Dynamics of a Quantum Phase Transition

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We present two approaches to the dynamics of a quench-induced phase transition in quantum Ising model. The first one retraces steps of the standard approach to thermodynamic second order phase transitions in the quantum setting. The second one is purely quantum, based on the Landau-Zener formula for transition probabilities in avoided level crossings. We show that the two approaches yield compatible results for the scaling of the defect density with the quench rate. We exhibit similarities between them, and comment on the insights they give into dynamics of quantum phase transitions.

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Phase transitions were traditionally analyzed with a focus on *equilibrium* scalings of various properties in the vicinity of the critical point. The first substantial break with this was motivated by the physics of the early Universe: Kibble [1] noted that cosmological phase transitions in a variety of field theoretic models lead to formation of topological defects (such as monopoles or cosmic strings) and may have observational consequences. It was then pointed out [2] that analogs of cosmological phase transitions can be studied in the laboratory, and that the *equilibrium critical scalings predict* various aspects of the *non-equilibrium dynamics of symmetry breaking*, including the density of topological defects left behind [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 size $\hat{\xi}$ of domains that choose the same "broken symmetry vacuum" [3, 4]. When the nature of the broken symmetry phase (characterized by the homotopy group) permits for their formation, topological defects should appear with density of about one defect unit (e.g., one monopole or one $\hat{\xi}$-sized section of a string) per $\hat{\xi}$-sized domain. These predictions were tested, extended and refined with the help of numerical simulations [5, 6], and verified in a variety of increasingly sophisticated and reliable experiments in liquid crystals [7, 8], superfluids [9, 10, 11], superconductors [12, 13, 14], as well as other systems [15].

Majority of the experiments are consistent with KZM. Notable exception is the case of superfluid 4He, where initial reports of detection of KZM vortices [9] were retracted [10] after it turned out that vorticity was inadvertently induced by stirring. In view of various uncertainties it is still not clear if 4He experiments are at odds with KZM predictions re-evaluated in view of numerics. In any case, we have a nascent theory of the dynamics of second order phase transitions that – owing to its universality – spans with its range all the way from low temperature Bose - Einstein condensation to GUT-scales encountered in particle physics and cosmology.

This last remark points to a barely explored problem treated in this paper: Dynamics of quantum phase transitions. Quantum many-body systems (e.g., BEC's) can undergo thermodynamic phase transformation (such as Bose-Einstein condensation that follows evaporative cooling). There KZM developed to deal with thermodynamic phase transitions applies directly, although the dynamics of Bose condensation is explicitly quantum [16].

On the other hand, quantum phase transitions [17] exemplified by the insulator-superfluid Mott transition of bosons in a periodic lattice is a change of the character of the *ground state* of a system that occurs at a critical value of some parameter of its Hamiltonian (e.g., lowering of the amplitude of the optical lattice induces the insulator-superfluid transition). In contrast to thermodynamic transitions, quantum systems follow reversible Schrödinger dynamics. Therefore, scaling arguments that work in the thermodynamic transitions (where the order parameter is damped) need not necessarily work in the quantum case (but see [18, 19]). Yet, dynamics of quantum phase transitions is obviously interesting in its own right. Moreover, they have applications in quantum information processing [19, 20].

We will analyze quench-induced transition in quantum Ising model. According to Sachdev [17], it is one of two prototypical quantum phase transitions. Quantum Ising model represents chain of spins with the Hamiltonian:

$$H = -J(t)\sum_{l=1}^{N}\sigma_l^x - W\sum_{l=1}^{N-1}\sigma_l^z\sigma_{l+1}^z \ . \qquad (1)$$

Above, $\sigma_l^{x,z}$ are Pauli operators, W is the Ising coupling, and $J(t)$ is proportional to the external (e.g., magnetic) field that attempts to align spins with the x-axis.

