Phase Transition in Space: How Far Does a Symmetry Bend Before It Breaks?

Wojciech H. Zurek\textsuperscript{1} and Uwe Dorner\textsuperscript{2}

\textsuperscript{1}Theory Division, LANL, MS-B213, Los Alamos, NM 87545, USA
\textsuperscript{2}Clarendon Laboratory, University of Oxford, Parks Road, Oxford OX1 3PU, United Kingdom

We extend the theory of symmetry breaking dynamics in non-equilibrium second order phase transitions known as the Kibble-Zurek mechanism (KZM) to transitions where the change of phase occurs not in time, but in space. This can be due to a time-independent spatial variation of a field that imposes a phase with one symmetry to the left of where it attains critical value, while allowing spontaneous symmetry breaking to the right of that critical borderline. Topological defects need not form in such a situation. We show, however, that the size, in space, of the “scar” over which the order parameter adjusts as it “bends” interpolating between the phases with different symmetry follows from a KZM - like approach. As we illustrate on the example of a transverse quantum Ising model, in quantum phase transitions this spatial scale – the size of the scar – is directly reflected in the energy spectrum of the system: In particular, it determines the size of the energy gap.

PACS numbers: 03.65.-w, 73.43.Nq, 03.75.Lm, 32.80.Bx, 05.70.Fh

INTRODUCTION

Near the critical point of a second order phase transition both the relaxation time (which determines “reflexes” of the system) and the healing length (which sets the scale on which its order parameter “heals” in space, i.e., returns to its equilibrium value) diverge:

\begin{align}
\tau &= \tau_0/|\epsilon|^\nu, \quad (1) \\
\xi &= \xi_0/|\epsilon|^\nu. \quad (2)
\end{align}

Above, \(\epsilon\) is a dimensionless parameter which measures the distance from the critical point. For instance, when the transition is caused by the change of the temperature \(T\) or by varying the parameter \(g\) of a Hamiltonian, \(\epsilon\) is, respectively, given by:

\[\epsilon = (T - T_C)/T_C, \quad \epsilon = (g - g_C)/g_C, \quad (3)\]

where \(T_C\) and \(g_C\) are the critical values.

Divergences in \(\tau\) and \(\xi\) that appear near the critical point as a consequence of these two equations are often referred to as critical slowing down (for obvious reasons) and as critical opalescence (as the fluctuation on a scale \(\xi\) that becomes large in the vicinity of a critical point cause, in some systems, variations of the optical properties on scales \(\sim\xi\), which leads to opalescence). These divergences will play a crucial role in our discussion.

Phase transitions are usually investigated as equilibrium phenomena in homogeneous systems. But many intriguing questions arise when a system is driven at a finite pace from one phase to another. That this will inevitably happen in the cosmological setting was first pointed out by Kibble\textsuperscript{1}, who noted that because of relativistic causality – cosmological phase transitions in a variety of field theoretic models necessarily lead to formation of topological defects (such as monopoles or cosmic strings) and may have dramatic astrophysical consequences.

It was later pointed out by one of us\textsuperscript{2} that analogs of cosmological phase transitions can be studied in the laboratory, and that the equilibrium critical scalings – Eqs. (1) and (2) – can be used to predict various aspects of non-equilibrium dynamics of symmetry breaking, including the density of topological defects left behind by a non-equilibrium second order phase transition\textsuperscript{2,3,4}.

The resulting theory (known as “Kibble-Zurek mechanism” or KZM) uses critical scalings of the relaxation time and of the healing length to estimate the size \(\xi\) of the domains that choose the same broken symmetry\textsuperscript{2,3}. Owing to the universality of phase transitions, KZM can be applied on many energy scales, from the (cosmologically relevant) high energy settings (including experiments such as RHIC or LHC), all the way to Bose-Einstein condensates at ultra-low temperatures.

In all of these situations a frequent prediction is that the process of symmetry breaking will lead to the formation of topological defects. This is essentially inevitable when the broken symmetry phase (characterised by the homotopy group) permits their existence\textsuperscript{1,2,3,4}. Following the transition, topological defects should appear with the density of about one defect unit (e.g., one monopole or one \(\xi\)-sized section of a string) per \(\xi\)-sized domain. The value of \(\xi\) that results from this non-equilibrium process can be deduced from the equilibrium near-critical behaviour. Estimating this size is therefore essential.

Here we first summarise the key ideas and equations that lead to such estimates. We shall then investigate the behaviour of the order parameter in an inhomogeneous system, where the change between phases is imposed by a slowly varying externally controlled parameter, such as the field in the quantum Ising model. We shall calculate how far does the transition region between the two phases persist – how much does a symmetry that prevails on one side of the critical line “bend” before it breaks, spontaneously, on the other side.
DYNAMICS OF SYMMETRY BREAKING

We consider a second order phase transition that is traversed at a finite rate set by the quench timescale $\tau_Q$,

$$\epsilon = \frac{t}{\tau_Q}. \quad (4)$$

The system will be able to adjust its state adiabatically as long as the rate of change imposed from the outside is slow compared to its reaction time given by $\tau$, Eq. 14. This change from nearly adiabatic to approximately impulse behaviour will happen at an instant $\hat{t}$ when

$$\tau(\hat{t}) = \frac{\epsilon(\hat{t})}{\dot{\epsilon}(\hat{t})}, \quad \text{or} \quad \tau_0|\dot{\epsilon}(\tau)|^{-\tau_{\nu z}} = \hat{t}. \quad (5)$$

