Boundaries and Unphysical Fixed Points in Dynamical Quantum Phase Transitions

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We show that dynamic quantum phase transitions (DQPT) in many situations involve renormalization group (RG) fixed points that are unphysical in the context of thermal phase transitions. In such cases, boundary conditions are shown to become relevant to the extent of even completely suppressing the bulk transitions. We establish these by performing an exact RG analysis of the quantum Ising model on scale-invariant lattices of different dimensions, and by analyzing the zeros of the Loschmidt amplitude. Further corroboration of boundaries affecting the bulk transition comes from the three-state quantum Potts chain, for which we also show that the DQPT corresponds to a pair of period-2 fixed points.

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Dynamical quantum phase transitions (DQPT), a recent discovery of phase transitions, often periodic, in large quantum systems during time evolution [1–3], have generated a lot of interest because here time itself acts as the parameter inducing the transitions. Also, to be at a transition point, only time needs to be chosen properly without any requirement of fine-tuning of system parameters, unlike thermal transitions [4]. The signature of DQPT is the nonanalytic behavior of various quantities in time around critical times t_c's. These transitions have now been shown in many models, like the transverse-field Ising model (TFIM), spin chains, quantum Potts models, the Kitaev model, and many others [1,2,6–10], and also observed experimentally [11,12]. In spite of being a zero-temperature quantum phenomenon, DQPT is not determined by the quantum phase transitions of the system but rather seems related to the classical thermal criticalities of an associated system [10]. However, despite the use of many techniques so far, very few exact results are known on the scaling and universality in DQPT [10]. Moreover, the natures of the possible phases and the transitions remain to be properly classified, e.g., whether only equilibrium phases and transitions would suffice or there can be specialities of its own [10].

A general approach for phase transitions is the renormalization group (RG) framework [5] in terms of length-dependent effective parameters and their flows to the fixed points (FP), with the stable FPs determining the allowed phases, and the unstable ones (or separatrices) the phase transitions. In this Letter, we adopt an *exact* RG scheme for TFIM and the three-state quantum Potts chain (3QPC). Our exact results establish that there are DQPTs involving FPs that are *unphysical* in traditional thermal transitions. Second, we show that, for those unphysical FPs, boundary conditions (BC) are relevant and can even lead to a suppression of the transitions completely, unlike thermal cases where BCs do not affect the bulk transitions. Another surprising result is the emergence of a pair of period-2 FPs, never seen in the thermal context, that controls the DQPT in 3QPC, in contrast to the zero-temperature FP [2] for the Ising DQPT case. In short, our exact results bring out several distinctive features of DQPT, not to be found in equilibrium transitions.

If a quantum system, with Hamiltonian H, is prepared in a noneigenstate $|\psi_0\rangle$ and suddenly allowed to evolve, then the probability for the system to be in state $|\psi_0\rangle$ after time t is given by $P(t) = |L(t)|^2 \sim e^{-N\lambda(t)}$, where

$$L(t) = \langle\psi_0|e^{-itH}|\psi_0\rangle \sim e^{-Nf(t)}, \qquad (\hbar = 1), \quad (1)$$

is the Loschmidt amplitude with $f(t)$ and $\lambda(t) = 2\mathrm{Re}f(t)$ as the large-deviation rate functions [13] for a large system of $N(\to\infty)$ degrees of freedom. Often, $\lambda(t)$ and $f(t)$ show phase-transition-like nonanalyticities at time $t = t_c$. These phase transitions in time are the DQPTs [8,10].

TFIM is defined on a lattice as $H_{\mathrm{I}} = H + H_\Gamma$, where

$$H = -J\sum_{\langle jk\rangle}\sigma_j^z\sigma_k^z, \quad H_\Gamma = -\Gamma\sum_j \sigma_j^x, \quad (J,\Gamma > 0), \quad (2)$$

σ_j^α being the Pauli matrices ($\alpha = x, y, z$) at lattice site j, and $\langle jk\rangle$ denoting nearest neighbors [14]. The interaction favors an aligned state in the z direction [15], and H_Γ is the transverse field term that aligns the spins in the x direction. We may add a boundary term given by $H_B = -h(\sigma_1^z + \sigma_N^z)$, where the boundary field h acts only on the first and the Nth spins. Two special cases are $h = 0$ and $h \to \infty$ corresponding to open BC and fixed BC (both up in the z direction), respectively. For periodic BC in one dimension, $H_B = -J\sigma_1^z\sigma_N^z$.

