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Dynamics of a Quantum Phase Transition: Exact Solution of the Quantum Ising Model

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The Quantum Ising model is an exactly solvable model of quantum phase transition. This Letter gives an exact solution when the system is driven through the critical point at a finite rate. The evolution goes through a series of Landau-Zener level anticrossings when pairs of quasiparticles with opposite pseudomomenta get excited with a probability depending on the transition rate. The average density of defects excited in this way scales like a square root of the transition rate. This scaling is the same as the scaling obtained when the standard Kibble-Zurek mechanism of thermodynamic second order phase transitions is applied to the quantum phase transition in the Ising model.

Introduction.—A phase transition is a fundamental change in the state of a system when one of the parameters of the system passes through its critical point. The states on the opposite sides of the critical point are characterized by different types of ordering. In a second order phase transition the fundamental change is continuous and the critical point is characterized by diverging correlation length and relaxation time. This critical slowing down implies that no matter how slowly a system is driven through the transition its evolution cannot be adiabatic close to the critical point. If it were adiabatic, then the system would continuously evolve between the two types of ordering. However, ordering of the state after the transition is not perfect in the necessarily nonadiabatic evolution: the state is a mosaic of ordered domains whose finite size depends on the rate of the transition. This scenario was first described by Kibble [1] and then its underlying dynamical mechanism was proposed by Zurek [1] who predicted that the size of the ordered domains scales with the transition time τ_Q as τ_Q^w, where w is a combination of critical exponents. The Kibble-Zurek mechanism (KZM) of second order thermodynamic phase transitions was confirmed by numerical simulations of the time-dependent Ginzburg-Landau model [2] and tested by experiments in liquid crystals [3], superfluid helium 3 [4], superfluid helium 4 [5], and both high-T_c [6] and low-T_c [7] superconductors. KZM is a universal theory of the dynamics of second order phase transition whose applications range from the low temperature Bose-Einstein condensation [8] to the ultrahigh temperature transitions in the grand unified theories of high energy physics. However, the zero temperature quantum limit remains largely unexplored (but see Refs. [9–11]) and quantum phase transitions are in many respects qualitatively different from transitions at finite temperature. Most importantly time evolution is unitary; there is no damping that seems to play an essential role in KZM.

According to Sachdev [12] understanding of quantum phase transitions is based on two prototypical models. One is the Bose-Hubbard model with its transition from Mott insulator to superfluid and the other is the 1-dimensional quantum Ising model. Of the two only the Ising model is exactly solvable. It is defined by the Hamiltonian

$$H = -J \sum_{n=1}^{N} (g\sigma_n^x + \sigma_n^z \sigma_{n+1}^z). \tag{1}$$

with periodic boundary conditions

$$\vec{\sigma}_{N+1} = \vec{\sigma}_1. \tag{2}$$

The 1-dimensional quantum Ising model has the same critical properties as the 2-dimensional classical Ising model. Quantum phase transition takes place at the critical value $g = 1$ of external magnetic field. When $g \gg 1$, then the ground state is a paramagnet $|\rightarrow\rightarrow\rightarrow \ldots \rightarrow\rangle$ with all spins polarized up along the x axis. On the other hand, when $g \ll 1$, then there are two degenerate ferromagnetic ground states with all spins pointing either up or down along the z axis: $|\uparrow\uparrow\uparrow \ldots \uparrow\rangle$ or $|\downarrow\downarrow\downarrow \ldots \downarrow\rangle$. In adiabatic transition from paramagnet to ferromagnet the system would choose one of the two ferromagnetic states (with the possible help of an infinitesimal symmetry breaking field along the z axis, as usual in symmetry breaking phase transitions). However, when $N \rightarrow \infty$, then the energy gap at $g = 1$ tends to zero (quantum version of the critical slowing down) and it is impossible to pass the critical point without exciting the system. As a result the system ends in a quantum superposition of states like

$$|\ldots \uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow\downarrow\downarrow\uparrow\uparrow\uparrow\uparrow\uparrow\downarrow \ldots\rangle \tag{3}$$

with finite domains of spins pointing up or down and separated by kinks where the polarization of spins changes its orientation. Average size of the domains or, equivalently, average density of kinks depends on the transition rate. When the transition is slow, then the size is large, but when it is very fast, then the orientation of individual spins can become random, uncorrelated with their nearest neighbors. Transition time τ_Q can be unambiguously defined when we assume that close to the critical point at $g = 1$ the time-dependent field $g(t)$ driving the transition can be approximated by a linear quench

