## Dynamical Quantum Phase Transitions in the Transverse Field Ising Model

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A phase transition indicates a sudden change in the properties of a large system. For temperaturedriven phase transitions this is related to non-analytic behavior of the free energy density at the critical temperature: The knowledge of the free energy density in one phase is insufficient to predict the properties of the other phase. In this paper we show that a close analogue of this behavior can occur in the real time evolution of quantum systems, namely non-analytic behavior at a critical time. We denote such behavior a *dynamical phase transition* and explore its properties in the transverse field Ising model. Specifically, we show that the equilibrium quantum phase transition and the dynamical phase transition in this model are intimately related.

Phase transitions are one of the most remarkable phenomena occurring in many-particle systems. At a phase transition a system undergoes a non-analytic change of its properties, for example the density at a temperature driven liquid-gas transition, or the magnetization at a paramagnet-ferromagnet transition. What makes the theory of such equilibrium phase transitions particularly fascinating is the observation that a perfectly wellbehaved microscopic Hamiltonian without any singular interactions can lead to non-analytic behavior in the thermodynamic limit of the many-particle system. In fact, the occurrence of equilibrium phase transitions was initially a puzzling problem because one can easily verify no go theorems for finite systems, therefore the thermodynamic limit is essential [1].

Today the theory of equilibrium phase transitions is well established, especially for classical systems undergoing continuous transitions, where the powerful tool of renormalization theory bridges the gap from microscopic Hamiltonian to universal macroscopic behavior. On the other hand, the behavior of non-equilibrium quantum many-body systems is by far less well understood. Recent experimental advances have triggered a lot of activity in this field [2], like the beautiful experiments on the real time evolution of essentially closed quantum systems in cold atomic gases [3, 4]. The experimental setup is typically a quantum quench, that is a sudden change of some parameter in the Hamiltonian. Therefore the system is initially prepared in a non-thermal superposition of the eigenstates of the Hamiltonian which drives its time evolution.

From a formal point of view, there is a very suggestive similarity between the canonical partition function of an equilibrium system

$$Z(\beta) = \operatorname{Tr} e^{-\beta H} \tag{1}$$

and the overlap amplitude of some time-evolved initial quantum state  $|\Psi_i\rangle$  with itself

$$G(t) = \langle \Psi_i | e^{-iHt} | \Psi_i \rangle \tag{2}$$

This leads to the question whether some analogue of temperature ( $\beta$ )-driven equilibrium phase transitions in (1) exists in real time evolution problems. In the theory of equilibrium phase transitions it is well established that the breakdown of the high-temperature (small  $\beta$ ) expansion indicates a temperature-driven phase transition. Likewise, we propose the term *dynamical phase transition* for non-analytic behavior in time, that is the breakdown of a short time expansion in the thermodynamic limit at a critical time.

In this paper we study this notion of dynamical phase transition in the one dimensional transverse field Ising model, which serves as a paradigm for one dimensional quantum phase transitions [5]. It can be solved exactly, which permits us to establish the existence of dynamical phase transitions that are intimately related to the equilibrium quantum phase transition in this model. Our results in this specific model lead to numerous intriguing follow up questions like the existence of dynamical phase transition in other models, and which concepts from the theory of equilibrium phase transitions can be carried over to dynamical phase transitions.

## RESULTS

The key quantity of interest in this work is the partition function

$$Z(z) = \langle \Psi_i | e^{-zH} | \Psi_i \rangle \tag{3}$$

in the complex plane  $z \in \mathbb{C}$ . For imaginary z = it this just describes the overlap amplitude (2). For real z = Rit can be interpreted as the partition function of the field theory described by H with boundaries described by boundary states  $|\Psi_i\rangle$  separated by R [6]. In the thermodynamic limit one defines the free energy (apart from a different normalization)

$$f(z) = -\lim_{N \to \infty} \frac{1}{N} \ln Z(z)$$
(4)

where N is the number of degrees of freedom. Now subject to a few technical conditions one can show that the partition function (3) is an entire function of z since inserting an eigenbasis of H yields sums of terms  $e^{-zE_j}$ , which are entire functions of z. According to the Weierstrass factorization theorem an entire function with zeroes  $z_j \in \mathbb{C}$  can be written as

$$Z(z) = e^{h(z)} \prod_{j} \left( 1 - \frac{z}{z_j} \right)$$
(5)

