matter systems. Zurek pointed out, that some critical phenomena predicted by Kibble, can be tested in suitable experiments in the laboratory. This general description is usually referred as the Kibble–Zurek mechanism.
(KZM). It predicts the formation of smaller phase domains for faster quenches across the phase transition, and it describes the scaling with the quench speed of the number of topological defects formed after the transition crossing by means of simple analytic relations [1].

2.2 Quick Revision of Phase Transitions

Before we move forward with the theory of KZM, we shall make a quick revision of phase transitions. Phase transitions are usually characterized by the system undergoing a transition from a symmetric (disordered) state to a broken symmetry (ordered) state. The order parameter can be introduced in each state. The order parameter is usually zero in the disordered state and nonzero in ordered state. An example of symmetric, disordered state (water) and less symmetric, ordered state (ice) is shown in figure 1 [5]. The more symmetrical phase is on the high temperature side of a phase transition and the less symmetrical phase on the low temperature side. At low temperatures, the system tends to be confined to lower energy states. At higher temperatures, thermal fluctuations allow the system to access states in a broader range of energy [6].

![Figure 1: Schematic example of symmetry in water and ice][5]

As traditional classification implies, phase transitions can be divided into two classes, depending on the thermodynamic characteristics of the considered system during the transformation:

- **First order** phase transitions are transitions, that show a discontinuity for one of the first partial derivatives of the Gibbs free energy. A typical example is solid/liquid/gas transition, where the discontinuity is manifested as latent heat.

- **Second order** phase transitions are continuous phase transition in all the first partial derivatives of the free energy, but exhibit a discontinuity in a second derivative of the free energy. A typical example is the ferromagnetic phase transition in materials such as iron.

In this seminar the focus will be on second order phase transitions, where the transformation is driven by the variation of a thermodynamic variable, called control parameter $\lambda$, through a particular value, called critical point $\lambda_c$. 

2.3 Heuristic Example

Before we look into “brute” theory of KZM, let us consider an example: the paramagnetic to ferromagnetic transition with a temperature quench. The control parameter is the temperature \( T \) and the critical point is the Curie temperature \( T_c \). The simplest model of ferromagnetism and transition between order and disorder is the two dimensional ferromagnetic Ising model in the absence of magnetic field:

\[
H = -J \sum_{i,j} (s_{i,j} s_{i+1,j} + s_{i,j+1}s_{i,j}),
\]

where \( s_{i,j} \) represents a spin on 2-d lattice with classical \( z \) component \( \pm 1 \) and \( J \) is the interaction between two spins. The disordered and ordered states are represented by the paramagnetic and the ferromagnetic states, respectively.

The direction of spin is directly connected to order parameter. In the disordered, paramagnetic phase the spins choose random direction \( \uparrow = +1 \) or \( \downarrow = -1 \). In average the sum of all spin values is zero and therefore the order parameter is zero. In the ordered ferromagnetic phase, immediately after the phase transition at \( T = T_c \), a slight majority of spins randomly chooses one of the possible direction. Lower the temperature, more spins choose the direction of majority. At \( T = 0 \) all spins point in the same direction. The order parameter is equal to the average spin and at \( T = 0 \) takes value \( \pm 1 \) depending on the majority direction choice at the transition point. The order parameter dependency of temperature is seen in figure 2 [7].

\[
\beta = \frac{1}{k_B T_c}, \quad k_B T_c = 2,269
\]

Figure 2: Ising model order parameter dependency of temperature.

