Dynamical Quantum Phase Transitions in the Transverse-Field Ising Model

M. Heyl, A. Polkovnikov, and S. Kehrein

Phys. Rev. Lett. **110**, 135704 — Published 28 March 2013
DOI: 10.1103/PhysRevLett.110.135704

Dynamical Quantum Phase Transitions in the Transverse Field Ising Model

M. Heyl
Department of Physics, Arnold Sommerfeld Center for Theoretical Physics and Center for NanoScience, Ludwig-Maximilians-Universität München, Theresienstr. 37, 80333 Munich, Germany and Institut für Theoretische Physik, Technische Universität Dresden, 01062 Dresden, Germany

A. Polkovnikov
Department of Physics, Boston University, 590 Commonwealth Ave., Boston, MA 02215, USA

S. Kehrein
Department of Physics, Georg-August-Universität Göttingen, Friedrich-Hund-Platz 1, 37077 Göttingen, Germany

A phase transition indicates a sudden change in the properties of a large system. For temperature-driven 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 well-behaved 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 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

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

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 (β)-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 β) 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 key quantity of interest is the boundary 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 $z = R$ it 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 density (apart from a different normalization)

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

where N is the number of degrees of freedom. Now subject to a few technical conditions [1] one can show that for finite N 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 [7] an entire function with zeroes $z_j \in \mathbb{C}$ can be written as

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

with an entire function $h(z)$. Thus

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

and the non-analytic part of the free energy density 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 [8]. 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 [9].

We now work out these analytic properties explicitly for the one dimensional transverse field Ising model (with periodic boundary conditions)

$$H(g) = -\frac{1}{2}\sum_{i=1}^{N-1} \sigma_i^z \, \sigma_{i+1}^z + \frac{g}{2}\sum_{i=1}^{N} \sigma_i^x \tag{7}$$

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 point at $g = g_c = 1$. The Hamiltonian (7) can be mapped to a quadratic fermionic model [10–12]

$$H(g) = -\frac{1}{2}\sum_{i=1}^{N-1}\left(c_i^\dagger c_{i+1} + c_i^\dagger c_{i+1}^\dagger + \text{h.c.}\right) + g\sum_{i=1}^{N} c_i^\dagger c_i \tag{8}$$

Diagonalization yields the 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 for parameter 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 parameter g_1. In the sequel we will first analyze quench experiments in the setting of the fermionic model (8). A subtle difference occurs when thinking in terms of the spin model (7) since in the ferromagnetic phase the ground state of the spin model is twofold degenerate, while the fermionic model always has a unique ground state. We will say more about this later. Taking the ground state of the fermionic model in Eq. (8) as the initial state $|\Psi_i\rangle$ the free energy density (4) describing this sudden quench $g_0 \to g_1$ can be calculated analytically [13] yielding

$$f_{g_0,g_1}(z) = -\int_0^\pi \frac{dk}{2\pi} \ln\left(\cos^2\phi_k + \sin^2\phi_k \, e^{-2z\epsilon_k(g_1)}\right) \tag{9}$$

Here $\phi_k = \theta_k(g_0) - \theta_k(g_1)$, and $\tan(2\theta_k(g)) \overset{\text{def}}{=} \sin k/(g - \cos k)$, $\theta_k(g) \in [0, \pi/2]$. In (9) we have ignored an uninteresting additive contribution $z\,E_{GS}(g_1)/N$ that depends on the ground state energy of $H(g_1)$.

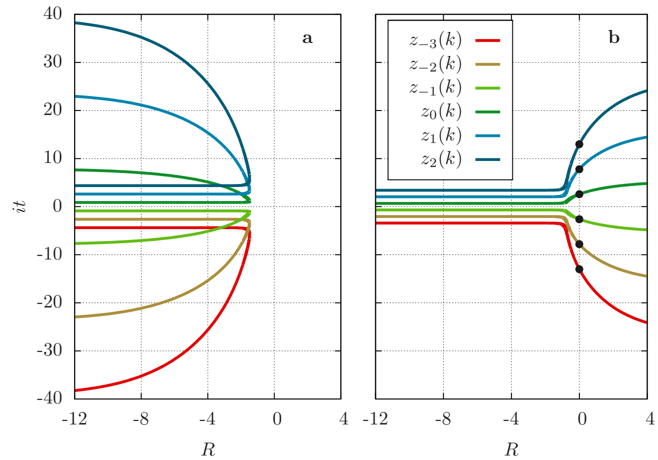

Figure 1: Lines of Fisher zeroes for a quench within the same phase $g_0 = 0.4 \;\to\; g_1 = 0.8$ (left) and across the quantum critical point $g_0 = 0.4 \;\to\; g_1 = 1.3$ (right). Notice that the Fisher zeroes cut the time axis for the quench across the quantum critical point, giving rise to non-analytic behavior at t_n^* (the times t_n^* are marked with dots in the plot).