with an entire function h(z). Thus

$$f(z) = -\lim_{N \to \infty} \frac{1}{N} \left[ h(z) + \sum_{j} \ln \left( 1 - \frac{z}{z_j} \right) \right]$$
(6)

and the non-analytic part of the free energy is solely determined by the zeroes  $z_j$ . A similar observation was originally made by M. E. Fisher [1], who pointed out that the partition function (1) is an entire function in the complex temperature plane. This observation is analogous to the Lee-Yang analysis of equilibrium phase transitions in the complex magnetic field plane [7]. For example in the 2d Ising model the Fisher zeroes in the complex temperature plane approach the real axis at the critical temperature  $z = \beta_c$  in the thermodynamic limit, indicating its phase transition [8].

We now work out these analytic properties explicitly for the one dimensional transverse field Ising model

$$H(g) = -\sum_{i=1}^{N-1} \sigma_i^z \, \sigma_{i+1}^z + g \sum_{i=1}^N \sigma_i^x \tag{7}$$

For magnetic field g < 1 the system is ferromagnetically ordered at zero temperature, and a paramagnet for g > 1[5]. These two phases are separated by a quantum critical



Figure 1: Left: Phase diagram of the transverse field Ising model.  $\Delta = |g - 1|$  is the excitation (mass) gap, which vanishes at the quantum critical point. Right: A quench across the quantum critical point (green arrow) generates a new non-equilibrium energy scale  $\epsilon_{k^*}$  (10), which is plotted here for a quench starting at  $g_0 = 0$ .



Figure 2: Lines of Fisher zeroes for a quench within the same phase  $g_0 = 0.4 \rightarrow g_1 = 0.8$  (left) and across the quantum critical point  $g_0 = 0.4 \rightarrow g_1 = 1.3$  (right). Notice that the Fisher zeroes cut the time axis for the quench across the quantum critical point, giving rise to non-analytic behavior at  $t_n^*$  (the times  $t_n^*$  are marked with dots in the plot).

point at  $g = g_c = 1$  (Fig. 1). The Hamiltonian (7) can be mapped to to a free fermion model [9–11] with dispersion relation  $\epsilon_k(g) = \sqrt{(g - \cos k)^2 + \sin^2 k}$ . In a quantum quench experiment the system is prepared in the ground state at magnetic field  $g_0$ ,  $|\Psi_i\rangle = |\Psi_{GS}(g_0)\rangle$ , while its time evolution is driven with a Hamiltonian  $H(g_1)$  with a different magnetic field  $g_1$ . Partition function (3) and free energy (4) describing this sudden quench  $g_0 \to g_1$ can be calculated analytically [12] (see Methods).

In the thermodynamic limit the zeroes  $z_j$  of the partition function in the complex plane coalesce on a family of lines, which are depicted in Fig. 2 for a quench within the same phase or across the quantum critical point. As expected there are no cuts across the real axis, otherwise one would have an equilibrium phase transition for a certain boundary separation. However, for a quench across the quantum critical point there are unavoidably non-analyticities on the time axis due to the limiting behavior of the lines of Fisher zeroes for  $R \to \pm \infty$ .

Now the free energy (4) is just the rate function of the return amplitude (2)

$$G(t) = \langle \Psi_i | \Psi_i(t) \rangle = \langle \Psi_i | e^{-iH(g_1)t} | \Psi_i \rangle = e^{-N f(it)}$$
(8)

Likewise for the return probability (Loschmidt echo)  $L(t) \stackrel{\text{def}}{=} |G(t)|^2 = \exp(-N l(t))$  one has l(t) = f(it) + f(-it). The behavior of the Fisher zeroes for quenches across the quantum critical point therefore translates into non-analytic behavior of the rate functions for return amplitude and probability at certain times  $t_n^*$ . For sudden quenches one can work out these times easily

$$t_n^* = t^* \left( n + \frac{1}{2} \right) , \quad n = 0, 1, 2, \dots$$
 (9)

