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Adiabatic dynamics of an inhomogeneous quantum phase transition: the case of a $z > 1$ dynamical exponent

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Abstract. We consider an inhomogeneous quantum phase transition across a multicritical point of the $XY$ quantum spin chain. This is an example of a Lifshitz transition with a dynamical exponent $z = 2$. Just like in the case $z = 1$ considered by Dziarmaga and Rams (2010 New J. Phys. 12 055007), when a critical front propagates much faster than the maximal group velocity of quasiparticles $v_q$, then the transition is effectively homogeneous: the density of excitations obeys a generalized Kibble–Zurek mechanism and scales with the sixth root of the transition rate. However, unlike for the case $z = 1$, the inhomogeneous transition becomes adiabatic not below $v_q$, but at a lower threshold velocity $\hat{v}$, proportional to the inhomogeneity of the transition, where the excitations are suppressed exponentially. Interestingly, the adiabatic threshold $\hat{v}$ is nonzero despite the vanishing minimal group velocity of low-energy quasiparticles. In the adiabatic regime below $\hat{v}$, the inhomogeneous transition can be used for efficient adiabatic quantum state preparation in a quantum simulator: the time required for the critical front to sweep across a chain of $N$ spins adiabatically is merely linear in $N$, while the corresponding time for a homogeneous transition across the multicritical point scales with the sixth power of $N$. What is more, excitations after the adiabatic inhomogeneous transition, if any, are brushed away by the critical front to the end of the spin chain.
1. Introduction

A quantum phase transition is a qualitative change in the ground state of a quantum system when one of the parameters in its Hamiltonian passes through a critical point. In a second-order transition, a continuous change is accompanied by a diverging correlation length and a vanishing energy gap. The vanishing gap implies that no matter how slowly a system is driven through the transition, its evolution cannot remain adiabatic near the critical point. As a result, after the transition the system is excited to a state with a finite correlation length $\xi_{\text{KZ}}$ whose size shrinks with the increasing rate of the transition. This scenario, known as the Kibble–Zurek (KZ) mechanism (KZM), was first described in the context of finite-temperature transitions [1, 2]. Although originally motivated by cosmology [1], KZM at a finite temperature was confirmed by numerical simulations of the time-dependent Ginzburg–Landau model [3] and successfully tested by experiments in liquid crystals [4], superfluid helium 3 [5], both high-$T_c$ [6] and low-$T_c$ [7] superconductors, and convection cells [8]. More recently, the spontaneous appearance of vortexes during Bose–Einstein condensation (BEC) driven by evaporative cooling was observed in [9]. However, the quantum zero-temperature limit, which is in many respects qualitatively different, remained unexplored until recently (see e.g. [10]–[20] and [21] for a review). The recent interest is motivated in part by adiabatic quantum computation or adiabatic quantum state preparation, where one would like to cross a quantum critical point as adiabatically as possible, and in part by condensed matter physics of ultracold atoms, where it is easy to manipulate parameters of a Hamiltonian in time and which, unlike their solid-state physics counterparts, are fairly well isolated from their environment. In fact, an instantaneous quench to the ferromagnetic phase in a spinor BEC resulted in finite-size ferromagnetic domains whose origin was attributed to the KZM [22]. However, since the transition rate was formally infinite in that experiment, the KZ scaling relation between the average domain size $\xi_{\text{KZ}}$ and the quench rate has not been verified.
The KZM argument is briefly as follows [2, 12]. When a transition is driven by varying a parameter \( g \) in the Hamiltonian across an isolated critical point at \( g_c \), then we can define a dimensionless distance from the critical point as

\[
\epsilon = \frac{g - g_c}{g_c}.
\]

(1)

When \( \epsilon \to 0 \), the correlation length \( \xi \) in the ground state diverges as \( \xi \sim |\epsilon|^{-\nu} \), and the energy gap \( \Delta \) between the ground state and the first excited state vanishes as \( \Delta \sim |\epsilon|^{-\nu} \). Setting \( h = 1 \) from now on, a diverging \( \Delta^{-1} \sim |\epsilon|^{-\nu} \) is the shortest time scale on which the ground state can adjust adiabatically to varying \( \epsilon(t) \). A generic \( \epsilon(t) \) can be linearized near the critical point \( \epsilon = 0 \) as

\[
\epsilon(t) \approx -\frac{t}{\tau_Q} + \mathcal{O}(t^2),
\]

(2)

where the coefficient \( \tau_Q \) is called a quench time. Assuming that the system was initially prepared in its ground state, its adiabatic evolution fails at an \( \hat{\epsilon}_{KZ} \) when time \( \hat{t}_{KZ} \) left to crossing the critical point equals the shortest time scale \( \Delta^{-1} \) on which the ground state can adjust. Solving this equality, we obtain

\[
\hat{\epsilon}_{KZ} \sim \tau_Q^{-1/(\nu+1)},
\]

(3)

\[
\hat{t}_{KZ} \sim \tau_Q^{\nu/(\nu+1)}.
\]

(4)

From \( \hat{\epsilon}_{KZ} \), the evolution becomes impulse, i.e. the state does not evolve but remains frozen in the ground state at \( \hat{\epsilon}_{KZ} \), until \( -\hat{\epsilon}_{KZ} \) when the evolution becomes adiabatic again. In this way, the ground state at \( \hat{\epsilon}_{KZ} \) with a KZ correlation length

\[
\hat{\xi}_{KZ} \sim \hat{\epsilon}_{KZ}^{-\nu} \sim \tau_Q^{\nu/(\nu+1)}
\]

(5)

becomes the initial excited state for the adiabatic evolution after \( -\hat{\epsilon}_{KZ} \). This \( \hat{\xi}_{KZ} \) determines the density of quasiparticles excited during a phase transition in, say, one dimension,

\[
d \sim \hat{\xi}_{KZ}^{-1} \sim \tau_Q^{-\nu/(\nu+1)},
\]

(6)

and, in general, expectation values of other operators according to their critical scaling dimensions. An operator \( O \) whose expectation value scales like \( \langle O \rangle \sim \hat{\xi}^\phi \) in the ground state near the critical point will scale like \( \langle O \rangle \sim \hat{\xi}_{KZ}^\phi \) right after the dynamical transition.