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$$g(t < 0) = -\frac{t}{\tau_Q} \qquad (4)$$

with variable quench time τ_Q. Density of kinks after the linear quench was estimated in Ref. [11] as

$$n \simeq \left(\frac{\hbar}{2J\tau_Q}\right)^{1/2} \qquad (5)$$

in an attempt to generalize KZM to quantum phase transitions. This is an order of magnitude estimate with an unknown $\mathcal{O}(1)$ prefactor. Results of numerical simulations in Ref. [11] for a chain of N spins were fitted with $n \sim \tau_Q^{-w}$. The fitted exponent w decreased with increasing N reaching $w = 0.58$ for $N = 100$. This is roughly consistent with the predicted $w = \frac{1}{2}$.

These encouraging results strongly motivate further study of the dynamics of quantum phase transition in the quantum Ising model. As this model is exactly solvable, the dynamics of its quantum phase transition also deserves to be solved exactly. In fact this is the only model, without any counterpart in the thermodynamic transitions, where KZM can be compared with an exact analytic solution. I begin by recalling relevant facts about the energy spectrum of the model.

Energy spectrum.—Here I assume N is even for convenience. After a Jordan-Wigner transformation [13],

$$\sigma_n^x = 1 - 2c_n^\dagger c_n, \qquad (6)$$

$$\sigma_n^z = -(c_n + c_n^\dagger)\prod_{m<n}(1 - 2c_m^\dagger c_m), \qquad (7)$$

introducing fermionic operators c_n which satisfy anticommutation relations $\{c_m, c_n^\dagger\} = \delta_{mn}$ and $\{c_m, c_n\} = \{c_m^\dagger, c_n^\dagger\} = 0$, the Hamiltonian (1) becomes [14]

$$H = P^+ H^+ P^+ + P^- H^- P^-, \qquad (8)$$

where

$$P^\pm = \frac{1}{2}\left[1 \pm \prod_{n=1}^N \sigma_n^x\right] = \frac{1}{2}\left[1 \pm \prod_{n=1}^N(1 - 2c_n^\dagger c_n)\right] \qquad (9)$$

are projectors on the subspaces with even $(+)$ and odd $(-)$ numbers of c quasiparticles and

$$H^\pm = -J\sum_{n=1}^N\left(c_n^\dagger c_{n+1} + c_{n+1}c_n + \frac{g}{2} - gc_n^\dagger c_n + \text{H.c.}\right) \qquad (10)$$

are corresponding reduced Hamiltonians. The c_n's in H^- satisfy periodic boundary conditions $c_{N+1} = c_1$, but the c_n's in H^+ must obey $c_{N+1} = -c_1$—what I call "antiperiodic" boundary conditions.

The parity of the number of c quasiparticles is a good quantum number and the ground state has even parity for any value of g. Assuming that a quench begins in the

ground state we can confine ourselves to the subspace of even parity. H^+ is diagonalized by Fourier transform followed by Bogoliubov transformation [14]. Fourier transform consistent with the antiperiodic boundary condition $c_{N+1} = -c_1$,

$$c_n = \frac{e^{-i\pi/4}}{\sqrt{N}}\sum_k c_k e^{ik(na)}, \qquad (11)$$

where the pseudomomenta k take "half-integer" values

$$k = \pm\frac{1}{2}\frac{2\pi}{Na}, \dots, \pm\left(\frac{N}{2} - \frac{1}{2}\right)\frac{2\pi}{Na}, \qquad (12)$$

transforms the Hamiltonian into

$$H^+ = J\sum_k\{2[g - \cos(ka)]c_k^\dagger c_k$$
$$+ \sin(ka)[c_k^\dagger c_{-k}^\dagger + c_{-k}c_k] - g\}. \qquad (13)$$