In the thermodynamic limit the zeroes of the partition function in the complex plane coalesce to a family of lines labeled by a number $n \in \mathbb{Z}$

$$z_n(k) = \frac{1}{2\epsilon_k(g_1)}\left(\ln\tan^2\phi_k + i\pi(2n+1)\right) \tag{10}$$

The limiting infrared and ultraviolet behavior of the Boboliubov angles

$$\phi_{k=0} = \begin{cases} 0 & \text{quench in same phase} \\ \pi/4 & \text{quench to/from quantum critical point} \\ \pi/2 & \text{quench across quantum critical point} \end{cases}$$
$$\phi_{k=\pi} = 0 \tag{11}$$

immediately shows that the lines of Fisher zeroes cut the time axis for a quench across the quantum critical point (Fig. 1) since then $\lim_{k\to 0} \text{Re}\; z_n(k) = \infty$, $\lim_{k\to\pi} \text{Re}\; z_n(k) = -\infty$. In fact, the limiting behavior (11) remains unchanged for general ramping protocols [15].

The free energy density (4) is just the rate function of the return amplitude $G(t) = \exp[-N\, f(it)]$. 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

$$t_n^* = t^* \left(n + \frac{1}{2}\right) \ , \quad n = 0, 1, 2, \ldots \tag{12}$$

with $t^* = \pi/\epsilon_{k^*}(g_1)$ and k^* determined by $\cos k^* = (1 + g_0\, g_1)/(g_0 + g_1)$. 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. [16] 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 non-equilibrium energy scale ϵ_{k^*} becomes very different from the mass gap, which is the only equilibrium energy scale of the final Hamiltonian.

The interpretation of the mode k^* follows from the observation $n(k^*) = 1/2$, where $n(k)$ is the occupation of the excited state in the momentum k-mode in the eigenbasis 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. [17].

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

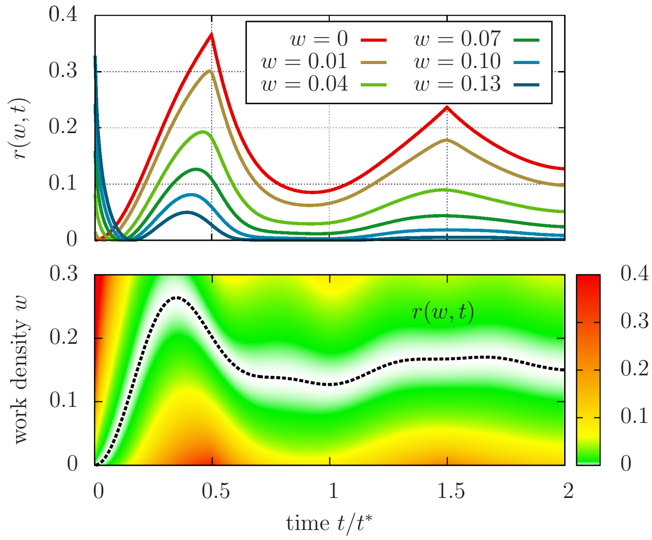

Figure 2: The bottom plot shows the work distribution function $r(w, t)$ for a double quench across the quantum critical point ($g_0 = 0.5$, $g_1 = 2.0$). The dashed line depicts the expectation value of the performed work, $r(w, t) = 0$. The top plot shows various cuts for fixed values of the work density 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. In this respect work density plays a similar role to temperature in the phase diagram of an equilibrium quantum phase transition.