Thus, the state of the system’s order parameter will in effect “freeze” at

$$\hat{t} = (\tau_0 \nu_{\tau z})^{-\frac{1}{1+\nu_{\tau z}}} = \hat{t}. \quad (6)$$

Its evolution will restart only $\hat{t}$ after the critical point is passed. The instant $\hat{t}$ plays a key role in the establishment of the fluctuations which seed structures (such as topological defects) in the broken symmetry phase 5.

The key instant $\hat{t}$ corresponds to

$$\dot{\epsilon} = \left(\frac{\tau_0}{\tau_Q}\right)^{\frac{1}{1+\nu_{\tau z}}} \quad (7)$$

which in turn sets the characteristic spatial scale given by the corresponding healing length

$$\xi = \xi_0 \left(\frac{\tau_Q}{\tau_0}\right)^{\frac{1}{1+\nu_{\tau z}}}. \quad (8)$$

This is the estimate of the size of regions that break symmetry in a more or less coordinated manner 2, 3. Our derivation subverts equilibrium properties of the system – its scaling in the vicinity of the critical point – to predict non-equilibrium consequences of the quench. The density of topological defects left behind in the wake of a phase transition is the best known (but not the only) example of such predictions of KZM.

These predictions were tested, extended and refined with the help of numerical simulations 6, 7, and verified in a variety of increasingly sophisticated and reliable experiments in liquid crystals 8, 9, superfluids 10, 11, 12, superconductors 13, 14, 15, as well as other systems 16. The majority of the experiments to date are consistent with KZM. The case of superfluid $^4$He may be an exception. There the initial reports of detection of KZM vortices 10 were retracted 11 after it turned out that the observed copious vorticity was inadvertently induced by stirring. It is still not clear if $^4$He behaviour is really at odds with the KZM predictions re-evaluated in view of the refined numerical estimates 7. One problem is that the decay of vortex tangle generated by KZM may be faster than that generated by stirring: KZM leads to anticorrelations between neighbouring vortices, so phase ordering kinetics is expected to proceed faster than when vortices are correlated, as when they originate from turbulent flows. An accessible recent summary of the experimental situation due to Kibble 17 is a highly recommended and up-to-date complement to this brief discussion. Further experiments that may allow for a better control of various parameters would be obviously welcome. Gaseous Bose-Einstein condensates are one recent and very promising proving ground 18, 19 that has already yielded some exciting results 20, 21, 22.

Recently, KZM theory was applied to quantum phase transitions 23, 24, 25, 26, 27, 28, 29, 30, 31, 32, 33, 34. There, the system is at $T = 0$, and the nature of its ground state changes discontinuously as a result of a continuous change of some parameter of its Hamiltonian. At the critical value of that parameter the gap – energetic price of the lowest excitations, given by the difference between the energy of the ground and the first excited state – is at its minimum, and it disappears in the limit of an infinite system. In a finite system the quantum phase transition is then described by an avoided level crossing. The basic observation due to Damski 27 is that KZM can be used to analyse the avoided level crossing process, and that it yields results in excellent agreement with Landau-Zener theory 35. As we shall see below, the analogy is based on the observation that, far away from the avoided level crossing, the quantum system usually starts its enforced evolution adiabatically, as was the case for second order phase transitions. However, it can only react on the relaxation timescale given by the inverse of the gap. Therefore, near the avoided crossing – where the gap closes – its reflexes deteriorate, and the impulse approximation in the immediate vicinity of a quantum critical point is appropriate. Below we give an illustration of KZM in action in the exactly solvable and paradigmatic quantum Ising model.

**QUENCH IN A QUANTUM ISING MODEL**

According to Sachdev 26 the quantum Ising model is one of two prototypical examples of quantum phase transitions. It represents a chain of spins with the Hamiltonian

$$H = -J(t) \sum_{i=1}^{N} \sigma^z_i - W \sum_{i=1}^{N-1} \sigma^z_i \sigma^z_{i+1} \quad (9)$$

where $\sigma_i^{x,z}$ are Pauli operators, $W$ is the Ising coupling, and $J(t)$ is due to the external (e.g., magnetic) field that attempts to align all spins with the $x$-axis. The phase transition from the paramagnetic state where all the spins are aligned with $x$ by the strong external field (e.g., $\uparrow, \downarrow, \ldots, \downarrow$) to the low-field ferromagnetic and degenerate (in the large $N$ limit) ground state that “lives”
in the Hilbert subspace spanned by the broken symmetry basis $|↑,↑,\ldots,↑\rangle$ and $|↓,↓,\ldots,↓\rangle$ takes place when $J(t) = W$. Therefore, as suggested by Eqs. (3) and (4), a key role is played by the relative coupling given by
\[ \epsilon(t) = J(t)/W - 1 = t/\tau_Q \]
and we assume that it depends linearly on $t$.