Here a is lattice spacing. Diagonalization of H^+ is completed by the Bogoliubov transformation

$$c_k = u_k\gamma_k + v_{-k}^*\gamma_{-k}^\dagger \qquad (14)$$

provided that Bogoliubov modes (u_k, v_k) are eigenstates of the stationary Bogoliubov–de Gennes equations

$$\epsilon u_k = +2J[g - \cos(ka)]u_k + 2J\sin(ka)v_k,$$
$$\epsilon v_k = -2J[g - \cos(ka)]v_k + 2J\sin(ka)u_k. \qquad (15)$$

There are two eigenstates for each k with eigenenergies $\epsilon = \pm\epsilon_k$, where

$$\epsilon_k = 2J\sqrt{[g - \cos(ka)]^2 + \sin^2(ka)}. \qquad (16)$$

The positive energy eigenstate

$$(u_k, v_k) \propto [g - \cos(ka)$$
$$+ \sqrt{g^2 - 2g\cos(ka) + 1}, \sin(ka)], \qquad (17)$$

normalized so that $|u_k|^2 + |v_k|^2 = 1$, defines the quasiparticle operator $\gamma_k = u_k^* c_k + v_{-k}c_{-k}^\dagger$, and the negative energy eigenstate $(u_k^-, v_k^-) = (-v_k, u_k)$ defines $\gamma_k^- = (u_k^-)^* c_k + v_{-k}^- c_{-k}^\dagger = -\gamma_{-k}^\dagger$. After the Bogoliubov transformation the Hamiltonian $H^+ = \frac{1}{2}\sum_k \epsilon_k(\gamma_k^\dagger \gamma_k - \gamma_k^{-\dagger}\gamma_k^-)$, equivalent to

$$H^+ = \sum_k \epsilon_k\left(\gamma_k^\dagger \gamma_k - \frac{1}{2}\right), \qquad (18)$$

is a simple-looking sum of quasiparticles with half-integer pseudomomenta. However, thanks to the projection $P^+ H^+ P^+$ in Eq. (8), only states with even numbers of quasiparticles belong to the spectrum of H.

Transition from paramagnet to ferromagnet.—In the linear quench Eq. (4) the system is initially prepared in its ground state at a large initial value of $g \gg 1$, but when g is ramped down to zero the state of the system gets excited

from its instantaneous ground state and, in general, its final state at $t = 0$ has a finite number of kinks. Comparing the Ising Hamiltonian Eq. (1) at $g = 0$ with the Bogoliubov Hamiltonian (18) at $g = 0$ we obtain a simple expression for the operator of the number of kinks

$$\mathcal{N} \equiv \frac{1}{2} \sum_{n=1}^{N} (1 - \sigma_n^z \sigma_{n+1}^z) = \sum_k \gamma_k^\dagger \gamma_k. \qquad (19)$$

The number of kinks is equal to the number of quasiparticles excited at $g = 0$. The excitation probability

$$p_k = \langle \psi(0) | \gamma_k^\dagger \gamma_k | \psi(0) \rangle \qquad (20)$$

in the final state can be found with the time-dependent Bogoliubov method.

The initial ground state is a Bogoliubov vacuum $|0\rangle$ annihilated by all quasiparticle operators γ_k which are determined by the asymptotic form of the (positive energy) Bogoliubov modes $(u_k, v_k) \approx (1, 0)$ in the regime of $g \gg 1$. When $g(t)$ is ramped down, then the quantum state $|\psi(t)\rangle$, in general, gets excited from the instantaneous ground state. The time-dependent Bogoliubov method makes an ansatz that $|\psi(t)\rangle$ is a Bogoliubov vacuum annihilated by a set of quasiparticle annihilation operators $\tilde{\gamma}_k$ defined by a time-dependent Bogoliubov transformation

$$c_k = u_k(t) \tilde{\gamma}_k + v_{-k}^*(t) \tilde{\gamma}_{-k}^\dagger \qquad (21)$$