Let us have a temperature quench and begin in the region \( T \gg T_c \). The system can follow the temperature change until temperature \( T \) is close to critical temperature \( T_c \) of phase transition. In the region \( T \sim T_c \) the system cannot follow the temperature change and the system is effectively frozen. The system stays frozen until temperature \( T \) is sufficiently smaller than \( T_c \) when the system can follow the change of temperature again. But important is what happens when the system is effectively frozen and cannot follow the temperature change, that is, when the system is driven through a phase transition. Regions of the system must randomly choose spin \( \uparrow \) or spin \( \downarrow \), therefore different regions choose different order parameter. Because some regions are too far away and cannot “communicate” with each other, domains are formed. The size and number of domains depend on the temperature quench rate.
The Ising model is only a simplification of a ferromagnetic material. In ferromagnetic systems the spins represent magnetic dipoles which point in all directions in the disordered state and the net magnetisation is zero. In the ordered state there is a tendency to have all magnetic dipoles aligned in the same direction and have the maximum net magnetisation. For a slow temperature quench one domain is formed and maximum net magnetisation is obtained. For a fast temperature quench, domains and domain walls are formed. A schematic representation of a paramagnetic to ferromagnetic phase transition with forming domains is shown in figure 3.

Figure 3: Schematic example of a ferromagnetic phase transition.

It is best to keep in mind, that this is only a heuristic example. It is impossible to perform such an experiment in a laboratory and measure the domain sizes and numbers (or any other topological defects formed at domain walls) due to the temperature gradients that arise in the material. There are more suitable experiments of verifying KZM which will be represented later on.

2.4 Theory
2.4.1 Equilibrium

Let us make a step back to the second order phase transition theory and look into the order parameter fluctuations. Statistical fluctuations of the order parameter play a key role in mentioned phase transitions. The length scale over which fluctuations of the order parameter are correlated is called correlation length $\xi$. At the transition, when the control parameter is close to the critical point ($\lambda \sim \lambda_c$), the correlation length can be described with a power law with critical exponent $\nu$:

$$\xi \sim |\lambda - \lambda_c|^{-\nu}.$$  

(1)

The divergence of $\xi$ corresponds to singularities in other thermodynamic quantities. For example: heat capacity $C$, order parameter $m$ and susceptibility $\chi$. The quantities or their derivatives all diverge at the critical point. Their definitions are as follows:

$$C \sim |\lambda - \lambda_c|^{-\alpha}, \quad m \sim |\lambda - \lambda_c|^{\beta}, \quad \chi \sim |\lambda - \lambda_c|^{-\gamma}.$$  

(2)
For example, in a ferromagnet the control parameter \( \lambda \) is the temperature \( T \) in quantities \([2]\). It turns out that in all second order phase transitions thermodynamic quantities and correlation length abide as power law functions of the control parameter at \( \lambda \sim \lambda_c \). \( \nu, \alpha, \beta, \gamma,... \) are known as critical exponents. There are a total of six critical exponents, but only two are independent. It is experimentally proven that widely different systems, with critical temperatures differing by orders of magnitudes, approximately possess the same set of critical exponents. This phenomenon is known as universality \([1, 6, 8]\).

### 2.4.2 Non-Equilibrium Dynamics

So far a stationary system was considered. The system is point by point at its equilibrium. However, this adiabatic description is not realistic in experiments where the transition is crossed changing the control parameter at a finite rate. In order to describe the dynamical properties of the system one can introduce another characteristic quantity called relaxation time \( \tau \) which sets the timescale for the relaxation of the order parameter to its equilibrium value. Similar to the correlation length the relaxation time \( \tau \) scales with the control parameter \( \lambda \) as a power law diverging at the critical point of a second order phase transition with a critical exponent \( \mu \):

\[
\tau \sim |\lambda - \lambda_c|^{-\mu}.
\] (3)

The result of the divergence of relaxation time (3) is critical slowing down. In this regime the system takes a lot of time to relaxate back to equilibrium if a slight disturbance is applied. This regime is the reason that phase transitions in experiments are always crossed in a non-adiabatic way \([1]\).