Note that when \( \tau_Q \) is large enough, then \( \hat{\epsilon}_{KZ} \) is small and the linearization in equation (2) is self-consistent: the KZM physics happens very close to the critical point between \( -\hat{\epsilon}_{KZ} \) and \( +\hat{\epsilon}_{KZ} \).

Recently, the quantum KZ paradigm has been generalized to transitions that happen in space rather than in time [27]–[30] and to inhomogeneous transitions that happen in time but are inhomogeneous in space [30, 31]. They are described in more detail in sections 2 and 3, respectively. In an inhomogeneous transition, how fast the critical front, i.e. the place where the control parameter \( \epsilon \) is zero, moves in space is important. In [30], we considered an example of the quantum Ising chain that is a representative of a universality class with the dynamical exponent \( z = 1 \). This exponent means that at the critical point the dispersion of low-energy quasiparticles is linear with a unique quasiparticle velocity \( v_q \). Reference [30] demonstrates that when a critical front is moving with a velocity \( v \gg v_q \), then the transition proceeds as it were effectively homogeneous and the homogeneous estimate (6) applies. On the other hand,
when \( v \ll v_q \), the excitations are exponentially suppressed and the transition is effectively adiabatic.

This picture becomes slightly more complex when \( z > 1 \), like in the Lifshitz transition with \( z = 2 \). When \( z > 1 \), there is a nonlinear low-energy quasiparticle dispersion at the critical point \( \omega \sim k^z \) and no unique quasiparticle velocity. However, similar causality arguments as for \( z = 1 \) lead to a more general conclusion that the transition is effectively homogeneous when \( v \gg v_q \), with \( v_q \) being the maximal group velocity of quasiparticles at the critical point (equal to the unique quasiparticle velocity when \( z = 1 \)). Indeed, when the critical front is much faster than \( v_q \), then even the fastest quasiparticles are not able to communicate any information across the front and the transition is effectively homogeneous. However, we also demonstrate that the condition \( v \ll v_q \) is not enough for an inhomogeneous transition to become adiabatic when \( z > 1 \), but at the same time one does not need to go as far as below the minimal quasiparticle group velocity, which is zero when \( z > 1 \). The inhomogeneous transition turns out to be adiabatic below a finite threshold velocity \( \hat{v} \), proportional to the inhomogeneity of the transition, which can be obtained from a variation in the simple KZ argument. In this paper, we both present the general physical arguments and support them by a solution of a transition across a multicritical point of the \( XY \) model \([33]\). The solution demonstrates that the general arguments are robust despite their simplicity, while the general discussion suggests that the conclusions are applicable beyond this particular example.

This paper is organized as follows. In section 2, we provide experimental motivation and a generalized KZ argument for an inhomogeneous transition. It is here that we obtain the general estimate for \( \hat{v} \). In section 3, we do the same for a static transition in space and then we use the general results for a static transition to derive again the same estimate for \( \hat{v} \) as in section 2. In this way, the general \( \hat{v} \) is arrived at from two different angles. In order to test the general predictions, we introduce the transverse field \( XY \) model in section 4. In section 5, we review an exact solution for a homogeneous transition in this model \([33]\), and in section 5.1 that for a homogeneous transition in a finite chain of \( N \) spins. The last transition becomes adiabatic when the transition time \( \tau_Q \) is much longer than \( N^6 \). In section 6, we consider a transition in space and confirm the general predictions of section 3 in the \( XY \) model. Section 7 is devoted to an inhomogeneous transition in the \( XY \) model. In section 7.1 the effectively homogeneous case of \( v \gg v_q \) is studied, and in sections 7.2 and 7.3, the adiabatic regime of \( v \ll \hat{v} \) is studied. In section 7.2, \( \hat{v} \) is shown to be proportional to the inhomogeneity of the transition at the critical front. It is argued there that the adiabatic quantum state preparation by an inhomogeneous transition requires time proportional to the number of spins \( N \), i.e. for large \( N \) the inhomogeneous transition is much faster than the adiabatic homogeneous transition. This conclusion is further strengthened in section 7.3, showing that eventual (exponentially small) quasiparticle excitations in the adiabatic inhomogeneous transition are brushed away by the critical front to the end of the spin chain. Finally, the concluding section 8 provides a summary of our results.

2. Inhomogeneous transition

As already pointed out in the finite-temperature context \([23]\) (see also \([24]\) for recent applications), in a realistic experiment it is difficult to make \( \epsilon \) exactly homogeneous throughout a system. For instance, in the superfluid \(^3\)He experiments \([5]\), the transition was caused by neutron irradiation of helium 3. Heat released in each fusion event, \( n + ^3\)He \( \rightarrow ^4\)He,
created a bubble of normal fluid above the superfluid critical temperature $T_c$. As a result of quasiparticle diffusion, the bubble was expanding and cooling with local temperature $T(t, r) = \exp\left(-r^2/2Dt\right)/(2\pi Dt)^{3/2}$, where $r$ is the distance from the center of the bubble and $D$ is the diffusion coefficient. Since this $T(t, r)$ is hottest in the center, the transition back to the superfluid phase, driven by an inhomogeneous parameter

$$\epsilon(t, r) = \frac{T(t, r) - T_c}{T_c},$$

proceeded from the outer to the central part of the bubble with a critical front $r_c(t)$, where $\epsilon = 0$, shrinking with a finite velocity $v = dr_c/dt < 0$.