with the initial condition $[u_k(-\infty), v_k(-\infty)] = (1, 0)$. The Bogoliubov modes $[u_k(t), v_k(t)]$ must satisfy the Heisenberg equation $i\hbar \frac{d}{dt} c_k = [c_k, H^+]$ with the constraint $\frac{d}{dt} \tilde{\gamma}_k = 0$ equivalent to $\tilde{\gamma}_k |\psi(t)\rangle = 0$. The Heisenberg equation is equivalent to the dynamical version of the Bogoliubov–de Gennes equation (15):

$$i\hbar \frac{d}{dt} u_k = +2J[g(t) - \cos(ka)] u_k + 2J \sin(ka) v_k,$$
$$\qquad (22)$$
$$i\hbar \frac{d}{dt} v_k = -2J[g(t) - \cos(ka)] v_k + 2J \sin(ka) u_k.$$

At any value of g Eqs. (22) have two instantaneous eigenstates. Initially the mode $[u_k(t), v_k(t)]$ is the positive energy eigenstate, but during the quench it gets "excited" to a combination of the positive and negative mode. At the end of the quench at $t = 0$ when $g = 0$ we have

$$[u_k(0), v_k(0)] = \alpha_k(u_k, v_k) + \beta_k(u_k^-, v_k^-) \qquad (23)$$

and consequently $\tilde{\gamma}_k = \alpha_k \gamma_k - \beta_k \gamma_k^\dagger$. The final state which is, by construction, annihilated by both $\tilde{\gamma}_k$ and $\tilde{\gamma}_{-k}$ is

$$|\psi(0)\rangle = \prod_{k>0} (\alpha_k + \beta_k \gamma_k^\dagger \gamma_{-k}^\dagger) |0\rangle. \qquad (24)$$

Pairs of quasiparticles with pseudomomenta $(k, -k)$ are excited with probability

$$p_k = |\beta_k|^2, \qquad (25)$$

which can be found by mapping Eq. (22) to the Landau-Zener (LZ) problem (similarity between KZM and LZ problem was first pointed out by Damski in Ref. [15]). The transformation

$$\tau = 4J\tau_Q \sin(ka)\left(\frac{t}{\tau_Q} + \cos(ka)\right) \qquad (26)$$

brings Eq. (22) to the standard LZ form [16]

$$i\hbar \frac{d}{d\tau} u_k = -\frac{1}{2}(\tau \Delta_k) u_k + \frac{1}{2} v_k,$$
$$\qquad (27)$$
$$i\hbar \frac{d}{d\tau} v_k = +\frac{1}{2}(\tau \Delta_k) v_k + \frac{1}{2} u_k,$$

with $\Delta_k^{-1} = 4J\tau_Q \sin^2(ka)$. Here the time τ runs from $-\infty$ to $\tau_{\text{final}} = 2J\tau_Q \sin(2ka)$ corresponding to $t = 0$. Tunneling between the positive and negative energy eigenstates happens when $\tau \in (-\Delta_k^{-1}, \Delta_k^{-1})$. τ_{final} is well outside this interval, $\tau_{\text{final}} \gg \Delta_k^{-1}$, for long wavelength modes with $|ka| \ll \frac{\pi}{4}$. For these modes time τ in Eq. (27) can be extended to $+\infty$ making them fully equivalent to LZ equations [16].

In slow transitions only long wavelength modes can get excited. For these modes we can use the LZ formula [16] for excitation probability:

$$p_k \simeq e^{-\frac{\pi}{2\hbar\Delta_k}} \approx e^{-2\pi(J\tau_Q/\hbar)(ka)^2}. \qquad (28)$$

This calculation is self-consistent when the width of the obtained Gaussian distribution $ka = (4\pi J\tau_Q/\hbar)^{-1/2}$ is much less than $\frac{\pi}{4}$ or, equivalently, for slow enough quenches with $\tau_Q \gg \frac{4\hbar}{\pi^3 J}$. With the LZ formula (28) we can calculate the number of kinks in Eq. (19) as

$$\mathcal{N} = \sum_k p_k. \qquad (29)$$

There are at least two interesting special cases. (1) When $N \to \infty$, i.e., in the limit of proper phase transition, the sum in Eq. (29) can be replaced by an integral. Expectation value of density of kinks becomes

$$n = \lim_{N \to \infty} \frac{\mathcal{N}}{N} = \frac{1}{2\pi} \int_{-\pi}^{\pi} d(ka) p_k = \frac{1}{2\pi} \frac{1}{\sqrt{2J\tau_Q/\hbar}}. \qquad (30)$$