The TFIM is prepared in a product state $|\psi_0\rangle$ [16] with all spins aligned in the x direction, e.g., by $\Gamma \to \infty$. At time $t = 0$, we set $\Gamma = 0$. So, the magnet evolves with H of Eq. (2) and any boundary term mentioned above. This is the particular sudden quench we use in this Letter. By expressing $|\psi_0\rangle$ in terms of the eigenstates of H, the Loschmidt amplitude and the rate function per bond can be expressed as [10,15],

$$L(y) = 2^{-N} \sum_C y^{-E_C/2J}, \qquad f(y) = -N_B^{-1} \ln L(y), \qquad (3)$$

respectively, where $y = e^{2zJ}$, N_B is the number of bonds, and, for generality, z is taken as a complex number. $L(y)$ is an analytic continuation of the partition function of the traditional nearest neighbor Ising model [17] defined for $1 \leq y < \infty$ on the real positive axis ($z = \beta$ being the inverse temperature). The quantum time evolution in Eq. (1) is given by the unit circle $|y| = 1$ ($y = e^{i2Jt}$) in the complex y plane. A phase transition—defined as the point of nonanalyticity of f—is expected along the unit circle if there are zeros or limit points of zeros of $L(y)$ on the path [17]. An isolated zero on the circle, in contrast, just indicates orthogonality of the evolved and the initial states. The S^1 (circle) topology guarantees (via winding numbers) that, if there are zeros on the circle, there will be periodic transitions in time.

In one-dimensional TFIM and 3QPC, similar DQPT occurs, viz., linear kinks in $f(t)$, despite the absence of any thermal transitions [1,7]. For the two-dimensional TFIM, DQPT was found to be the same as the two-dimensional Ising critical point [2]. However, the generality of these results has not yet been established. In this context, we focus on a class of exactly solvable models that would help us in alienating the specialities of DQPT.

We choose scale-invariant lattices for which the real space renormalization group (RSRG) can be implemented exactly. The lattices are constructed hierarchically by replacing a bond iteratively by a diamondlike motif of b branches [18,19] as shown in Fig. 1. Such lattices appear naturally in approximate RSRG for usual lattices. Three cases are considered here, (a) $b = 1$ corresponding to a one-dimensional lattice, (b) $b = 2$, which is two dimensional but not a Bravais lattice, and (c) $b = 3$ as a fractal-type lattice.

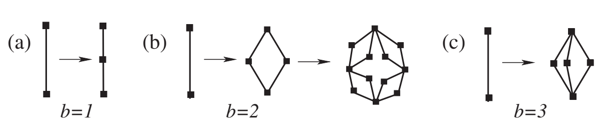

FIG. 1. Construction of hierarchical lattices. The sites are represented by squares. Replace each bond by a motif of b branches. (a) $b = 1$, (b) $b = 2$ (diamondlike motif), and (c) $b = 3$. Three generations are shown for $b = 2$.

The hierarchical structure of the lattice allows us to calculate $L(y)$ via a real space renormalization group approach, by decimating spins on individual motifs [18,20]. Let us define $Z_n = 2^N L_n$ and $f_n = (2b)^{-n} \ln Z_n$ for the nth generation. Note that $f_n(y)$ is related to $f(y)$ of Eq. (3) by $f = f_n(1) - f_n(y)$. Z_n and f_n satisfy the following recursion relations (see Supplemental Material [21])

$$Z_n(y) = \zeta(y_1) Z_{n-1}(y_1), \qquad \zeta(x) = 2^b x^{1/2}, \qquad (4a)$$

$$f_n(y) = (2b)^{-1} f_{n-1}(y_1) + (2b)^{-1} g(y_1), \qquad (4b)$$

with $g(x) = \ln \zeta(x)$, and the RG flow equation

$$y_1 = 2^{-b}(y + y^{-1})^b. \qquad (4c)$$

The boundary conditions (BC) are encoded in Z_1 as,

$$Z_1 = \begin{cases} 2(y^{1/2} + y^{-1/2}), & \text{(Open BC)} \\ y^{1/2}, & \text{(Fixed BC)}(\uparrow\uparrow), \end{cases} \qquad (4d)$$

with $f_1 = \ln Z_1$.

Equation (4c) has FPs at $y = 1$ (infinite-temperature FP, paramagnetic phase), $y = \infty$ (zero-temperature FP, ordered phase), and a b-dependent unstable FP at $y = y_c$ (for $b > 1$) representing the critical point. For any odd $b > 1$, there are additional "unphysical" FPs at $y = -1$, $-y_c$ ($\pm\infty$ to be identified). There is no y_c for $b = 1$, as there is no thermal phase transition for the one-dimensional Ising model. The zeros of $L_n(y)$ can be determined from those of L_{n-1} via Eqs. (4a) and (4c), starting from the BC-dependent roots of $L_1(y) = 0$. In the $n \to \infty$ limit, the zeros then belong to the set of points that do not flow to infinity, thereby constituting the Julia set of the transformation [20]. These sets, obtained by *MATHEMATICA*, are shown for $b = 1$, 2, and 3 in Figs. 2 and 3.