All the relevant properties depend on the size of the gap $\Delta$ between the ground state and the first excited state. In an infinite system the gap is given by:
\[ \Delta = 2|J(t) - W| = 2W|\epsilon(t)| . \]
The spectrum (and the gap) of a finite quantum Ising system are illustrated in Fig. 1. The gap sets the energy scale and is reflected in the relaxation time and the healing length
\[ \tau = \hbar/\Delta = \hbar/2W|\epsilon(t)| = \tau_0/|\epsilon(t)| , \]
\[ \xi = 2W a/\Delta(t) = a/|\epsilon(t)| = \xi_0/|\epsilon(t)| , \]
the latter given by the product of $\tau$ and the speed of sound $c = 2Wa/\hbar$ (see [36]), where $a$ is the distance between spins. The divergence of $\tau$ and $\xi$ is the critical slowing down and the analogue of critical opalescence, respectively.

The instants $\pm \hat{t}$ when the behaviour switches from adiabatic to impulse happen when the reaction time of the system, Eq. (12), is the same as the timescale on which its Hamiltonian is altered (given by $\epsilon(t)/\dot{\epsilon}(t) = t$), i.e.
\[ \tau(\hat{t}) = \tau_0/|\epsilon(\hat{t})| = \epsilon(\hat{t})/\dot{\epsilon}(\hat{t}) = \hat{t}, \]
and thus
\[ \hat{t} = \sqrt{\tau_0/\tau_0} = \sqrt{\tau_0\hbar/2W}. \]
As before, for $t < -\hat{t}$, the state of the system will continue to adjust adiabatically to changes imposed by the decreasing $J(t)$. However, at $t = -\hat{t}$ before the critical point the evolution will cease, and it will re-start only at $t = +\hat{t}$ after the transition, with the initial state similar to the one “frozen out” at $-\hat{t}$.

Using the relative coupling $\hat{\epsilon}$ associated with $\hat{t}$ we get
\[ \hat{\epsilon} \equiv \epsilon(\hat{t}) = \dot{\hat{t}}/\tau_Q = \sqrt{\tau_0/\tau_Q}, \]
\[ \hat{\xi} \equiv \xi_0/\hat{\epsilon} = \xi_0\sqrt{\tau_Q/\tau_0} = a\sqrt{2W\tau_Q/\hbar} . \]
Following KZM, we now predict appearance of $O(1)$ defects per $\hat{\xi}$. Their density should be approximately
\[ \hat{n}_{KZM} \propto a/\hat{\xi} = \sqrt{\hbar/2W\tau_Q} \]
per spin. This is only an estimate: Simulations of classical second order phase transitions yield defect densities that scale with $\tau_Q$ in accordance with this reasoning, but are lower than the relevant power of $\hat{\xi}$ of Eq. (17) so that a “unit of defect” is often separated by $\sim \text{10-15}\;\hat{\xi}$; see e.g. [6, 7].

There is a fundamental difference between quantum and thermodynamic phase transitions. In the thermodynamic case ‘real’ fluctuations exist above the critical point. They can initiate the symmetry breaking process – in effect, choose how symmetry breaks in domains that appear after the transition. In the case of quantum phase transition there are only ‘quantum fluctuations’, but they are virtual, so one cannot be certain that they will have an analogous effect on the post-transition state. Therefore, an explicitly quantum approach to the quantum Ising model is needed.

As we have already noted, a key feature of a quantum phase transition is the gap $\Delta$. Actually, as can be seen in Fig. the relevant gap (i.e. the gap between the ground and the first accessible state) is not the symmetric $\Delta$ but rather $2\Delta$ on the approaching side. Nevertheless, in the quantum Ising model the gap disappears at the critical point when the system is infinite. When $N < \infty$, this critical gap becomes small, but does not disappear, (see Fig. 1). This is important, and allows us to propose a purely quantum approach: Instead of density of defects in an infinite system we can compute (as a function of quench timescale $\tau_Q$) the length of the spin chain that, with probability $p$ of about a half, can remain defect-free (in a ground state) after the quench. An excited state would (most likely) contain just a single excitation (e.g., a kink). Therefore, the inverse of the length that limits the excitation probability to approximately $\sim 0.5$ should correspond to about half of the kink density.

The two lowest accessible levels of $H$ in the vicinity of the critical point (Fig. 1) exhibit an avoided level crossing

\[ \text{FIG. 1: Energies of lowest excitations of the Ising chain for } N = 20 \text{ with open (rather than periodic) boundary conditions. The ground and the first accessible excited state that define the gap are marked with a thicker line.} \]
and we can calculate the excitation probability of the system driven through this avoided crossing using the Landau-Zener formula (LZF),

\[ p \approx e^{-\frac{n^2\Delta^2}{2h|v|}}. \]  

Equation (19) translates into a condition for the rate of quench

\[ |v| \leq \frac{\pi \Delta^2}{2h|\ln p|}. \]  

Using \( v = |\Delta| = 2J(t) = 2W/\tau_Q \) [see Eq. (10)] and \( \Delta = 4\pi W/N \) for the gap upon “closest approach” we get

\[ |v| = |\Delta| = \frac{2W}{\tau_Q} \leq \frac{\pi(4\pi W/N)^2}{2h|\ln p|}. \]  

This relates the size \( \tilde{N} \) of a chain that will remain defect-free with the probability 1-p to the quench rate:

\[ \tilde{N} \leq 2\pi \sqrt{\frac{\pi W\tau_Q}{h|\ln p|}}. \]  

This LZF estimate is (surprisingly) accurate for \( p < 0.5 \) even though there are many levels in the spectrum of the quantum Ising model. Such accuracy was surprising when this analysis was first presented [22]. Dziarmaga has soon after demonstrated that this is no accident – in effect, the phase transition in the quantum Ising model can be decomposed into a collection of independent avoided level crossings.