The density scales like $\tau_Q^{-1/2}$ in agreement with KZM. It is a factor of $\frac{1}{2\pi} \approx 0.159$ less than the simple estimate in Eq. (5) based on KZM [11]. The results of numerical simulations in Ref. [11] are best fitted with a prefactor of 0.16 which is consistent with the exact number. (2) For a finite chain we can ask what is the fastest τ_Q when still no kinks get excited. This critical τ_Q^{ad} marks a crossover between adiabatic and nonadiabatic regimes. In other words we can ask what the probability is for a finite chain to stay in the ground state. As different pairs of quasiparticles $(k, -k)$ evolve independently, the probability to stay in the ground state is the product

$$\mathcal{P}_{GS} = \prod_{k>0}(1 - p_k). \qquad (31)$$

Well on the adiabatic side only the pair $(\frac{\pi}{N}, -\frac{\pi}{N})$ is likely to get excited and we can approximate

$$\mathcal{P}_{GS} \approx 1 - p_{\frac{\pi}{N}} \approx 1 - \exp\left(-2\pi^3 \frac{J\tau_Q}{\hbar N^2}\right). \qquad (32)$$

Again, numerical results in Ref. [11] are consistent with this formula: the best fit gives 59 in place of the $2\pi^3 \approx 62$. A quench in a finite chain becomes nonadiabatic when τ_Q is less than $\tau_Q^{ad} = \frac{\hbar N^2}{2\pi^3 J}$ which grows with the system size like N^2. In other words, the size N of a defect-free chain grows like $\tau_Q^{1/2}$ in consistency with Eq. (30).

Transition from ferromagnet to paramagnet.—Again, close to the critical point at $g = 1$ the external field can be approximated by a linear quench $g(t > 0) = \frac{t}{\tau_Q}$. The initial state is the even parity ground state at $g = 0$ and the final state $|\psi(t)\rangle$ is, in general, excited with respect to the polarized ground state at a large final $g \gg 1$. We want to know how many spins in the final state are flipped with respect to the polarization in the ground state or, more precisely, the expectation value of the operator of the number of flips $\mathcal{F} = \frac{1}{2}(N - \sum_{n=1}^{N} \sigma_n^x)$. We note that when $g \gg 1$, then $H \approx -Jg\sum_{n=1}^{N} \sigma_n^x = -Jg(N - 2\mathcal{F})$, but on the other hand $H^+ \approx 2Jg\sum_k \hat{\gamma}_k^\dagger \hat{\gamma}_k - JgN$, and consequently

$$\mathcal{F} = \sum_k \hat{\gamma}_k^\dagger \hat{\gamma}_k. \qquad (33)$$

At large $g \gg 1$ the number of flips is the number of excited quasiparticles. Formal similarity of Eqs. (33) and (19) allows us to proceed in the same way as in the paramagnet to ferromagnet transition. We soon arrive at Eq. (27) but with τ replaced by $-\tau$ on the right hand side. In analogy to Eq. (30) we find density of flipped spins

$$f = \frac{1}{2\pi} \frac{1}{\sqrt{2J\tau_Q/\hbar}} \qquad (34)$$

and the probability for a finite chain to stay in the ground state is again given by Eq. (31).

Conclusion.—This Letter gives an exact analytic solution when the quantum Ising model is driven through its quantum critical point at a finite transition rate. The evolution goes through a series of Landau-Zener level anticrossings when pairs of quasiparticles with opposite pseudomomenta get excited, with a probability depending on the transition rate. The average density of defects excited in this way scales like a square root of the transition rate. This scaling is the same as the scaling obtained when the standard Kibble-Zurek mechanism of thermodynamic second order phase transitions is extended to the quantum phase transition in the Ising model.

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