### 2.4.3 Linear Quench

Everything is set for the Kibble-Zurek Mechanism (KZM). Let us consider a second order phase transition with a linear quench of the control parameter \( \lambda \) in the vicinity \( \lambda_c \), starting from \( \lambda > \lambda_c \) in the disordered phase, to some value \( \lambda < \lambda_c \) of ordered phase. The control parameter \( \lambda \) varies at the vicinity \( \lambda \sim \lambda_c \) linearly as

\[
\lambda(t) = \lambda_c(1 - \epsilon(t)),
\] (4)

where \( \epsilon \) is the reduced control parameter defined as

\[
\epsilon = \frac{\lambda_c - \lambda}{\lambda_c} = \frac{t}{\tau_q}.
\] (5)

Here \( \tau_q \) is the quench time which characterizes the speed of the transition. Note, that \( \epsilon \) vanishes at the critical point. The time \( t \) takes value \(-\tau_q < t < \tau_q\).

A slight redefinition of equations (4) and (3) (correlation length \( \xi \) and relaxation time \( \tau \) respectively) has to be made and is as follows

\[
\xi = \xi_0|\frac{\lambda - \lambda_c}{\lambda_c}|^{-\nu} = \xi_0|\epsilon(t)|^{-\nu},
\] (6)

\[
\tau = \tau_0|\frac{\lambda - \lambda_c}{\lambda_c}|^{-\mu} = \tau_0|\epsilon(t)|^{-\mu},
\] (7)
where $\xi_0$ and $\tau_0$ are constants determined by the system. A characteristic velocity of a system can be defined

$$c(\lambda) = \frac{\xi(\lambda)}{\tau(\lambda)} = \frac{\xi_0}{\tau_0} |\epsilon(t)|^{\mu-\nu}. \quad (8)$$

The characteristic velocity tells us the limit how fast the information of order parameter can propagate through the system. Hence, after the transition the distance over which information can propagate is the sonic horizon

$$h(t) = \int_0^t c(\lambda(t'))dt' = \frac{1}{1+\mu-\nu} \xi_0 \tau_0 |\epsilon(t)|^{1+\mu-\nu}. \quad (9)$$

Thus, at symmetry breaking, if two regions are further away than the sonic horizon, the order parameter can take different random values in those two regions and domain walls (or other topological defects) are formed [9].

The typical size of domains can be estimated from Zurek correlation length $\xi_Z$ introduced in equation (12). When they form can be estimated from Zurek relaxation time $\tau_Z$ introduced in equation (13). Sonic horizon (9) becomes equal to the correlation length (6) when

$$\epsilon = \epsilon_Z = \left(1 + \mu - \nu \right) \frac{\tau_0}{\tau_q} \frac{1}{1+\mu}. \quad (10)$$

The time when this happens is the Zurek time

$$t_Z = \left(1 + \mu - \nu \right) \frac{\tau_0}{\tau_q} \frac{1}{1+\mu}. \quad (11)$$

At the Zurek time $t_Z$ the correlation length (6) equals the Zurek correlation length

$$\xi(t_Z) = \xi_Z = \xi_0 \left(\frac{\tau_q}{\tau_0}\right)^{\frac{-\mu}{1+\mu}} \quad (12)$$

and the relaxation time (7) equals the Zurek relaxation time

$$\tau(t_Z) = \tau_Z = \left(\frac{1}{1+\mu - \nu} \frac{\tau_q}{\tau_0}\right)^{\frac{-\mu}{1+\mu}}. \quad (13)$$

![Figure 4: Schematic representation of the frozen regime dependent of $\tau_Z$.](image)
Domains or other topological defects form when relaxation time in the equation $\tau(t) > \tau_Z$. In this regime the system is frozen and cannot follow the change of the control parameter. In the other regime, when $\tau < \tau_Z$ the system can follow the change of the control parameter adiabatically. For slower quenches the frozen-out stage is narrower than for faster quenches. For an infinite long quench, the frozen-out stage vanishes. This is shown schematically on figure 4 where the frozen regime represents the darkened part. Correlation length behaves qualitatively the same and a similar graph $\xi(\epsilon)$ as a figure 4 can be plotted.