A similar scenario is generic in ultracold atom gases in magnetic/optical traps [25, 26]: a trapping potential results in an inhomogeneous density of atoms $\rho(\vec{r})$ and a critical point $g_c$ depends on the atomic density $\rho$. Thus even a transition driven by a perfectly homogeneous $g(t)$ is inhomogeneous,

$$\epsilon(t, \vec{r}) = \frac{g(t) - g_c[\rho(\vec{r})]}{g_c[\rho(\vec{r})]},$$

with a surface of critical front, where $\epsilon = 0$, moving at a finite speed.

According to the KZM, in a homogeneous symmetry-breaking transition, a state after the transition is a mosaic of finite ordered domains of average size $\hat{\xi}_{KZ}$. Within each finite domain, orientation of the order parameter is constant but uncorrelated to orientations in other domains. In contrast, in an inhomogeneous symmetry-breaking transition [23], the parts of the system that cross the critical point earlier may be able to communicate their choice of orientation of the order parameter to the parts that cross the transition later and bias them to make the same choice. Consequently, the final state may be correlated at a range longer than $\hat{\xi}_{KZ}$ or even end up being the ground state, and the final density of excited quasiparticles may be lower than the KZ estimate in equation (6) or even zero.

From the point of view of testing the KZM, this inhomogeneous scenario, when relevant, may sound like a negative result because an imperfect inhomogeneous transition suppresses the KZM. However, from the point of view of adiabatic quantum computation or adiabatic quantum state preparation, it is the KZM itself that is a negative result: no matter how slow the homogeneous transition is, there is a finite density of excitations (6) that decays only as a fractional power of transition time $\tau_Q$. From this perspective, the inhomogeneous transition may be a practical way of suppressing KZ excitations and preparing the desired final ground state adiabatically.

To estimate when the inhomogeneity may actually be relevant, in a similar way as in equation (2) and [30], we linearize the parameter $\epsilon(t, n)$ in both $n$ and $t$ near the critical front where $\epsilon(t, n) = 0$,

$$\epsilon(t, n) \approx \alpha(n - vt).$$

Here, $n$ is position in space, e.g. lattice site number, $\alpha$ is the gradient/inhomogeneity of the transition and $v$ is velocity of the critical front. When watched locally at a fixed $n$, the inhomogeneous transition in equation (9) appears to be the homogeneous transition in equation (2) with a local

$$\tau_Q = \frac{1}{\alpha v}.$$
The part of the system where \( n < v t \), or equivalently \( \epsilon(t, n) < 0 \), is already in the broken symmetry phase. An outcome of the transition depends on \( v \).

On the one hand, there cannot be efficient communication across the critical point when it is moving faster than quasiparticles near the critical point,

\[
v \gg v_q, \tag{11}\]

Here, \( v_q \) is the maximal group velocity of quasiparticles at \( \epsilon = 0 \) or, in general, a Lieb–Robinson velocity [32]. It is a constant that does not depend on the inhomogeneity \( \alpha \). In this ‘homogeneous regime’ the inhomogeneous transition is effectively homogeneous and the final density of excitations after the transition is given by equation (6) with the local \( \tau_0 = 1/\alpha v \).

On the other hand, the KZM provides the relevant scales of length and time, \( \xi_{\text{KZ}} \) and \( \tilde{t}_{\text{KZ}} \), respectively, whose combination [23],

\[
\tilde{v} \simeq \frac{\xi_{\text{KZ}}}{\tilde{t}_{\text{KZ}}} \simeq \alpha^{v(z-1)/(1+z)}, \tag{12}\]

is a relevant scale of velocity. Here, we used equations (4) and (5) and equation (10), which is valid for small \( \alpha \). Indeed, when \( v \ll \tilde{v} \), the system has enough time to adjust adiabatically on the relevant length \( \xi_{\text{KZ}} \) and the density of excitations is less than in the homogeneous KZM. This is an ‘adiabatic regime’ of the inhomogeneous transition.

In general, the adiabatic threshold \( \tilde{v} \) depends on the inhomogeneity \( \alpha \) as distinct from the constant \( v_q \). However, in a special case of \( z = 1 \), or linear quasiparticle dispersion at the critical point, the two velocities are the same: \( \tilde{v} \simeq v_q \). This (quite generic) special case was studied recently in [30, 31]. In this paper, we consider an example of a more general class of critical points with \( z > 1 \), or nonlinear quasiparticle dispersion, when the adiabatic threshold \( \tilde{v} \) in equation (12) scales with a positive power of \( \alpha \) and, for small enough \( \alpha \), can be clearly distinguished from the homogeneous threshold \( v_q \): \( \tilde{v} \ll v_q \).

However, before we proceed with the example, in the next section we rederive equation (12) from a slightly different perspective.

3. Kibble–Zurek mechanism (KZM) in space

The authors of [27]–[30] considered a ‘phase transition in space’ where \( \epsilon(n) \) is inhomogeneous but time-independent. In the same way as in equation (9), this parameter can be linearized as

\[
\epsilon(n) \approx \alpha (n - n_c), \tag{13}\]

near the static critical front at \( n = n_c \) where \( \epsilon = 0 \). The system is in the broken symmetry phase where \( n < n_c \) and in the symmetric phase where \( n > n_c \). In the first ‘local approximation’, we would expect that the order parameter behaves as if the system were locally homogeneous: it is nonzero for \( n < n_c \) only, and when \( n \rightarrow n_c^- \) it tends to zero as \( (n_c - n)^\beta \) with the critical exponent \( \beta \). However, this first approximation is in contradiction with the basic fact that the correlation (or healing) length \( \xi \) diverges as \( \xi \sim |\epsilon|^{-\nu} \) near the critical point and the diverging \( \xi \) is the shortest length scale on which the order parameter can adjust to (or heal with) the changing \( \epsilon(n) \). Consequently, when approaching \( n_c^- \), the local approximation \( (n_c - n)^\beta \) must break down when the local correlation length \( \xi \sim \alpha^{-v/(1+z)} \) equals the distance remaining to the critical point \( (n_c - n) \). Solving this equality with respect to \( \xi \), we obtain

\[
\xi_{\text{SP}} \sim \alpha^{-v/(1+z)}. \tag{14}\]
Beginning from \( n - n_c \simeq -\xi_{\text{SP}} \), the ‘evolution’ of the order parameter in \( n \) becomes ‘impulse’, i.e. the order parameter does not change until \( n - n_c \simeq +\xi_{\text{SP}} \) in the symmetric phase, where it begins to follow the local \( \epsilon(n) \) again and decays to zero on the same length scale of \( \xi_{\text{SP}} \).