performed follows from the distribution function

$$P(W, t) = \sum_j \delta\left(W - (E_j - E_{GS}(g_0))\right) |\langle E_j|\Psi_i(t)\rangle|^2 \tag{13}$$

where the sum runs over all eigenstates $|E_j\rangle$ of the initial Hamiltonian $H(g_0)$. It obeys a large deviation form $P(W, t) \sim e^{-N\, r(w,t)}$ 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 $r(w, t)$: According to the Gärtner-Ellis theorem [18] it is just the Legendre transform

$$-r(w, t) = \inf_{R\in\mathbb{R}} \left(wR - c(R, t)\right) \tag{14}$$

where

$$c(R, t) \ = \ -\int_0^\pi \frac{dk}{2\pi} \ln\Big(1 + \sin^2(2\phi_k) \sin^2(\epsilon_k(g_1)t) \times (e^{-2\epsilon_k(g_0)R} - 1)\Big) \tag{15}$$

is the rate function for the cumulant generating function of the work distribution function, $C(R, t) = \int dW\, P(W, t)\, e^{-RW} = e^{-N\, c(R,t)}$. In Fig. Fig. 2 we show $r(w, t)$ for a quench across the quantum critical point. For $w = 0$ it 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. 2 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 being replaced by the work density w, motivates us to call this behavior dynamical *quantum* phase transitions. Notice that experimentally the work density can be lowered by *post-selection* [14].

So far we have analyzed the quench dynamics in terms of the fermionic model (8). When thinking in terms of the transverse field Ising model (7), all results carry over for quenches starting in the paramagnetic phase since then the spin ground state is unique. Specifically, one finds the non-analytic behavior in the Loschmidt echo *and* the work distribution function for quenches from the paramagnetic to the ferromagnetic phase. For quenches originating in the ferromagnetic phase, the Loschmidt echo calculated above corresponds to working in the Neveu-Schwarz sector [22], which amounts to an unphysical superposition of spin up and spin down ground states in the spin language. However, looking at the experimentally relevant quantity work distribution function, one derives the same result in the thermodynamic limit as above when starting from either of the two degenerate ferromagnetic ground states. Specifically, one obtains the non-analytic behavior in $P(w = 0, t)$ at the critical times (12) for quenches from the ferromagnetic to the paramagnetic phase [14].

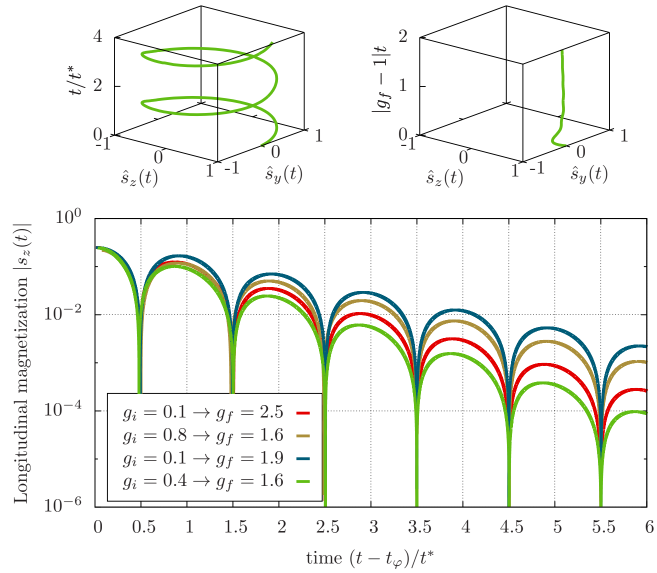

Figure 3: Dynamics of the magnetization after the quench. The bottom plot shows the longitudinal magnetization for various quenches across the quantum critical point. The time axis is shifted by a fit parameter t_φ and one can see that the period of the oscillations is the time scale t^* (12). The upper plots show the magnetization dynamics in the $y-z$-plane for a quench across the quantum critical point $g_0 = 0.3 \to g_1 = 1.4$ (left) and a quench in the ordered phase $g_0 = 0.3 \to g_1 = 0.8$ (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 Larmor 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 [20].

Interestingly, the non-equilibrium time scale (12) also plays a role in the dynamics of a local observable after the quench. We have calculated the longitudinal magnetization by numerical evaluation of Pfaffians [19]. For quenches within the ordered phase it is known analytically [20, 21] 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. 3. 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. A conjecture consistent with our observation was also formulated in Ref. [22]. A better understanding of this observation will be the topic of future work. At low energies the oscillatory decay transforms into real-time nonanalyticities at the Fisher times using the concept of post-selection allowing to observe the dynamical phase transitions in local observables [14].

Summing up, 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 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*. Very recent numerical results in Ref. [23] show that the dynamical phase transitions in the Ising model are stable against weak integrability breaking perturbations and indicate that the appearance of the real-time nonanalyticities seem to be a generic feature also in other systems as long as the respective quenches cross the equilibrium critical points. 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 [24, 25], or qualitative changes in the ensemble of trajectories as a function of the conjugate field of a dynamical order parameter [26].