2.4.4 Main Prediction of KZM

The KZM predicts the typical average size of a domain that form in the freeze-out stage as $\xi_Z$ in equation (12). Moreover, the density of defects $n$ that form at domain walls can be estimated as

$$n \sim \frac{\xi_d^d}{\xi_Z^D} = \frac{1}{\xi_Z^{D-d}} \left( \frac{\tau_0}{\tau_q} \right)^{(D-d) \frac{\nu}{\nu+\mu}},$$

where $D$ and $d$ are the dimensions of space and defects respectively. For example, $D = 3$ and $d = 1$ for space and vortex lines respectively in a 3D superfluid. Thus KZM predicts “larger” domains in smaller numbers for slow quenches and “smaller” domains in larger numbers for fast quenches but it fails to predict the precise values. Usually the predicted density of defects in (14) is overestimated and a factor $f \approx 5 - 10$ to multiply $\xi_Z$ is used. However, if one were able to check the power law above, one could claim that the KZM holds and show that the non-equilibrium dynamics across the phase transition is also universal.

3 Experiments

The predictions of the KZM have been tested in numerous numerical experiments under varying conditions. Laboratory experiments are fewer and their results are less conclusive. Chronologically, the experiments in superfluid helium were one of the first experiments to test KZM.

3.1 Helium 4

Zurek initially suggested testing the predictions of the mechanism in superfluid $^4$He. The reason is the fact, that both liquid $^4$He and many models of the early universe can be described in a mathematically similar manner (using Ginzburg-Landau theory). He pointed out in particular that the cosmological symmetry-breaking transition, expected on the basis of grand unified theories (GUTs) to have occurred $\sim 10^{-34}$ s after the big bang, is in many ways closely analogous to the lambda (superfluid) transition in liquid $^4$He. In each case a complex order parameter is used which is on average zero above the transition temperature and takes on a finite average value in the broken symmetry state.
below it. Therefore the order parameter of liquid $^4\text{He}$ (superfluid wave function) plays a similar role to that of the Higgs field in cosmological case [11].

Zurek suggested an experiment, where a rapid expansion of normal liquid He I through the lambda transition to superfluid He II would be made. Consequently, because of the fast transition, vortexes as defects should appear. Such an experiment was indeed performed. A sample of isotopically purified liquid $^4\text{He}$ was held within an isolated experimental cell, which could be compressed or expanded. The formation of vortexes was measured with attenuation of the second sound, which is strongly damped by vortexes. Second sound is a thermal wave in which the normal and superfluid components oscillate in antiphase. A pulse of second sound produced by the heater, planted in the cell, travels to the bolometer where it induces a signal in the form of a transient jump of temperature. The signal intensity is reduced by the presence of any vortexes in the intervening liquid. Expansion trajectories were determined by making quasistatic adjustments of the chamber volume with measurements of resultant changes in the pressure and temperature of the sample. Some trajectories are shown on the relevant part of $^4\text{He}$ phase diagram [5] [11].

![Figure 5: Relevant part of the $^4\text{He}$ phase diagram with calculated $\bullet$ and measured $\circ$ points of isentropes by expanding normal fluid He I to superfluid He II [11].](image)

In the experiment fast expansions followed the quasistatic ones shown on figure 5 to a good approximation. The vortexes did appear in the experiment, but it was anticipated that the vortexes would decay faster. The cause of long decay of vortexes could be the vorticity produced by hydrodynamic effects on the walls of the cell. To overcome these problems, the apparatus of the experiment was redesigned to minimize the hydrodynamic effects, and the experiment repeated. Disappointingly the result was null. No vortexes were detected. One possible explanation for this is that the vortexes produced may simply disappear too fast to be seen [9] [11].