A direct consequence of this ‘KZM in space’ is that a nonzero order parameter penetrates into the symmetric phase to a depth \( \delta_n \sim \xi_{\text{SP}} \), as if the critical point were effectively ‘rounded off’ on the length scale of \( \xi_{\text{SP}} \). This rounding off also results in a finite energy gap, \( \Delta_{\text{SP}} \sim \xi_{\text{SP}} \alpha_{z}(1+\nu) \), in contrast to the local approximation, where we would expect gapless excitations near the critical point. The finite gap in turn should prevent excitation of the system even when the critical point \( n_c \) in equation (13) moves with a finite velocity: \( n_c(t) = vt \). The excitation is suppressed up to a threshold velocity, \( \hat{v} \sim \frac{\xi_{\text{SP}}}{\Delta_{\text{SP}}^{-1}} \sim \alpha_{z}(1+\nu) \), which is a ratio of the relevant length \( \xi_{\text{SP}} \) to the relevant time \( \Delta_{\text{SP}}^{-1} \). This \( \hat{v} \) is the same as that in equation (12).

In the following sections, we test the general predictions in the \( XY \) model.

4. Transverse field \( XY \) chain

The ferromagnetic transverse field \( XY \) quantum spin chain is

\[
H = -\sum_{n=1}^{N} h_n \sigma_n^z - \sum_{n=1}^{N-1} \left( J_n^x \sigma_n^x \sigma_{n+1}^x + J_n^y \sigma_n^y \sigma_{n+1}^y + J_n^z \sigma_n^z \sigma_{n+1}^z \right),
\]

where \( \sigma^{x,y,z} \) are spin-1/2 Pauli matrices. Here, we consider a path in the parameter space \( (J^x, J^y, h) = (\frac{1-\epsilon}{2}, \frac{1+\epsilon}{2}, 1+\epsilon) \) parametrized by the anisotropy of the ferromagnetic couplings \( \epsilon \in [-1,1] \). The parameter \( \epsilon \) will be driven from the initial \( \epsilon = 1 \) to the final \( \epsilon = -1 \), when Hamiltonian (18) becomes the simple Ising chain,

\[
H_{\text{final}} = -\sum_{n=1}^{N-1} \sigma_n^x \sigma_{n+1}^x.
\]

In the thermodynamic limit, a homogeneous system has a second-order quantum phase transition (multicritical point) at \( \epsilon = 0 \), which separates a paramagnetic phase where \( \epsilon > 0 \) from a ferromagnetic phase where \( \epsilon < 0 \). Nonadiabaticity of this dynamical transition will be quantified by the average number of quasiparticle/kink excitations in the final ferromagnetic state.

In a more general inhomogeneous system that we will consider in this paper, it is natural to parametrize

\[
J_n^x = \frac{1-\epsilon_n^{1/2}}{2}, \quad J_n^y = \frac{1+\epsilon_n^{1/2}}{2}, \quad h_n = 1 + \epsilon_n,
\]

where \( \epsilon_n(t) \) is a continuous function of \( n \) and, in general, time.
After the Jordan–Wigner transformation to spinless fermionic annihilation operators $c_n, \quad \sigma_n^x = (c_n - c_n^\dagger)iS_n, \quad \sigma_n^z = (c_n + c_n^\dagger)S_n, \quad \sigma_n^= = 1 - 2c_n^\dagger c_n$, where $S_n = \prod_{m<n} (1 - 2c_m^\dagger c_m)$, Hamiltonian (18) becomes

$$H = \sum_n \left[ - (c_n^\dagger c_{n+1} + \text{h.c.}) - \epsilon_{n+1/2} (c_{n+1}c_n + \text{h.c.}) + (1 + \epsilon_n) \left( 2c_n^\dagger c_n - 1 \right) \right]. \quad (20)$$

This quadratic $H$ is diagonalized to $H = \sum_m \omega_m \gamma_m^\dagger \gamma_m$ by a Bogoliubov transformation $c_n = \sum_{m=0}^{N-1} (u_{nm} \gamma_m + v_{nm} \gamma_m^\dagger)$ with $m$ numerating $N$ eigenmodes of the stationary Bogoliubov–de Gennes equations,

$$\omega u_n^\pm = 2(1 + \epsilon_n)u_n^\mp - (1 \mp \epsilon_{n+1/2})u_{n+1}^\mp - (1 \pm \epsilon_{n+1/2})u_{n-1}^\mp,$$

with $\omega \geq 0$. Here, $u^\pm \equiv u \pm v$.

The Hamiltonian (18) and (20) commutes with a parity operator,

$$P = \prod_{n=1}^{N} \sigma_n^z = \prod_{n=1}^{N} (2c_n^\dagger c_n - 1). \quad (22)$$

The even parity of the initial ground state at $\epsilon = 1$ is conserved during the dynamical transition.