with  $t^* = \pi/\epsilon_{k^*}(g_1)$  and  $k^*$  determined by

$$\cos k^* = \frac{1 + g_0 g_1}{g_0 + g_1} \tag{10}$$

We conclude that for any quench across the quantum critical point the short time expansion for the rate function of the return amplitude and probability breaks down in the thermodynamic limit, analogous to the breakdown of the high-temperature expansion at an equilibrium phase transition. In fact, the non-analytic behavior of l(t)at the times  $t_n$  has already been derived by Pollmann et al. [13] for slow ramping across the quantum critical point. For a slow ramping protocol  $\epsilon_{k^*}(g_1)$  becomes the mass gap  $m(g_1) = |g_1 - 1|$  of the final Hamiltonian, but in general it is a new energy scale generated by the quench and depending on the ramping protocol. In the universal limit for a quench across but very close to the quantum critical point,  $g_1 = 1 + \delta$ ,  $|\delta| \ll 1$  and fixed  $g_0$ , one finds  $\epsilon_{k^*}(g_1)/m(g_1) \propto 1/\sqrt{|\delta|}$ . Hence in this limit the nonequilibrium energy scale  $\epsilon_{k^*}$  becomes very different from the mass gap, which is the only equilibrium energy scale of the final Hamiltonian (compare Fig. 1).

The interpretation of the mode  $k^*$  follows from the observation  $n(k^*) = 1/2$  (see methods), where n(k) is the occupation of the excited state in the momentum k-mode in the basis of the final Hamiltonian  $H_f(g_1)$ . Modes  $k > k^*$  have thermal occupation n(k) < 1/2, while modes  $k < k^*$  have inverted population n(k) > 1/2 and therefore formally negative effective temperature. The mode  $k^*$  corresponds to infinite temperature. In fact, the existence of this infinite temperature mode and thus of the Fisher zeroes cutting the time axis periodically is guaranteed for arbitrary ramping protocols across the quantum critical point. For example, for slow ramping across the quantum critical point the existence of this mode and the negative temperature region in relation to spatial correlations was discussed in Ref. [23].



Figure 3: The bottom plot shows the work distribution function r(w,t) for a double quench across the quantum critical point  $(g_0 = 0.5, g_1 = 2.0)$ . The dashed line depicts the expectation value of the work performed, r(w,t) = 0. The top plot shows various cuts for fixed values of the work density w. The line w = 0 is just the Loschmidt echo: Its non-analytic behavior at  $t_n^*$  becomes smooth for w > 0, but traces of the non-analytic behavior extend into the work density plane.

One measurable quantity in which the non-analytic behavior generated by the Fisher zeroes appears naturally is the work distribution function of a double quench experiment: We prepare the system in the ground state of  $H(g_0)$ , then quench to  $H(g_1)$  at time t = 0, and then quench back to  $H(g_0)$  at time t. The amount of work W performed follows from the distribution function

$$P(W,t) = \sum_{j} \delta \left( W - (E_{j} - E_{GS}(g_{0})) \right) |\langle E_{j} | \Psi_{i}(t) \rangle|^{2}$$
(11)

where the sum runs over all eigenstates  $|E_j\rangle$  of the initial Hamiltonian  $H(g_0)$ . P(W, t) obeys a large deviation form [14]

$$P(W,t) \sim e^{-N r(w,t)} \tag{12}$$

with a rate function  $r(w,t) \geq 0$  depending on the work density w = W/N. In the thermodynamic limit one can derive an exact result for r(w,t) (Methods section). Its behavior for a quench across the quantum critical point is shown in Fig. 3. For w = 0 the rate function just gives the return probability to the ground state, r(w = 0, t) = l(t), therefore the non-analytic behavior at the Fisher zeroes shows up as non-analytic behavior in the work distribution function. However, from Fig. 3 one can see that these non-analyticities at w = 0 also dominate the behavior for w > 0 at  $t_n^*$ , corresponding to more likely values of the performed work. The suggestive similarity to the phase diagram of a quantum critical point, with temperature



Figure 4: Dynamics of the magnetization after the quench. The bottom plot shows the longitudinal magnetization for various quenches across the quantum critical point. The time axis is shifted by a fit parameter  $t_{\varphi}$  and one can see that the period of the oscillations is the time scale  $t^*$  (9). The upper plots show the magnetization dynamics in the y-z-plane for a quench across the quantum critical point  $g_0 = 0.3 \rightarrow g_1 = 1.4$  (left) and a quench in the ordered phase  $g_0 = 0.3 \rightarrow g_1 = 0.8$  (right). For better visibility the magnetization is normalized to unit length:  $\hat{s}_{y,z}(t) \stackrel{\text{def}}{=} s_{y,z}(t)/\sqrt{s_y^2(t) + s_z^2(t)}$ . Notice the Lamor precession for the quench across the quantum critical point, while the dynamics for the quench in the ordered phase is asymptotically just an exponential decay [16].

being replaced by the work density w, motivates us to call this behavior dynamical quantum phase transitions.