Phase transition from the state with spins aligned with x (e.g., $|\rightarrow,\rightarrow,\ldots,\rightarrow\rangle$) to the low-field ground state (spanned by the broken symmetry states $|\uparrow,\uparrow,\ldots,\uparrow\rangle$ and $|\downarrow,\downarrow,\ldots\downarrow\rangle$ that is doubly degenerate in the large N

limit) takes place when $J(t) = W$, so *relative coupling*:

$$\epsilon(t) = J(t)/W - 1 \tag{2}$$

is expected to play a role similar to relative temperature $\frac{T(t)}{T_C} - 1$ in the behavior of the system near critical T_C. Indeed, all of the relevant properties are depend on the size of the *gap* Δ between the ground state and the first excited state. In the infinite system the gap:

$$\Delta = 2|J(t) - W| = 2W|\epsilon(t)| \ . \tag{3}$$

sets energy scale that is reflected in the *relaxation time*:

$$\tau = \hbar/\Delta = \hbar/2W|\epsilon(t)| = \tau_0/|\epsilon(t)| \ . \tag{4}$$

Divergence of τ at the critical point is analogous to *critical slowing down* in the usual phase transitions. Similarily, *healing length* ξ is given by the product of the speed of sound c and relaxation time:

$$\xi = 2Wa/\Delta(t) = a/|\epsilon(t)| = \xi_0/|\epsilon(t)| \ , \tag{5}$$

where $c = 2Wa/\hbar$ (see [17]), and a is the distance between spins. Divergence of ξ near the critical point is the analogue of *critical opalescence*.

Scaling behavior of τ and ξ suggests using the same approach to estimate size of the broken symmetry domains (regions aligned spins) that worked in thermodynamic phase transitions [2, 3]: As either quantum or thermodynamic system approaches phase transition, its "reflexes" (measured by the relaxation time τ) deteriorate, until – at the critical point, where $\tau(\epsilon = 0) = \infty$ – it cannot react at all. Nevertheless, when quench starts far away from the critical point where τ is still small, the system will be initially able to adjust to the changes imposed by e.g. slowly varying $J(t)$. This division into quasi - adiabatic and nearly impulse regimes of the quench works in thermodynamic phase transitions [2]. We shall first review it and then try it out on the quantum case.

The instant $\hat{t}$ when behavior changes from adiabatic to impulse is of key importance. This happens when the reaction time of the system (given by Eq. (4)) is the same as the timescale on which its Hamiltonian is altered. To calculate $\hat{t}$, we assume that the external bias field changes linearly with time so that relative coupling is:

$$\epsilon(t) = J(t)/W - 1 = t/\tau_Q \ . \tag{6}$$

The relative coupling changes on a timescale:

$$\epsilon(t)/\dot{\epsilon}(t) \ = \ t \ . \tag{7}$$

So, the switch between adiabatic and impulse occurs at instants $\pm\hat{t}$ when the relaxation time is equal to t, or:

$$\tau(\hat{t}) = \ \tau_0/|\epsilon(\hat{t})| \ = \ \epsilon(\hat{t})/\dot{\epsilon}(\hat{t}) = \hat{t}. \tag{8}$$

Thus, using Eqs. (4), (6) and (7), we arrive at:

$$\hat{t} = \sqrt{\tau_Q \tau_0} = \sqrt{\tau_Q \hbar/2W} \tag{9}$$

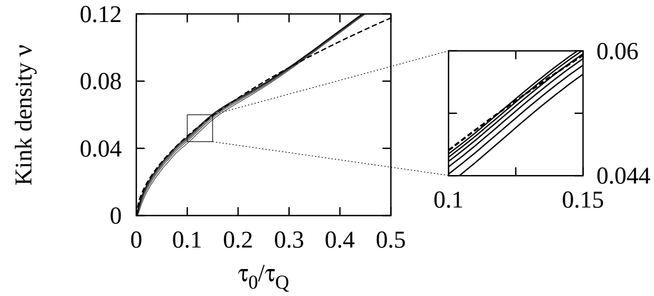

FIG. 1: Number of kinks per spin in quantum Ising model after a quench starting in a ground state at $J = 5$ and ending at $J = 0$, plotted as a function of dimensionless quench rate $\tau_0/\tau_Q = \hbar v/4W^2$ for $N = 50, 60, 70, 80, 90, 100$ (solid lines; bottom to top). Scaling $\hat{\nu}_{KZM} \sim \sqrt{\tau_0/\tau_Q}$, Eq. (12), is predicted by the Kibble-Zurek mechanism. It is consistent with the simulations (see [19] for details of the numerical method). Agreement improves with the size of the system: for 100 spins a fit gives $\nu \sim \tau_Q^{-0.58}$ (dashed line). As in the classical case [5] Eq. (12) is an overestimate; best fit is $\nu \simeq 0.16\hat{\nu}_{KZM}$.