We can now directly compare KZM, Eq. (18), and LZF predictions for defect density:

\[ \tilde{n}_{LZF} \simeq \frac{1}{N} = \frac{1}{2\pi} \sqrt{\frac{2|\ln p|}{\pi}} \times \tilde{n}_{KZM}. \]  

The two estimates exhibit the same scaling with the quench rate and with the parameters of \( H \), Eq. (9). LZF predicts fewer defects than “raw KZM” (\( \tilde{n}_{LZF} \simeq 0.14 \times \tilde{n}_{KZM} \) when \( p \) is set – somewhat arbitrarily – to 0.5). This is not a big surprise – as seen in the numerical simulations, confirmed by the experiments and verified analytically in specific models, Eqs. (17) and (18) provide correct scalings, but tend to overestimate densities (see e.g. [3, 28]). Fig. 2 indicates that this conclusion holds also for the quantum Ising model.

Figure 2 also shows that the kink density scales approximately as \( \sim 1/\sqrt{\tau_Q} \), Eq. (18), in the region of the validity of KZM, i.e. for \( \hat{t} \) less than 1 (so that quench is quasi-adiabatic at the beginning and at the end, but impulse near the critical point, i.e., when at least one defect is expected). The prefactor which is approximately 0.16 [0.12 if the steeper slope on the approach in Fig. 1 is taken] is not far from the previous experience [6]. For very slow quenches (\( \hat{t} > h/\Delta \), the expected range of validity of KZM. For sufficiently slow quenches LZF provides reliable predictions. Very fast quenches are “all impulse”, levelling off of the expected number of kinks, as is indeed seen.

FIG. 2: (a) Number of kinks per spin in the quantum Ising model after a quench starting in the ground state at \( J = 5W \) and ending at \( J = 0 \), plotted as a function of the quench rate \( \tau_0/\tau_Q = \hbar v/4W^2 \) for \( N = 50, 60, 70, 80, 90, 100 \) (solid lines; bottom to top). The scaling \( \tilde{n}_{KZM} \sim \sqrt{\tau_0/\tau_Q} \) predicted by KZM is consistent with the simulations (see [27] for details of the numerical method). Agreement improves with the size of the system: for 100 spins a fit gives \( n \sim \tau_Q^{0.58} \) (dashed line). As in the classical case [6] Eq. (18) is an overestimate; the best fit is \( n \approx 0.16\tilde{n}_{KZM} \). (b) Total number of kinks for \( N = 50, 60, 70, 80, 90, 100 \) spins (dashed lines, bottom to top) after a quench as a function of the quench rate \( \tau_0/\tau_Q = \hbar v/4W^2 \). Both the scaling \( \tilde{n}_{KZM} \sim 1/\sqrt{\tau_Q} \) predicted by KZM (solid, straight lines), Eq. (13), and the LZF estimate \( p \) (solid, bend lines) when less than one kink is expected are valid. The straight lines are linear fits in the range (0.025,0.25) yielding slopes between 0.66 and 0.58. Numerical data include these used in (a) but we now go beyond the expected range of validity of KZM. For sufficiently slow quenches LZF provides reliable predictions. Very fast quenches are “all impulse”, levelling off of the expected number of kinks, as is indeed seen.
predict the same scaling of the size of broken symmetry domains with quench time.

The importance of the behaviour of the gap (and, in particular, of the smallest gap \( \Delta \)) for the quantum estimate of defect density is – in addition to the broader theme of connections between KZM and LZF – our principal general conclusion at this point. We shall return to discuss the gap in the quantum Ising model and utility of extensions of KZM and LZF to more complicated behaviours of the near-critical gap below.

### STATICS OF SYMMETRY BREAKING

Consider now a situation where the all-important dimensionless \( \epsilon \) is \textit{time-independent}, but depends on the location in space instead. We suppose – in analogy with Eqs. [10] – that in the vicinity of the critical point \( \epsilon(x) \) is approximately linear:

\[
\epsilon = \frac{x}{\lambda_Q} = \alpha x .
\]

Clearly, sufficiently far from \( x = 0 \) the order parameter will settle into an equilibrium state corresponding to the local value of \( \epsilon \). We are however left with an interesting question: How far – and how – does the influence of the critical point propagate?