## 5. Homogeneous transition

When $N \to \infty$ and $\epsilon_n = \epsilon$ is homogeneous, it is convenient to make a Fourier transform $u_k^\pm = N^{-1/2} \sum_{n=1}^{N} u_n^\pm e^{-ikn}$ with pseudomomentum $k \in (-\pi, \pi]$. Equation (21) becomes

$$\frac{\omega_k}{2} \left[ \begin{array}{c} u_k^+ \\ u_k^- \end{array} \right] = \left[ \sigma^x (1 + \epsilon - \cos k) - \sigma^y \epsilon \sin k \right] \left[ \begin{array}{c} u_k^+ \\ u_k^- \end{array} \right], \quad (23)$$

with eigenfrequencies

$$\omega_k = 2\sqrt{(1 + \epsilon - \cos k)^2 + \epsilon^2 \sin^2 k}. \quad (24)$$

We can expand $\omega_0 \approx 2|\epsilon| \equiv |\epsilon|^v$ for small $\epsilon$, and $\omega_k \approx k^2 \equiv |k|^z$ for $\epsilon = 0$ and small $k$, to identify the critical exponents

$$z = 2, \quad v = 1/2. \quad (25)$$

With these exponents, the general equation (6), valid for an isolated quantum critical point, would predict the density of excitations after the homogeneous transition in equation (2) to scale as $d \approx \epsilon_Q^{-1/4}$. However, as shown in [33] and outlined below, the multicritical nature of the critical point results in a different scaling exponent and the KZM requires careful generalization here [21, 33].

The correct scaling can be obtained by mapping our time-dependent problem,

$$\frac{i}{2} \frac{d}{dt} \left( \begin{array}{c} u_k^+ \\ u_k^- \end{array} \right) = \left[ \sigma^x \left( 1 - \frac{t}{t_Q} - \cos k \right) + \sigma^y \frac{t}{t_Q} \sin k \right] \left( \begin{array}{c} u_k^+ \\ u_k^- \end{array} \right), \quad (26)$$

to the standard Landau–Zener (LZ) model [35],

$$\frac{i}{\tau'} \frac{d}{dt'} \left( \begin{array}{c} u_k^+ \\ u_k^- \end{array} \right) = \left[ \frac{t'}{\tau} \sigma + \Delta^\prime \sigma_\perp \right] \left( \begin{array}{c} u_k^+ \\ u_k^- \end{array} \right), \quad (27)$$

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where \( t' = t + \tau_Q (\cos k - 1)/(1 + \sin^2 k) \) is shifted time, \( \sigma = (\sigma^+ \sin k - \sigma^-)/\sqrt{1 + \sin^2 k} \) and \( \sigma_\perp = (\sigma^+ + \sigma^- \sin k)/\sqrt{1 + \sin^2 k} \) are two orthogonal spin components, \( \tau = \tau_Q / 2\sqrt{1 + \sin^2 k} \) is the LZ transition time, and \( \Delta' = 2 \sin k (1 - \cos k) / \sqrt{1 + \sin^2 k} \) is the minimal gap at the anticrossing center when \( t' = 0 \).

In the adiabatic limit, \( \tau_Q \gg 1 \), only the long-wavelength modes \( k \approx 0 \) get excited with the LZ probability

\[
p_k = \exp(-\pi \tau (\Delta')^2) \approx \exp(-\pi \tau_Q k^6/2),
\]

and the density of quasiparticle excitations after crossing the multicritical point is

\[
d = \int_{-\pi}^{\pi} \frac{dk}{2\pi} p_k = d_0 \tau_Q^{-1/6},
\]

where \( d_0 = 2^{1/6} \Gamma(7/6) \pi^{-7/6} = 0.274 \) and \( \Gamma(\cdots) \) is the gamma function.

The correct exponent \( 1/6 \) can be made compatible with the general equation (6), as follows. The instantaneous quasiparticle frequency in equations (27) is \( \omega'_k = \sqrt{(\epsilon')^2 + (\Delta')^2} \), where \( \epsilon' = t'/\tau \) is the relevant distance from the anticrossing center. We can expand \( \omega'_k \sim |k|^3 \equiv |k|^{\nu'} \) at \( \epsilon' = 0 \) and small \( k \), \( \omega'_k \sim |\epsilon'| \equiv |\epsilon'|^{\nu} \) at small \( \epsilon' \), to identify the exponents relevant for a homogeneous transition as

\[
z' = 3, \quad \nu' = 1/3.
\]

Using these relevant exponents in the general equation (6) gives the correct exponent 1/6 in the exact equation (29). Note that both \( z \) in equation (25) and \( z' \) in equation (30) are greater than 1.

Moreover, when transition is in space, then equation (16) with exponents (30) predicts the gap

\[
\tilde{\Delta}_{SP} \simeq \alpha^{3/4},
\]

while the ‘canonical’ exponents (25) give \( \tilde{\Delta}_{SP} \simeq \alpha^{2/3} \). In section 6, we will see that equation (31) is indeed the correct gap in a transition in space.

However, depending on the choice of \( \nu \) or \( \nu' \) in equation (14), we obtain either \( \tilde{\Delta}_{SP} \simeq \alpha^{1/3} \) or \( \tilde{\Delta}_{SP} \simeq \alpha^{1/4} \), of which only the former will turn out to be relevant for a transition in space, but even it is not a unique scale of length there. Nevertheless, since both \( z > 1 \) and \( z' > 1 \), we expect the adiabatic threshold velocity \( \hat{v} \) in an inhomogeneous transition to scale with a positive power of the inhomogeneity \( \alpha \); compare the general equation (17).

5.1. Adiabatic regime of homogeneous transition

Since a finite chain of \( N \) spins has a finite energy gap at the critical \( \epsilon = 0 \), the homogeneous transition becomes adiabatic above a finite \( \tau_Q \) when scaling relation (29) crosses over to exponential decay.