In the beginning of the quench, for $t < -\hat{t}$, the state of the system will continue to adjust to the changes imposed by the decreasing $J(t)$. However, at $t = -\hat{t}$ before the critical point the evolution will cease, and will re-start only at $t = +\hat{t}$ after the transition, presumably with initial state similar to the one "frozen out" at $-\hat{t}$.

In thermodynamic phase transitions fluctuations of the order parameter from before at $\hat{t}$ give rise to domains with the size $\hat{\xi}$ given by the healing length at $-\hat{t}$. Using the relative coupling $\hat{\epsilon}$ associated with $\hat{t}$ we get:

$$\hat{\epsilon} \equiv \epsilon(\hat{t}) = \hat{t}/\tau_Q = \sqrt{\tau_0/\tau_Q}; \tag{10}$$

$$\hat{\xi} \equiv \xi_0/\hat{\epsilon} = \xi_0\sqrt{\tau_Q/\tau_0} = a\sqrt{2W\tau_Q/\hbar} \ . \tag{11}$$

Note that this scaling differs from $\hat{\xi} = \xi_0/\sqrt{\hat{\epsilon}} = \xi_0(\tau_Q/\tau_0)^{\frac{1}{4}}$ that obtains in non-relativistic mean-field theories for thermal second order phase transitions [2, 3].

Following KZM, we now predict appearance of $O(1)$ defects per $\hat{\xi}$. Their density should be approximately:

$$\hat{\nu}_{KZM} \simeq a/\hat{\xi} = \sqrt{\hbar/2W\tau_Q} \tag{12}$$

per spin. This is an estimate: Simulations of classical second order transitions yield defect densities that scale with τ_Q in accordance with this reasoning, but that are lower than the relevant power of $\hat{\xi}$ of Eq. (11) so that a "unit of defect" is separated by ∼10-15 $\hat{\xi}$; see e.g. [5].

This paradigm should not be uncritically 'transferred' to quantum phase transitions: In thermodynamic case 'real' (thermal) fluctuations exist above the critical point: One can imagine they choose how symmetry breaks in domains that appear after transition. It is hard to make this argument for quantum phase transitions. There are 'quantum fluctuations', but one cannot be certain they will have analogous effect on the post-transition state.

Yet, Fig. 1 shows that number of kinks per spin – kink density ν created in quantum Ising model by a quench scales approximately as $\sim 1/\sqrt{\tau_Q}$, Eq. (12), in the region of the validity of KZM, i.e. for $\hat{\epsilon}$ less than 1 (so that quench is quasi - adiabatic at the beginning and at the end, but impulse near critical point, i.e., at least one defect is expected). The prefactor (~ 0.16) is also not far from the previous experience [5]. KZM paradigm works! Yet, in view of doubts about quantum fluctuations, an explicitly quantum approach would be most useful.

Salient feature of the quantum phase transition is the behavior of the gap Δ. In quantum Ising model the gap disappears at the critical point in accord with Eq. (3) when the system is infinite. When $N < \infty$, this critical gap becomes small, but does not disappear, (see Fig. 2a). This is of key importance for the remainder of our considerations: Instead of calculating density of defects in an infinite system we shall compute (as a function of quench timescale τ_Q) size of the system that can remain defect free (in a ground state) after a quench.

Eigenstates of H, Eq. (1), that lie above the ground state on the broken symmetry ($W > J$) side of the transition represent spin chain in which the direction of symmetry breaking changes once, twice, etc. [17]. Thus, they represent system with one, two, etc. "kinks". Behavior of the lowest levels of H in the vicinity of the critical point (Fig. 2a) suggests avoided level crossing. Hence, it appears that phase transition dynamics in quantum Ising model can be treated using Landau-Zener formula [22]: LZF gives the probability of exciting the system driven through avoided level crossing:

$$p \simeq e^{-\frac{\pi\hat{\Delta}^2}{2\hbar|v|}} \tag{13}$$

Above $\hat{\Delta}$ is the energy gap between the two levels on their closest approach, and v is velocity with which quench is imposed on the system: That is, far away from the "point of the nearest approach" $v = \dot{\Delta}$. Indeed, similarities between LZF and KZM were noted by Damski [21].