Interestingly, the non-equilibrium time scale (9) also plays a role in the dynamics of a local observable after the quench. We have calculated the longitudinal magnetization (which is the equilibrium order parameter of the transverse field Ising model)

$$s_z(t) = \frac{1}{N} \sum_{j=1}^{N} \langle \Psi_i(t) | \sigma_j^z | \Psi_i(t) \rangle$$
(13)

by numerical evaluation of Pfaffians [15] (for details see the Methods section). For quenches within the ordered phase it is known analytically [16, 17] that the order parameter decays exponentially as a function of time, which is expected since in equilibrium one only finds long range order at zero temperature (g < 1). For a quench across the quantum critical point an additional oscillatory behavior is superimposed on this exponential decay, see Fig. 4. Notice that the behavior of the magnetization remains perfectly analytic, but the period of its oscillations agrees exactly (within numerical accuracy) with the period  $t^*$  of Fisher times. We have no proof for this observation, but have verified it numerically in many different quenches across the quantum critical point (a conjecture consistent with our observation was also formulated in Ref. [18]). A better understanding of this observation will be the topic of future work.

## CONCLUSIONS

We have shown that ramping across the quantum critical point of the transverse field Ising model generates periodic non-analytic behavior at certain times  $t_n^*$ . This breakdown of the short time expansion for the rate function of the return amplitude is reminiscent of the breakdown of a high temperature expansion for the free energy at an equilibrium phase transition. We have therefore denoted this behavior dynamical phase transition. Notice that there are other related but not identical notions of dynamical phase transitions, for example a sudden change of the dynamical behavior of an observable as a function of some control parameter [19, 20], or qualitative changes in the ensemble of trajectories as a function of the conjugate field of a dynamical order parameter [21]. Our definition implies non-analytic behavior at some critical time, which comes about due to the distribution of Fisher zeroes in the complex plane.

For quenches within the same phase (including to/from the quantum critical point) the lines of Fisher zeroes lie in the negative half plane, Re  $z_j(k) \leq 0$  (Fig. 2). Hence the knowledge of the equilibrium free energy f(R) on the positive real axis completely determines the time evolution by a simple Wick rotation. This is no longer true for a quench/ramping protocol across the quantum critical point since then the lines of Fisher zeroes cut the complex plane into disconnected stripes, Fig. 2: Knowing f(R) for  $R \ge 0$  does not determine the time evolution for  $t > t_0^*$ . In this sense non-equilibrium time evolution is no longer described by equilibrium properties, at least for the return amplitude. We conjecture that this is due to the athermal mode occupation for  $k < k^*$  that cannot be achieved by any equilibrium Gibbs state with positive temperature. A related observation was recently made in Ref. [23] regarding negative spatial correlations which are not possible in any thermal state.

The key question for future work will be the robustness of the dynamical quantum phase transition with respect to perturbations; specifically perturbations which are irrelevant in the renormalization sense, but break the integrability of the model. At present it is unclear whether some concept of universality can be carried over from the theory of equilibrium phase transitions. Also one would like to study other models to see what kind of quantum quenches can give rise to dynamical phase transitions.

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## METHODS

Free energy and Fisher zeroes. The analytic solvability of the transverse field Ising model relies on the Jordan-Wigner transformation and a Bogoliubov rotation [9–11], which map the Hamiltonian (7) to a free fermion model

$$H_f(g) = \sum_k \epsilon_k(g) \left(\gamma_k^{\dagger} \gamma_k - \gamma_{-k} \gamma_{-k}^{\dagger}\right)$$
(14)

with dispersion relation  $\epsilon_k(g) = \sqrt{(g - \cos k)^2 + \sin^2 k}$ and  $k = 2\pi n/N$ ,  $n = 1 \dots N/2$ . The key property we make use of for describing quenches is the simple structure of the initial ground state  $|\Psi_i\rangle = |\Psi_{GS}(g_0)\rangle$  in terms of eigenoperators  $\gamma_k^{\dagger}$ ,  $\gamma_k$  of the final Hamiltonian  $H_f(g_1)$ [12]

$$|\Psi_{GS}(g_0)\rangle = \frac{1}{\mathcal{N}} \exp\left(\sum_{k>0} B(k) \gamma_k^{\dagger} \gamma_{-k}^{\dagger}\right) |0\rangle \qquad (15)$$