Indeed, in a periodic chain the quasimomenta are quantized as \( k = \pm \frac{\pi}{N}, \pm \frac{3\pi}{N}, \ldots \) to satisfy anti-periodic boundary conditions for the Jordan–Wigner fermions in the subspace of even parity. The \( p_k = \exp(-\pi \tau_Q k^6/2) \) in equation (28) is a probability to excite a pair of quasiparticles with momenta \((k, -k)\). When \( \tau_Q \) is large enough, then only the longest wavelength pair \((\frac{\pi}{N}, -\frac{\pi}{N})\) has non-negligible excitation probability \( p_{\pi/N} = \exp(-\pi^7 \tau_Q / 2N^6) \).
but even this probability becomes exponentially small when \( \tau_Q \) is deep enough in the adiabatic regime,

\[
\tau_Q \gg \frac{2}{\pi^7} N^6. \tag{32}
\]

The transition time required for a homogeneous transition to become adiabatic grows with the sixth power of the number of spins.

The adiabatic condition (32) can also be obtained in a more intuitive way from equation (5); compare the similar argument in [12]. Indeed, the average distance between excitations scales as \( \xi_{KZ} \sim \tau_Q^{1/6} \) and, consequently, the \( \tau_Q \) required for the whole chain of \( N \) spins to remain defect-free scales as \( N^6 \). This simple argument applies to an open chain as well.

In [34], a nonlinear generalization \( \epsilon(t) = \text{sign}(-t)\sqrt{t/|t_Q|} \) of the linear quench (2) was proposed to improve adiabaticity. Indeed, a similar argument as in section 1 yields \( \alpha_r \sim \tau_Q^{-r'/(1+r'z')}} \) as a generalization of equation (6). When \( r \gg 1/z'v' = 1 \), then \( \alpha_r \sim \tau_Q^{-1/z'} = \tau_Q^{-3/3} \) is much less than \( \alpha_1 \sim \tau_Q^{-1/6} \) after a linear quench for long enough \( \tau_Q \). In a finite chain, the nonlinear quench becomes adiabatic when

\[
\tau_Q \gg N^3, \tag{33}
\]

but this is still cubic in \( N \).

6. Transition in space in the XY model

In this section, we take the size of an open chain \( N \to \infty \) to avoid boundary effects and consider a smooth static slant,

\[
\epsilon_n = \tanh \left[ \alpha(n - n_c) \right] \approx \alpha(n - n_c), \tag{34}
\]

interpolating between \( \epsilon = 1 \) and \( \epsilon = -1 \), which is shown in figure 1. The slant (34) can be linearized near the critical point \( n_c \) as in the general equation (13).
We are interested in the low-frequency part of the quasiparticle spectrum where, presumably, we can make a long-wavelength approximation and treat $n$ as a continuous variable,

$$u_{n\pm 1} \approx u_n \pm \frac{d}{dn} u_n + \frac{1}{2} \frac{d^2}{dn^2} u_n. \quad (35)$$

We also expect that the low-frequency quasiparticle modes are localized near the critical point $n_c$, where we can use the linearization in equation (34).

Indeed, after rescaling,

$$n - n_c = \alpha^{-1/3} x, \quad \omega = \alpha^{3/4} \Omega, \quad (36)$$

equations (21) become

$$\alpha^{1/12} \Omega \left( \frac{u^+}{u^-} \right) - \sigma^x \left[ -\frac{d^2}{dx^2} + 2x \right] \left( \frac{u^+}{u^-} \right) = \alpha^{1/3} i \sigma^y \left[ 1 + 2x \frac{d}{dx} \right] \left( \frac{u^+}{u^-} \right). \quad (37)$$

To leading order in $\alpha \ll 1$, their two eigenmodes of lowest frequency are

$$\Omega_0 = 0,$$

$$u_0^+ \propto e^{-1/2u^{1/3}x^2} A(x), \quad u_0^- \propto 0, \quad (38)$$

and

$$\Omega_1 = \sqrt{8 \Gamma(5/4) / \Gamma(3/4)} = 2.43,$$

$$u_1^+ \propto e^{-(1/2)u^{1/3}x^2} \frac{dA}{dx}(x), \quad u_1^- \propto e^{-(1/2)u^{1/3}x^2} - \frac{2A(x)}{\alpha^{1/12} \Omega_1}, \quad (39)$$

where $A(x) = Ai[2^{1/3}x]$ and $Ai$ is the (oscillating) Airy function.

The lowest energy relevant (even parity) excitation of the two quasiparticles $\gamma_0$ and $\gamma_1$ has a finite gap,

$$\Delta_{SP} = \omega_0 + \omega_1 = \alpha^{3/4} \Omega_1 \simeq \alpha^{3/4}, \quad (40)$$

in agreement with the general equation (31) for the choice $z' = 1/\nu' = 3$ in equation (30).

However, the modes (38) and (39) do not have a unique scale of length. They penetrate into the paramagnetic phase, where $n > n_c$ and $x > 0$, to a depth

$$\delta n \simeq \alpha^{-1/3} \quad (41)$$

determined by the $x \to +\infty$ asymptote of the Airy function $A(x) \sim \exp(-2\sqrt{3}x^{3/2}/3)$ and equation (36). Consequently, this $\delta n$ is also the penetration depth of ferromagnetic magnetization into the paramagnetic phase (see figure 2). However, on the ferromagnetic side, where $n < n_c$ and $x < 0$, the same modes (38) and (39) extend to a depth

$$\Delta n \simeq \alpha^{-1/2}, \quad (42)$$

limited by the Gaussian envelope $e^{-1/2u^{1/3}x^2} \equiv e^{-1/2\alpha(n-n_c)^2}$. This envelope damps oscillations of the Airy function $A(x)$, which take place on the shorter scale $\delta n \simeq \alpha^{-1/3}$. An overall width of the modes (38) and (39) is set by the longer scale $\Delta n$.