There is an intriguing analogy between the freeze-out in time we have discussed in the preceding section and the freeze-out in space we are led to consider here: When \( \epsilon \) changes in space slowly compared to the local healing length given by \( \xi = \xi_0/|\epsilon|^{\nu} \), Eq. [2], the order parameter will be able to adjust in space to the changes of \( \epsilon \) – i.e., there should be a well-defined local value of the order parameter, local healing length \( \xi \), and local relaxation time \( \tau \), etc. However, very close to \( x = 0 \) the system cannot “heal” fast enough: The healing length becomes large, much larger than \( x \). Consequently, the critical opalescence – the divergence of \( \xi = \xi_0/|\epsilon|^{\nu} \) – will open up a “scar” in the order parameter that does not properly heal. Our aim now is to describe the consequences. To find out the size of the scar we write down the spatial analogue of Eq. [4],

\[
\xi(\hat{x}) = \frac{\epsilon(x)}{\partial_x \epsilon(x)} \bigg|_{x=\hat{x}} ,
\]

for the “adiabatic-impulse” borderline point, \( \hat{x} \). Thus,

\[
\xi_0 \frac{\hat{x}}{\lambda_Q} |^{-\nu} = \hat{x} .
\]

Consequently, and in accord with previous discussion, we conclude that the order parameter will in effect “freeze” (or, to put it differently, that the scar opened up by the transition through the critical region will heal) at a distance

\[
\hat{x} = (\xi_0 \lambda_Q)^{\frac{1}{1+\nu}} = \hat{\xi} .
\]

from the critical point. The distance \( \hat{x} \) corresponds to

\[
\hat{\epsilon} = \left( \frac{\xi_0}{\lambda_Q} \right)^{\frac{1}{1+\nu}} .
\]

We are really done – there is just a spatial \( x \), rather than both \( x \) and \( t \), as before. But let us (as a consistency check) repeat and take a few more steps, and use this estimate of \( \hat{\epsilon} \) to calculate the characteristic spatial scale given by the corresponding healing length,

\[
\hat{\xi} = \xi_0 \left( \frac{\lambda_Q}{\xi_0} \right)^{\frac{\nu}{1+\nu}} .
\]

We know this already [see Eq. (27)]. This is now the estimate of the size of the scar – the size of the region that is “still thinking” about how to break symmetry. Earlier, our derivation of the freezeout time and of the resulting analysis of the dynamics of symmetry breaking subverted equilibrium properties of the system – its scaling in the vicinity of the critical point – to predict non-equilibrium consequences of the quench. We have now repeated this subversive strategy in a new setting, by using the healing length (that is, strictly speaking, defined in a \textit{homogeneous} system) to find out consequences of inhomogeneity that must be there in the vicinity of the critical point if the phase transition takes place in space. The structure of the scar in the order parameter that connects the two phases is now of interest \textit{per se}.

There are two specific values of \( \nu \) that are often encountered: As we have seen in the preceding section, for quantum Ising model \( \nu = 1 \). Therefore,

\[
\hat{x} = \sqrt{\xi_0 \lambda_Q} = \hat{\xi}
\]

and the size of the scar is simply a geometric average of the two relevant lengths in the problem. We shall see below that, as a consequence, in the quantum Ising model the presence of such a scar widens a critical gap. In a mean field theory we have \( \nu = 1/2 \). Consequently,

\[
\hat{x} = (\xi_0^2 \lambda_Q)^{\frac{1}{2}} = \hat{\xi} .
\]

The thickness of the boundary between the two layers is a compromise that involves the characteristic healing length of the order parameter on one hand, and the typical scale of the externally imposed inhomogeneity of the Hamiltonian on the other. The extent to which each of them has its say depends on the scaling exponent \( \nu \). The most obvious test of these predictions would then explore variations of the order parameter in the vicinity of an externally imposed inhomogeneity.

### OPENING A GAP WITH A WEDGE OF A FIELD

To illustrate our considerations with a concrete example we return to the quantum Ising model we have already
FIG. 3: Illustration of the spatially dependent field $J(x)$ in the transverse quantum Ising model we consider. The parameter $J(x)$ corresponds to $J(l)$ from Hamiltonian (b) but now depends on position, $J(l) \rightarrow J(x)$. The spins are located at positions $x_i = (l - 1)a$ with $l = 1, \ldots, N$.

employed in the previous section. The Hamiltonian we shall use now has the same form as before, Eq. (30), but the field $J$, which before was the same for every spin, now has a form illustrated in Fig. 3. As a result, sufficiently far to the left of $\tilde{x}$ the system will be in a paramagnetic phase, while to the right a ferromagnetic phase should be dominant.