Using LZF we can compute size $\tilde{N}$ of the spin chain that will likely remain in the ground state in course of the quench. In the adiabatic limit ($v \approx 0$) Eq. (13) predicts (in accord with the adiabatic theorem) that the system stays in the same energy eigenstate (i.e., probability of switching levels is then vanishingly small). To quantify this we use fidelity, $f = |\langle\psi_{ACTUAL}|\psi_{GROUND}\rangle|^2$. Given the nature of ground and excited states, f gives probability that no defect – no excited state – is produced. It follows that $p_{CHANGE} \simeq \exp\{-\frac{\pi\hat{\Delta}^2}{2\hbar|v|}\} \leq 1 - f$. Hence:

$$\frac{\pi\hat{\Delta}^2}{2\hbar|v|} \geq \ln\frac{1}{1-f} \tag{14}$$

for $f \sim 1$ assures a nearly defect - free quench (i.e., quench resulting in defects with probability 1-f). This translates into a condition for the rate of quench:

$$|v| \leq \frac{\pi\hat{\Delta}^2}{2\hbar|\ln(1-f)|} \ . \tag{15}$$

Employing notations used here or in [19] $v = |\dot{\Delta}| = 2\dot{J}(t) = 2W/\tau_Q$, we relate v to quench time, Eq. (6).

The first *accessible* level has one kink. It gets to within $\hat{\Delta} = 3\pi W/N$ above the ground state. (Lowest excited state is inaccessible – it has a different parity than the ground state.) With the above inputs we get:

$$|v| = |\dot{\Delta}| = \frac{2W}{\tau_Q} \leq \frac{\pi(3\pi W/\tilde{N})^2}{2\hbar|\ln(1-f)|} \tag{16}$$

relating size $\tilde{N}$ of defect-free chain to the quench rate:

$$\tilde{N} \leq \frac{3\pi}{2}\sqrt{\frac{\pi W\tau_Q}{\hbar|\ln(1-f)|}} = \frac{3\pi W}{2}\sqrt{\frac{2\pi}{\hbar v|\ln(1-f)|}} \tag{17}$$

Figs. 2b & c show that LZF is (surprisingly) accurate for $f > 0.5$ even if there are many levels in Fig. 2a: when quench is slow, only the closest accessible level counts.

We can compare KZM and LZF predictions for defect density:

$$\tilde{\nu}_{LZF} \simeq \frac{1}{\tilde{N}} = \frac{2}{3\pi}\sqrt{\frac{2|\ln(1-f)|}{\pi}} \times \hat{\nu}_{KZM} \tag{18}$$

The two estimates exhibit the same scaling with the quench rate and with the parameters of H, Eq. (1). LZF predicts fewer defects than "raw KZM estimate" ($\tilde{\nu}_{LZF} \simeq 0.14 \times \hat{\nu}_{KZM}$ when f is set – somewhat arbitrarily – to 0.5). This is no surprise: as seen in the numerical simulations, confirmed by the experiments and verified analytically in specific models, Eqs. (11) and (12) provide correct scalings, but tend to overestimate densities (see e.g. [5, 14]). Fig. 1 indicates that this conclusion holds also for quantum Ising model.

We note while $\hat{\nu}_{KZM}$ and $\tilde{\nu}_{LZF}$ are closely related, they answer somewhat different questions. In particular, $\hat{\nu}_{KZM}$ does not depend on f. However, when less than one defect is expected in a chain of length N, defect number is $\simeq 1 - f$ and can be computed using LZF. Fig. 3 shows that – in this case – LZF and KZM complement, and jointly cover a wide range of quench rates.

We have investigated dynamics of quantum phase transitions in the Ising model. We have found that quantum analogue of KZM based on critical scalings predicts correctly results of numerical simulations. As expected, KZM scaling holds when $\hat{\epsilon} < 1$ – when quench starts and ends in the adiabatic regime, but becomes impulse near the critical point. For very slow quenches ($\hat{t} > \hbar/\hat{\Delta}$, or $\tau_Q > (\frac{2N}{3\pi})^2\tau_0$) that – for a system of fixed size N are nowhere convincingly 'impulse' – LZF is surprisingly accurate. We conclude that the two approaches work well in complementary regimes of quench rates, and predict