Thus in the case of a finite chain size $N$, the results of this section require $\Delta n \ll N$ or, equivalently, a lower bound $\alpha \gg N^{-2}$.
Figure 2. Phase transition in space. In panel (A), ferromagnetic magnetization $X_n = \langle \sigma_n^x \rangle$ is shown as a function of distance from the critical point $n - n_c$ for different values of the gradient $\alpha$. This ferromagnetic magnetization penetrates into the paramagnetic phase where $n - n_c > 0$. In panel (B), the same magnetization as in panel (A), but rescaled by its value at the critical point $X_{n_c}$, is shown as a function of the rescaled distance $x = (n - n_c)\alpha^{1/3}$. The six rescaled plots collapse, demonstrating that the magnetization penetrates into the paramagnetic phase to a depth $\delta n \simeq \alpha^{-1/3}$ predicted in equation (41).

7. Inhomogeneous transition in the XY model

In this section, we make the critical front in equation (34) and figure 1 sweep from $n_c \to -\infty$ to $n_c \to +\infty$ at a constant velocity $v$,

$$\epsilon_n(t) = \tanh [\alpha(n - vt)] \approx \alpha(n - vt)$$

(see figure 1). Near the critical point at $n = vt$, the slant (43) can be linearized as in the general equation (9).

7.1. The homogeneous regime of inhomogeneous transition

We can obtain quasiparticle group velocity at the critical point $\epsilon = 0$ from the dispersion (24). The group velocity is maximized for $k = \pm \pi/2$ by

$$v_q = 2.$$  

(44)

When $v \gg v_q$, there is no causal connection across the critical point and the inhomogeneous transition proceeds as if it were effectively homogeneous with a quench time $\tau_Q = 1/\alpha v$. In this
regime we expect the ‘homogeneous’ 1/6-scaling in equation (29) to apply and a rescaled final density of kinks to scale as
\[ \alpha^{-1/6} d \sim v^{1/6} \] (45)
with velocity of the critical front \( v \).

To verify this prediction, we simulated time-dependent Bogoliubov–de Gennes equations,
\[
i \frac{d}{dt} u_n^\pm = 2(1 + \epsilon_n) u_n^\mp - (1 \mp \epsilon_{n+1/2}) u_{n+1}^\mp - (1 \pm \epsilon_{n+1/2}) u_{n-1}^\mp,\] (46)
in an open chain of \( N \) spins. The results are shown in figure 3, and in the homogeneous regime \( v \gg 2 \) they are consistent with the prediction (45).

7.2. The adiabatic regime of inhomogeneous transition

In this section, we consider the adiabatic limit of small front velocity \( v \) when only the lowest relevant excited state has non-negligible excitation probability. The state is the even parity state occupied by the lowest two quasiparticles: \( \gamma_0 \) and \( \gamma_1 \). When the critical point \( n_c \) is in the bulk of the finite lattice, then these quasiparticles are described by the Bogoliubov modes (38) and (39) and the energy gap for this excitation is given by equation (40).

In the adiabatic limit, the even parity subspace of the Hilbert space can be truncated to an effective two-level system,
\[ |\psi(t)\rangle = a(t)|0\rangle + b(t)|1\rangle,\] (47)
where \( |0\rangle \) is the instantaneous ground state in the even subspace for an instantaneous position \( n_c \) of the critical point and \( |1\rangle = \gamma_1^\dagger \gamma_0^\dagger |0\rangle \) is the instantaneous first excited state for the same \( n_c \).
The amplitudes $a, b$ solve a generalized LZ problem,

$$i \frac{d}{dt} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} 0 & ivZ \\ -ivZ & \Delta \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix},$$

with initial conditions $a(-\infty) = 1$ and $b(-\infty) = 0$. Here, $\Delta = \omega_0 + \omega_1$ is an instantaneous gap and

$$Z \equiv \langle 1 | \frac{d}{dn_c} | 0 \rangle = \sum_{n=1}^{N} (v_{n1}, u_{n1}) \frac{d}{dn_c} \left( \begin{array}{c} u_{n0} \\ v_{n0} \end{array} \right).$$

Generic $\Delta(n_c)$ and $Z(n_c)$ are shown in figures 4(A) and (B), respectively.

In the adiabatic limit of small excitation probability $|b(\infty)|^2 \ll 1$, our numerical simulations of the LZ equations (48) are well described by a simple LZ-like formula,

$$|b(\infty)|^2 = \exp \left( -c \frac{\alpha}{v} \right),$$

\textit{Figure 4.} Parameters $\Delta$ and $Z$ of the LZ problem in equation (48) for a lattice size $N = 400$ and different values of the small gradient $\alpha$. In panel (A), the instantaneous relevant gap $\Delta = \omega_0 + \omega_1$ is shown as a function of $n_c$. The bulk value of the gap, when $1 \ll n_c \ll N$, is estimated in equation (40) as $\Delta_{SP} \simeq \alpha^{3/4}$.