Our task is to characterise the state of such a system. In a homogeneous quantum Ising spin system the correlation function given by

$$\zeta(k) = \langle \sigma^{-}_{l-k}\sigma_{l}^{\uparrow}\rangle$$

is a well defined object, whose behaviour is thoroughly explored [36]. Indeed, the decay of such correlation functions is used to define the coherence length (which is in effect often equal to the healing length we have employed earlier). In a homogeneous system $\langle \sigma^{-}_{l-k}\sigma_{l}^{\uparrow}\rangle$ obviously does not depend on the “reference spin” $l$: Each spin “lives” in an identical neighbourhood, so $\zeta(k)$ is translationally invariant with respect to $l$. But when a system is inhomogeneous – for example when a phase transition occurs at some point within the system – the correlation function will obviously depend on where the reference spin $l$ is. We therefore consider a conditional correlation function,

$$\mu(k|l) = \langle \sigma^{-}_{l-k}\sigma_{l}^{\uparrow}\rangle.$$  

It depends explicitly on the location of the reference spin $l$. Formally, $\zeta(k)$ is given by $\mu(k|l)$ averaged over all $l$. In a homogeneous case $\mu(k|l)$ is independent of $l$, so this averaging is trivial. On the other hand, in an inhomogeneous system we are investigating here, such averaging would be counterproductive: The averaging would obscure precisely the signature we are looking for, i.e., the imprint made by the inhomogeneity of the Hamiltonian on the state of the system.

In Fig. 4(a) we show $\mu(k|l)$ for the fixed reference spin $l$ located in the ferromagnetic region. The behaviour of $\mu(k|l)$ seen there is a good illustration of our previous discussion: For spins located in the ferromagnetic region $\mu(k|l) \approx 1$. However, when $k$ assumes values such that $l-k$ falls within the paramagnetic region, the correlation function vanishes, $\mu(k|l) \approx 0$. The transition between these two extremes is our focus of interest. We can characterise the size of the “scar” by quantifying the width of the transition regime. The most obvious way to do this is through the inverse of the slope of $\mu(k|l)$ where $\mu(k|l) = \frac{1}{2}$. The resulting width of the transition region is plotted in Fig. 4(b). Evidently, the behaviour predicted by the KZM-like discussion for the quantum Ising model, Eq. (30), is reflected in the correlations between spins. Such correlation functions should be experimentally accessible, and may be a good way to test our predictions.

We note that some of the effects of the inability of the order parameter to adjust to the inhomogeneous variations of the Hamiltonian may become apparent even if the system does not cross “all the way” into the other phase. For instance, just coming close to the critical point may lead to the structures with sizes that can be estimated using the above approach. Similarly, when the same phase is separated by a narrow strip when the parameter that controls its phase crosses the critical point (i.e., a strip
in space within which ε has a different sign than outside it), an extension of the above discussion should be applicable. There should be therefore lots of opportunities to experimentally test the above equations, and plenty of variations of the homogeneity - inhomogeneity theme. One such obvious variation involves adopting a nonlinear spatial dependence of ǫ on x – i.e., a dependence that is different from Eq. (24). But there are clearly many more. We shall not attempt to enumerate them here.

Let us instead point out a less obvious consequence of a spatial inhomogeneity that will be especially important in quantum phase transitions: Its effect on the gap. The spectrum of an inhomogeneous Ising system as a function of the location of the point ˜x – the place where J(x) becomes 0, see Fig. 3 – is shown in Fig. 5. When this figure is compared with Fig. 1, the spectrum of a homogeneous system, two striking differences in the behaviour of the gap emerge. (i) Instead of a sharp “corner” where J/W = 1, there is now a plateau which extends over a range of values of ˜x. (ii) Moreover, this plateau is lifted above where it was (at ∼ 4πW/N) for a chain of N spins. In short, the sharp gap minimum we had before becomes now a wider, extended “bottleneck”. The spatial structure induced by the inhomogeneity in the state of the system should have an effect on their energetics. Indeed, one could venture a guess (based on “general principles”) that the size of the gap – which is the property of the whole inhomogeneous spin chain – will change with the size of the scar, ˜x. One could moreover speculate (and here the “general principles” are becoming too general for comfort) that the size of the gap should be inversely proportional to (some power of) ˜x. We shall now pose this very same question more precisely, and arrive at the estimate of the basic parameters of the “bottleneck” more directly.

The inhomogeneous Ising system we are dealing with can be typically divided into three regions: A ferromagnetic domain (where the Ising coupling W dominates), a paramagnetic domain (where J(x) is large) and what’s in between these two – the near-critical domain, where |J(x) − W| is small. The energetic price of excitations in either ferromagnetic or paramagnetic domains is large compared to the size of the gap, which (we remind the reader) in a near-critical chain of L spins is given by ∆L ∼ 4πW/L.

Our aim is to compute the size of the bottleneck gap in the inhomogeneous case of Fig. 3. We shall do that by a self-consistent estimate suggested by the above division of the whole inhomogeneous system into three domains. We first note that the energetic price of the excitations outside the near-critical regime is prohibitively large whenever these regimes are well defined, so such excitations will not be relevant for the calculation of the size of the gap (which is defined as the “price” of the least energetically expensive excitation). On the other hand, the near-critical domain should be able to support collective excitations that – when the size of that domain is L – should be able to support collective eigenstates with energies given by ∆L ∼ 4πW/L. Thus, all we have to do is to find that size L. One might be at this stage tempted to venture a guess that L ∼ ˜x, but let us proceed cautiously, and follow a line of reasoning based on energetics we have outlined above. To this end we propose a self-consistency condition,

\[ |J(x) − W| < ∆, \tag{34} \]

which in effect defines the near-critical domain. A plot that illustrates this inequality is shown in Fig. 6.