### 3.2 Helium 3

There are a number of advantages in using $^3\text{He}$ rather than $^4\text{He}$. One is that because the correlation length is much longer, a continuum Ginzburg-Landau description is much
more accurate than in $^4$He. Moreover, the energy needed to generate a vortex is larger relative to the thermal energy, therefore it is easier to avoid extrinsic vortex formation [9].

The greatest advantage might be the fact, that one can induce a temperature rather than pressure-driven transition. $^3$He is a rather efficient absorber of slow neutrons via the reaction

$$n + ^3\text{He} \rightarrow p + ^3\text{H} + 764 \text{ keV}. \quad (15)$$

The experiment (in Grenoble) was done using reaction (15) where small portions of superfluid helium $^3$He-B (the superfluid phase B and normal phase are shown in figure 6) were heated and changed to normal fluid phase. These regions of helium in the normal phase are then rapidly cooled back by the surrounding superfluid $^3$He-B. During this process it is expected that a random tangle of vortexes is generated [12].

![Figure 6: The relevant part of the $^3$He phase diagram in absence of magnetic field [12].](image)

The experiment was essentially calorimetry. The total thermal energy released in $^3$He-B following each neutron-absorption event was measured. Some of the measurements are seen in the left panel of figure 7. An energy deficit from 764 keV was noticed. From the energy deficit dissipations of around 25 keV due to scintillations in $^3$He-B were estimated.

Energy $E = (764 - 25) \text{ keV}$ is deposited at a single point in the fluid. The energy creates a sphere of normal fluid which subsequently cools via quasiparticle diffusion with diffusion constant $D$ of normal fluid $^3$He at $T_c$. As the sphere cools, the volume of normal fluid first expands and then shrinks to zero. The maximum radius of the normal fluid sphere is estimated to be

$$R \simeq 0.4 \cdot (E/CT_c)^{1/3} \quad (16)$$

where $C$ is the normal fluid heat capacity just above $T_c$ [12]. The quench time is estimated to be

$$\tau_q \simeq R^2/4D. \quad (17)$$

From calculated $\tau_q$ and given system correlation length $\xi_0$ theoretical prediction $\xi_Z$ is calculated using critical exponents $\mu = 1$ and $\nu = 1/2$. Theoretical ratio $\xi_Z/\xi_0$ is seen in the right panel of figure 7.
The deficit energy minus 25 keV is used for vortex creation. Estimated vortex energy is seen in the right figure.[6] The energy per length is given

\[ E_L \simeq \frac{\rho}{4\pi} \left( \frac{\hbar}{2m_3} \right)^2 \ln\left( \frac{\xi_Z}{\xi_0} \right) \]  

where \( \rho \) is \( ^3 \)He superfluid density and \( m_3 \) \( ^3 \)He atom mass \[12\]. With the equation (18) vortex length is computed from vortex energy. It is assumed that vortex length is evenly distributed over the maximum volume of normal fluid sphere. From the evenly distributed vortex length the ratio \( \xi_Z/\xi_0 \) is obtained. Experimental results are seen in the right panel of figure.[7] Although there is a difference of factor 2 and a difference in the pressure dependency between measured and theoretical values, the experiment and theory are in good agreement if large simplifications in the analysis are considered. The main problem is the lack of knowledge how the energy of initial reaction (15) is converted into thermal energy.

![Figure 7: The Grenoble experiment data and results \[12\].](image)

### 4 Conclusion

The Kibble-Zurek theory is itself a rather simplified model and should only be expected to give the correct order of defect number. Since the first experiments on liquid helium, some of the predictions for the KZM were observed in many different systems, such as nonlinear optical systems, thin-film superconductors, ring-shaped Josephson junctions, ferromagnetic spinor BECs, multiferroic crystals, atomic Mott insulators and others. All confirmed the basic idea, that defects are formed during rapid phase transition. The best evidence so far, that Zurek predictions of defect numbers are sound, comes from the \( ^3 \)He experiments though the others are reasonably consistent.
References