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. 1). 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. 1: Knowing $f(R)$ for $R \geq 0$ does not determine the time evolution for $t > t_0^*$. In this sense non-equilibrium time evolution is no longer described by equilibrium properties.

The authors thank L. D'Alessio, M. Kolodrubetz and D. Huse for valuable discussions. The authors also acknowledge the support of the Deutsche Forschungsgemeinschaft via SFB-TR 12, the German Excellence Initiative via the Nanosystems Initiative Munich (M.H. and S.K.), the NSF under grants DMR-0907039, PHY11-25915, the AFOSR under grant FA9550-10-1-0110, the Sloan and Simons Foundations (A.P.). S.K. thanks the Boston University visitors program, A.P. and S.K. thank the Kavli Institute for Theoretical Physics at UCSB for their hospitality and NSF PHY11-25915.

[1] M. E. Fisher, in: *Boulder Lectures in Theoretical Physics, Vol. 7* (University of Colorado, Boulder, 1965).
[2] A. Polkovnikov, K. Sengupta, A. Silva, and M. Vengalattore, *Rev. Mod. Phys.* **83**, 863 (2011).
[3] M. Greiner, O. Mandel, T. Esslinger, T. Hänsch, and I. Bloch, *Nature* **419**, 51 (2002).
[4] T. Kinoshita, T. Wenger, and D. Weiss, *Nature* **440**, 900 (2006).
[5] S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, 2011).
[6] A. LeClair, G. Mussardo, H. Saleur, and S. Skorik, *Nucl. Phys.* B **453**, 581 (1995).
[7] J. B. Conway, *Functions of One Complex Variable* (Springer, New York, 1995).
[8] C. Yang and T. Lee, *Phys. Rev.* **87**, 404 (1952).
[9] W. van Saarloos and D. Kurtze, *J. Phys.* A **17**, 1301 (1984).
[10] E. Lieb, T. Schultz, and D. Mattis, *Ann. Phys.* **16**, 407 (1961).
[11] P. Pfeuty, *Ann. Phys.* **57**, 79 (1970).
[12] E. Barouch, B. McCoy, and M. Dresden, *Phys. Rev.* A **2**, 1075 (1970).
[13] A. Silva, *Phys. Rev. Lett.* **101**, 120603 (2008).
[14] See Supplementary material for details about Loschmidt echos for symmetry broken initial states and post-selection.
[15] For a general ramping protocol $g(t)$ with $g(t=0) = g_0, g(t=\tau) = g_1$ we define $|\Psi_i\rangle = |\psi(\tau)\rangle$ and $|\psi(t)\rangle$ is the solution of the Schroedinger equation: $i\,\partial_t\,|\psi(t)\rangle = H(g(t))\,|\psi(t)\rangle$, $|\psi(t=0)\rangle = |\Psi_{GS}(g_0)\rangle$
[16] F. Pollmann, S. Mukerjee, A. Green, and J. Moore, *Phys. Rev.* E **81**, 020101 (R) (2010).
[17] M. Kolodrubetz, B. Clark, and D. Huse, *Phys. Rev. Lett.* **109**, 015701 (2012).
[18] H. Touchette, *Phys. Rep.* **478**, 1 (2009).
[19] E. Barouch and B. McCoy, *Phys. Rev.* A **3**, 786 (1971).
[20] P. Calabrese, T. Essler, and M. Fagotti, *Phys. Rev. Lett.* **106**, 227203 (2011).
[21] D. Schuricht and F. Essler, *J. Stat. Mech.* P04017 (2012).
[22] P. Calabrese, F. Essler, and M. Fagotti, *J. Stat. Mech.* P07016 (2012).
[23] C. Karrasch and D. Schuricht, arXiv:1302.3893.
[24] M. Eckstein, M. Kollar, and P. Werner, *Phys. Rev. Lett.* **103**, 056403 (2009).
[25] B. Sciolla and G. Biroli, *J. Stat. Mech.* **11**, P11003 (2011).
[26] J. Garrahan and I. Lesanovsky, *Phys. Rev. Lett.* **104**, 160601 (2010).
[27] B. McCoy, E. Barouch, and D. Abraham, *Phys. Rev.* A **4**, 2331 (1971).