At this point the relevant ∆ is not known. But (as |J(x) − W| is small in the near-critical domain) it is natural to employ ∆L ∼ 4πW/L, where now L stands for the number of spins that contribute to the collective state that defines the gap, i.e., the spins that fit inside the near-critical domain. Using J(x)/W = −α(x− ˜x) of Fig. 3, we solve the above equation to obtain the extent, in space, of the near-critical domain that defines the size of the
FIG. 7: The size of the smallest gap between the ground state and the first accessible excited state — the level of the plateau in Fig. 6 — as a function of the slope $\alpha = 1/\lambda Q$ for $N = 50$ spins. The dotted line is a fit to the data between $\alpha a = 0.01$ and $\alpha a = 0.2$ leading to $\Delta L/W = 2.72(\alpha a)^{0.49}$. The horizontal, dashed line corresponds to the minimum gap of a homogeneous spin chain.

The horizontal, dashed line corresponds to the minimum gap $\alpha a = 50$ spins. The dotted line is a fit to the data between $N = 0$ and $N = 50$ spins. The dotted line is a fit to the data between $\alpha a = 0.01$ and $\alpha a = 0.2$ leading to $\Delta L/W = 2.72(\alpha a)^{0.49}$.

To a gradual realignment of the spins. The border between the paramagnetic and ferromagnetic phases has a structure that can be characterized by the correlations between spins, which change between the two patterns of alignment. We have seen that this change is gradual, and happens (as was predicted by our theory) on the scale inversely proportional to the square root of the gradient of the field. The simple theory leading to Eq. (35) results in correct scaling behavior. As expected, a more specific calculation based on the quantum Ising model leads to a different prefactor, Eqs. (35) and (36). In effect, we now have two different measures of the size of the scar, one based on the correlations, Fig. 4, and the other on the size of the gap. We do not know which one of them (if any) is "correct", but we point out that they can differ.

Existence of the "transition scar" has a dramatic effect on the eigenspectrum of the system. In particular, instead of the simple avoided level crossing where the minimum gap helps set the probability that the system will remain in its ground state we are now dealing with an extended "bottleneck gap". Parameters of this bottleneck gap are (including a prefactor, somewhat in contrast with the case of the scar size estimates) in a surprisingly good accord with the theory.

One is now tempted to consider quantum phase transitions that occur both in space and in time. For thermodynamic phase transitions this situation can be treated by the KZM-based approach of Kibble and Volovik [38]. Their conclusion was, in effect, that when the critical line moves through space with velocities in excess of $\hat{v} = \xi/\tau$, the quench that leads to spontaneous symmetry breaking will proceed as if it were homogeneous, and KZM estimates of defect densities relevant for homogeneous quenches will apply. On the other hand, in the limit of slowly propagating phase fronts defect production will be suppressed, as the symmetry breaking choices made by the order parameter will be simply propagated with the phase front. This conclusion seems to be only weakly influenced by the spatial gradient of $\epsilon$, and is now supported by numerical studies (see e.g. [39]).

Our preliminary numerical simulations of the same problem in the quantum case indicate that there the situation is more complicated. Part of the problem can
be traced to the fact that the dynamics of a quantum phase transition is strictly reversible. Thus, the energy deposited in the order parameter stays in the order parameter, and – e.g., in the quantum Ising model – has “nowhere to go” except into the kinks. As a result, the rate of creation of kinks now depends on the spatial gradient of \(\varepsilon\), and does not become suppressed as dramatically as before when the front velocity falls below \(\dot{v}\). Moreover, in quantum phase transitions, the limit when less than a single kink is expected in the whole system is explicitly quantum, and (as we have seen earlier) different than (although compatible with) the KZM scaling. However, in an inhomogeneous case the simple Landau-Zener formula (suitable for gaps of Fig. 1) is obviously inapplicable. We have tried out its natural generalisation (which approximates the spectrum of Fig. 8 with two obvious avoided level crossings connected with a plateau (see Fig. 8a). The fit is imperfect. The resulting prediction of the probability of a kink, Fig. 8a, is also not very satisfying. But this calculation (while it predicts spurious oscillations, and overestimates the rate by about an order of magnitude) does capture one essential feature: The dependence of the probability \(p\) on the quench rate \(1/\tau_Q\) is now no longer exponential, as it was in the original LZF, but it becomes quadratic. Such quadratic dependence appears automatically, if rather surprisingly – given the exponential nature of LZF, Eq. (19) – in the avoided level crossing problem when the transition starts at the place of the nearest approach of the two levels \(2\), \(3\), rather than far away from the avoided crossing, as is usually assumed \([34]\). The behaviour we observe may be due to the asymmetry of the gap. In effect, as the slanted potential of Fig. 8 traverses the spin chain, the system will generally approach the plateau of the bottleneck gap with a slope that is quite different from the slope on the other end of the gap, where it exits. Therefore, recent study \([28]\) - showing that when avoided level crossing is traversed starting at the minimum of the gap, the probability of excitation \(p\) on the quench rate \(1/\tau_Q\) is no longer exponential but that it becomes quadratic – becomes relevant. For instance, in the case of the asymmetric gap of Fig. 8, one can imagine that the system is delivered essentially in its ground state to the bottleneck of the gap. While \(\dot{x}\) moves along the flat part of the gap, the Hamiltonian of the system is unchanged, so no transitions happen. However, as the gap opens up, now with a steep slope, one is really starting an avoided level crossing transition from a system that is still in its ground state near the end of the plateau. Clearly, conclusions of Refs. \([28, 30]\) apply.