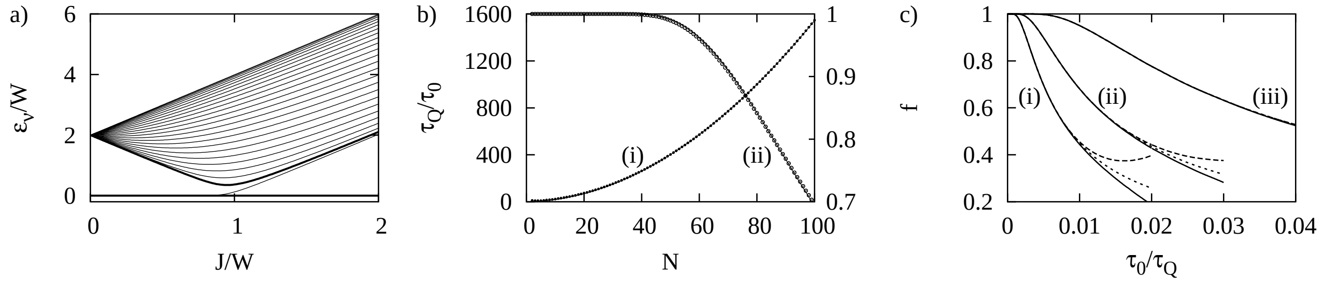

FIG. 2: (a) Energies ε_ν of elementary excitations for $N = 25$. The ground and the first accessible excited state are marked with a thicker line. (b) (i) Quench time $\tau_Q/\tau_0 = 4W^2/\hbar v$ that yields f of 99%, and (ii) the fidelity for a fixed $\tau_Q = 200\hbar/W = 400\tau_0$ as a function of the number of spins N in the quantum Ising chain. A power-law fit to the data corresponding to $\tau_{Q_{99\%}}$ gives a power of 1.93 (LZF yields 2, as would KZM). The best fit for the fidelity with Landau-Zener dependence $f = 1 - \exp\{\frac{-aW\tau_Q}{\hbar N^2}\}$ yields $a \simeq 59$, compared to theoretical $a = 9\pi^3/4 \simeq 69.8$. (c) Upper and lower bounds on fidelity as a function of $\tau_0/\tau_Q = \hbar v/4W^2$ for $N = 70$ (i), $N = 50$ (ii), $N = 30$ (iii). Fits to LZF lie between these bounds, and for $f > 0.6$ give $a \simeq 59$ (i), 57 (ii), 54 (iii).

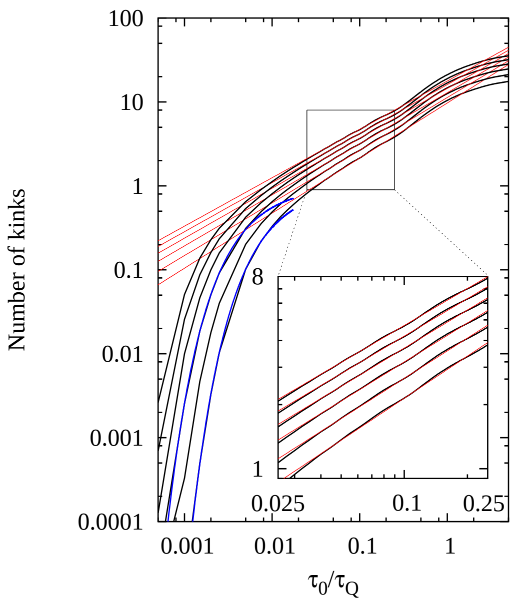

FIG. 3: Number of kinks with $N = 50, 60, 70, 80, 90, 100$ spins (bottom to top) after a quench as a function of dimensionless quench rate $\tau_0/\tau_Q = \hbar v/4W^2$. Both the scaling $\hat{\nu} \sim 1/\sqrt{\tau}_Q$ predicted by KZM (red lines), Eq. (12), and the LZF estimate $1 - f$ (blue lines) when less than one kink is expected are valid. The red lines are linear fits in the range (0.025,0.25) yielding slopes between 0.66 and 0.58. The blue lines are the fit results from Fig. 2c. Numerical data include these used in Fig. 1. They were obtained using the same method developed in [19], 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", leveling off of the expected number of kinks, as is indeed seen.

the same scaling of the size of broken symmetry domains with quench time.

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