Here  $|0\rangle$  is the vacuum of  $H_f(g_1)$ ,  $\mathcal{N}$  a normalization factor and the coefficients  $B(k) = i \tan \phi_k$  with the Bogoliubov angles  $\phi_k = \theta_k(g_0) - \theta_k(g_1)$ ,

$$\tan(2\theta_k(g)) \stackrel{\text{def}}{=} \frac{\sin k}{g - \cos k} , \ \theta_k(g) \in [0, \pi/2] .$$
 (16)

Therefore the partition function (3) is

$$Z(z) = \frac{1}{\mathcal{N}^2} \prod_{k>0} \left( 1 + |B(k)|^2 e^{-2z\epsilon_k(g_1)} \right)$$
(17)

leading to the free energy (4)

$$f_{g_0,g_1}(z) = -\int_0^\pi \frac{dk}{2\pi} \ln\left(\cos^2\phi_k + \sin^2\phi_k \, e^{-2z\epsilon_k(g_1)}\right)$$
(18)

Here we have ignored an uninteresting additive contribution  $z E_{GS}(g_1)/N$  that depends on the ground state energy of  $H(g_1)$  (in the notation of (5) one has  $h(z) = z E_{GS}(g_1)$ ). In the thermodynamic limit the zeroes of the partition function in the complex plane coalesce to a family of lines labelled by a number  $n \in \mathbb{Z}$ 

$$z_n(k) = \frac{1}{2\epsilon_k(g_1)} \left( \ln \tan^2 \phi_k + i\pi(2n+1) \right)$$
(19)

The limiting infrared and ultraviolet behavior of the Boboliuobv angles

$$\phi_{k=0} = \begin{cases} 0 & \text{quench in same phase} \\ \pi/4 & \text{quench to/from quantum critical point} \\ \pi/2 & \text{quench across quantum critical point} \end{cases}$$

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$$\phi_{k=\pi} = 0 \tag{20}$$

immediately shows that the lines of Fisher zeroes cut the time axis for a quench across the quantum critical point (Fig. 2) since then  $\lim_{k\to 0} \operatorname{Re} z_n(k) = \infty$ ,  $\lim_{k\to\pi} \operatorname{Re} z_n(k) = -\infty$ . In fact, the limiting behavior (20) remains unchanged for general ramping protocols g(t) with  $g(t = 0) = g_0, g(t = \tau) = g_1$ : For a general ramping protocol we define  $|\Psi_i\rangle = |\psi(\tau)\rangle$ , where  $|\psi(t)\rangle$ is the solution of the Schroedinger equation

$$i\frac{d}{dt}|\psi(t)\rangle = H(g(t))|\psi(t)\rangle , \quad |\psi(t=0)\rangle = |\Psi_{GS}(g_0)\rangle$$
(21)

*Work distribution function.* The cumulant generating function for the work distribution function for the double quench (11) follows via

$$C(R,t) = \int dW P(W,t) e^{-RW} = \langle \Psi_i | e^{iH(g_1)t} e^{-H(g_0)R} e^{-iH(g_1)t} | \Psi_i \rangle = e^{-N c(R,t)}$$
(22)

with

$$c(R,t) = -\int_0^{\pi} \frac{dk}{2\pi} \ln\left(1 + \sin^2(2\phi_k)\sin^2(\epsilon_k(g_1)t) \times (e^{-2\epsilon_k(g_0)R} - 1)\right)$$
(23)

According to the Gärtner-Ellis theorem [14] the work distribution function (11) depicted in Fig. 3 is just the Legendre transform

$$-r(w,t) = \inf_{R \in \mathbb{R}} \left( wR - c(R,t) \right)$$
(24)

Longitudinal magnetization. The local order parameter  $s_z(t)$  (13) is evaluated from the associated spin-spin correlation function

$$\rho_z(j,j') = \langle \Psi_i(t) | \sigma_j^z \, \sigma_{j'}^z | \Psi_i(t) \rangle \tag{25}$$

for j, j' away from the boundary of the chain via the cluster decomposition  $[22], [s_z(t)]^2 = \lim_{j \to \infty} \rho_z(j, j')$ . Expressing the Pauli matrices in terms of the Jordan-Wigner fermions, the spin-spin correlation function can be related to a Pfaffian [9] that can then be evaluated numerically. For our results in Fig. 4 we typically use N = 200.

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