While these preliminary insights are encouraging, more work is needed to gain a complete picture. In addition to the obvious intrinsic interest of this problem there are applications that may benefit from its thorough understanding. Let us mention one, slightly speculative: \textit{Adiabatic quantum computing} rests on the idea that a known ground state of a simple Hamiltonian can be adiabatically transformed into an initially unknown ground state that solves a problem encoded into the structure of another Hamiltonian. The rate at which this transition can be accomplished is limited by the size of the gap – faster transitions will result in errors appearing at the rate given by LZF, Eq. (19). This will severely limit the speed of the adiabatic computation – its duration will increase exponentially with the inverse of the size of the gap. But we have seen above that a gap can be widened, and the rate of transitions can be brought down from exponential to quadratic in \(1/\tau_Q\). It remains to be seen whether (and how) these changes can be used to suggest improvements in adiabatic quantum computing, but the preliminary results we have reached here are certainly suggestive.

This research was supported by the LDRD program.
funded by DoE at the Los Alamos National Laboratory. The research of UD was supported by a Marie Curie Intra-European Fellowship within the 6th European Community Framework Programme and by the EPSRC (UK) through the QIP IRC (GR/S82176/01) and EuroQUAM project EP/E041612/1.

[1] T. W. B. Kibble, J. Phys. A 9, 1387 (1976); Phys. Rep. 67, 183 (1980).
[2] W. H. Zurek, Nature 317, 505 (1985); Acta Physica Polonica B24, 1301 (1993).
[3] W. H. Zurek, Phys. Rep. 276, 177 (1996).
[4] T. W. B. Kibble, pp. 3-36 in Patterns of Symmetry Breaking, H. Arodz et al., eds. (Kluwer Academic, 2003).
[5] It is not yet clear however, whether these seeds are sown before or after the transition. There is numerical evidence that in thermodynamic transitions the instant \( t \) after the quench plays a dominant role \cite{A}. On the other hand, in quantum phase transitions both instants play a similar role \cite{B}, so that the effective power laws that follow are a compromise (usually “won” by the steeper dependence). Fortunately, when critical exponents are the same on both sides of the transition – as is the case in this paper – this distinction is of no importance.

[6] P. Laguna & W. H. Zurek, Phys. Rev. Lett. 78, 2519 (1997); Phys. Rev. D58, 5021 (1998); A. Yates & W. H. Zurek, Phys. Rev. Lett. 80, 5477 (1998); G. J. Stephens et al., Phys. Rev. D59, 045009 (1999); M. B. Hindmarsh and A. Rajantie, Phys. Rev. Lett. 85, 4660 (2000); G. J. Stephens, L. M. A. Bettencourt, and W. H. Zurek, ibid. 88, 137004 (2002).

[7] N. D. Antunes, L. M. A. Bettencourt, and W. H. Zurek, Phys. Rev. Lett., 82, 2824 (1999).
[8] I. L. Chuang et al., Science 251, 1336 (1991).
[9] M. I. Bowick et al., Science 263, 943 (1994).
[10] P. C. Hendry et al., Nature 368, 315 (1994).
[11] M. E. Dodd et al., Phys. Rev. Lett. 81, 3703 (1998).
[12] V. M. H. Ruutu et al. Nature 382, 334 (1996); C. Bäuerle et al., Nature 382, 332, (1996).
[13] R. Monaco et al., Phys. Rev. Lett. 89, 080603 (2002); Phys. Rev. B67, 104506 (2003); Phys. Rev. Lett. 96, 180604 (2006); arXiv:0707.0569 Phys. Rev. B 77, 054509 (2008).
[14] R. Carmi, E. Polturak, and G. Koren, Phys. Rev. Lett. 84, 4966 (2000).
[15] A. Maniv, E. Polturak, and G. Koren, Phys. Rev. Lett. 91, 197001 (2003).
[16] S. Ducci et al., Phys. Rev. Lett. 83, 5210(1999); S. Casado et al., Phys. Rev. E63, 057301 (2001); S. Casado et al., Eur. Phys. J. 146, 87 (2007).
[17] T. W. B. Kibble, Physics Today 60, (9), 47 (2007).
[18] J. R. Anglin & W. H. Zurek, Phys. Rev. Lett. 83, 1707 (1999).
[19] J. Dziarmaga et al., Phys. Rev. Lett. 88, 167001 (2002); and pp. 313-333 in Patterns of Symmetry Breaking, H. Arodz et al., eds. (Kluwer Academic, 2003); see also http://arxiv.org/abs/cond-mat/0403607.
[20] D. R. Scherrer et al., Phys. Rev. Lett., 98, 110402 (2007).
[21] L. E. Sadler et al., Nature, 443, 312 (2006).
[22] T. Lahaye et al., Nature 448, 672 (2007).