In panel (B), the parameter $Z$ in equation (49) is shown. Its bulk value can be estimated from equations (38), (39) and (49) as $Z \simeq \alpha^{1/4}$. In both panels (A) and (B), the crossover regions at both ends of the chain have a width $\Delta n \simeq \alpha^{-1/2}$ set by the Gaussian envelope of the modes (38) and (39). The additional oscillations at the left end have a length scale $\delta n \simeq \alpha^{-1/3}$ determined by the oscillatory Airy function $A(x)$ in the modes (38) and (39).
Figure 5. (A) Final excitation probability $|b(\infty)|^2$ in the generalized LZ problem, defined in equation (48) and figure 4, as a function of $\alpha/v$ for different values of the inhomogeneity $\alpha$. Here, the solid lines are the best fits of the LZ formula (50) to the numerical data points: $|b(\infty)|^2 = \exp(-c \frac{\alpha}{v})$. (B) Coefficients $c$ fitted in panel (A) as a function of $\alpha$. The solid line is the best fit $c = 3.12 + 4.50 \alpha^{1/3}$, demonstrating weak residual dependence on $\alpha^{1/3}$, which becomes negligible when $\alpha \to 0$ and $c \to 3.12$. (C) $|b(\infty)|^2$ as a function of $1/v$ for a fixed $\alpha = 2^{-7}$ and two different chain sizes $N = 200, 400$. In the adiabatic regime, the excitation probability does not depend on $N$, demonstrating that the excitation of the lowest two quasiparticles is a boundary effect. (D) $|b(\infty)|^2$ from the LZ model and corresponding excitation probabilities $P_0 = \langle \gamma_0^\dagger \gamma_0 \rangle$ and $P_1 = \langle \gamma_1^\dagger \gamma_1 \rangle$ from the exact Bogoliubov–de Gennes equations (46). All these three probabilities are the same, $|b(\infty)|^2 = P_0 = P_1$, in the adiabatic regime where only a pair of the lowest two quasiparticles $\gamma_0$ and $\gamma_1$ can get excited.

where $c = O(1)$ is a numerical prefactor. Indeed, the plots for different $\alpha$ that are collected in figure 5(A) nearly collapse. The collapse is not perfect because, as shown in figure 5(B), there is still a weak residual dependence $c \approx 3.12 + 4.50 \alpha^{1/3}$. However, when $\alpha \ll 1$ then $c \approx 3.12$ becomes independent of $\alpha$, as assumed in equation (50).

Furthermore, figure 5(C) shows that in the adiabatic regime the small excitation probability $|b(\infty)|^2$ does not depend on the chain size $N$. Not surprisingly, the excitation of the lowest two quasiparticles is a boundary effect determined by the behavior of $\Delta$ and $Z$ in figure 4 when the critical point $n_c$ is near the ends of the chain.

We can conclude that the excitation probability (50) is exponentially small when $v \ll \alpha$. This inequality identifies a threshold velocity,

$$\hat{v} \simeq \alpha,$$  

(51)

when the inhomogeneous transition becomes adiabatic. As anticipated for $z > 1$, the adiabatic threshold $\hat{v}$ is a positive power of the gradient $\alpha$. 

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Figure 6. Density distributions of kinks along a chain of $N = 200$ spins after an inhomogeneous transition in the adiabatic regime $v \ll \alpha$. These distributions were obtained from numerical simulations of the exact time-dependent Bogoliubov–de Gennes equations (46) with the critical front in figure 1. Residual (exponentially small) excitations are brushed away by the critical front to the right edge, leaving behind the defect-free bulk of the chain. The inset is a log-scale focus on the right edge. It shows that in the adiabatic regime all density distributions for different $v$ are the same up to an overall $v$-dependent amplitude set by the LZ excitation probability in equation (50).

7.3. Residual edge excitations after adiabatic transition

In the adiabatic limit $v \ll \alpha$, only the lowest two quasiparticles $\gamma_0$ and $\gamma_1$ can get excited. Since the inhomogeneous transition is between two gapped phases, these low-frequency modes are localized either near the critical point $n_c$ when $n_c$ is in the bulk of the spin chain or at one of the ends of the chain when $n_c$ is near this end. For instance, the ‘bulk’ modes in equations (38) and (39) are localized within the distance $\Delta n \simeq \alpha^{-1/2}$ from the critical point.

Consequently, as the critical front in figure 1 passes across the chain, these instantaneous low-frequency modes follow the moving front to the right end of the chain. Indeed, a few generic final density distributions of kinks along the spin chain are shown in figure 6. These (exponentially small) probabilities of kink excitation are localized near the right end of the chain. Residual excitations, if any, are brushed away to the right end, leaving behind a defect-free bulk of the chain.

8. Conclusion

Let us itemize what we know about the dynamics of quantum phase transitions across the multicritical point of the $XY$ chain, which is an example of a transition with $z > 1$:

- The density of excitations after a homogeneous transition in an infinite chain decays with the sixth root of the transition time $\tau_Q$. 

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• Consequently, the transition time required for a homogeneous transition in a finite chain of $N$ spins to be adiabatic scales like $N^6$.
• Quasiparticles excited by a homogeneous transition are uniformly scattered along a spin chain.
• In an inhomogeneous transition, when the critical front propagates much faster than the maximal quasiparticle group velocity $v_q = 2$, then the transition is effectively homogeneous.
• When a critical front moves much slower than the adiabatic threshold velocity $\hat{v} \simeq \alpha$, then the average number of excitations is exponentially suppressed and does not depend on $N$.
• Quasiparticles excited in the adiabatic regime, if any, are brushed away by the critical front to the end of a spin chain, leaving behind the defect-free bulk of the chain.
• The minimal time required for the adiabatic inhomogeneous transition to be completed is $N/\hat{v}$. It is a mere linear function of $N$ instead of the $N^6$ in the homogeneous case.

The main difference between the case $z = 1$ in [30] and $z > 1$ considered here is that in the former case the adiabatic threshold velocity $\hat{v}$ is the same as the homogeneous threshold velocity $v_q$, $\hat{v} = v_q$ when $z = 1$, while in the latter case the adiabatic threshold is less than the homogeneous one, $\hat{v} < v_q$ when $z > 1$, and is proportional to the inhomogeneity of the transition. When $z > 1$, the KZ adiabatic threshold $\hat{v}$ is nonzero despite vanishing minimal quasiparticle group velocity.

Putting the results for $z > 1$ together with those of [30] for $z = 1$, we can conclude that for large $N$ an inhomogeneous transition is a more efficient method of adiabatic quantum state preparation than a straightforward homogeneous transition. The time required for an adiabatic transition is much shorter, and also any residual (exponentially small) excitations are brushed away to the end of the spin chain.

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