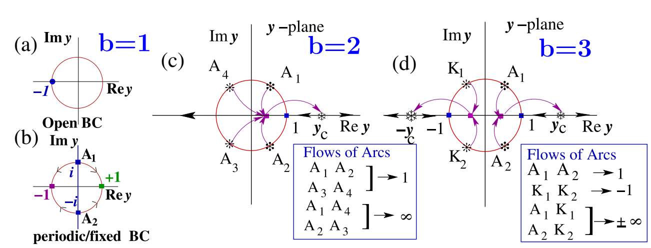

FIG. 2. Zeros of $L(y)$ in the complex-y plane, and RG flows. The red circle is the unit circle (UC) for time evolution. For $b = 1$, (a) only one zero at $y = -1$ for open BC, while (b) the zeros populate the imaginary axis for periodic or fixed BC. (c) For $b = 2$, the zeros meet the UC at four points, A_p, $p = 1, 2, 3, 4$. Under RG, UC flows to the positive real axis, taking each A_p to $y_c = 3.38298\ldots$. (d) For $b = 3$, the four meeting points are of two types; A_1, A_2 flow to $y_c = 2.05817\ldots$, while K_1, K_2 to $-y_c < 0$. See Fig. 3.

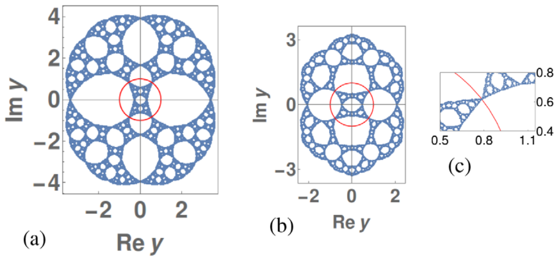

FIG. 3. Zeros of $L(y)$ as Julia sets in the complex-y plane for (a) $b=2$ and (b) $b=3$. See Fig. 2. The zeros pinch the UC at four points. (c) For $b=3$, zoomed view of the region near A_1 of Fig. 2(d).

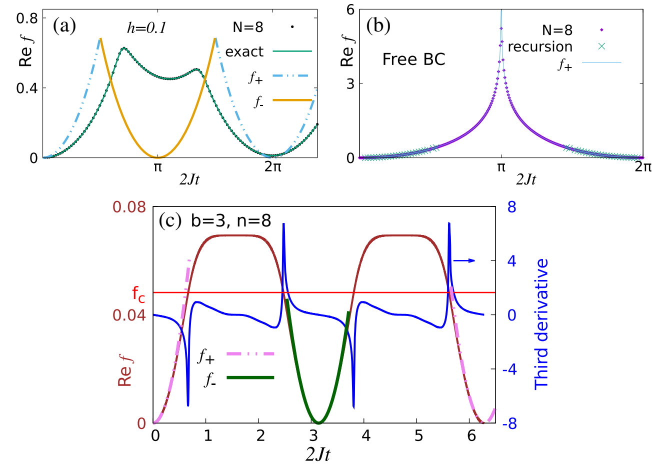

FIG. 4. Rate function Re$f(y=e^{i2Jt})$ vs $2Jt(=\theta)$. (a) $b=1$: for a chain of $N=8$ sites with boundary field $h=0.1$. Re$f(y)$ from a direct time evolution (using MATLAB) (discs) agrees with Eq. (6) (solid green line). The $N\to\infty$ limit is shown by the blue dash-dot (f_+) and orange dashed (f_-) lines, with DQPT at A_1, $\theta=\pi/2$, and A_2, $\theta=3\pi/2$ [Fig. 2(d)]. (b) Same as (a) but without the boundary field ($h=0$): time evolution data from MATLAB agree with f_+ (solid line) and with the values (green crosses) from Eq. (4b) [which fails for $\theta\in(\pi/2,3\pi/2)$]. (c) For $b=3$: f (thin brown line) from Eq. (4b) for $n=8$ with $++$ spins at the two boundary points. The intersections of the horizontal line at f_c (the critical value of f, Supplemental Material [21]) with f locates the transition points $A_{1,2}$ and $K_{1,2}$ [Fig. 2(d)]. At these points $d^3(\mathrm{Re}f)/dt^3$ diverges (solid blue line). Around $\theta=0$ and π, $f(y)$ matches with f_+ (magenta dash-dot) and f_- (green dashed lines), respectively.

The y, y^{-1} symmetry in Eq. (4c) ensures that if y^* is a FP, then $1/y^*$ flows to y^*. Therefore, there are four special points on the unit circle which flow to the nontrivial FPs, and are, necessarily, members of the Julia set. These four points on the unit circle in Figs. 2(c), 2(d), and 3 are the four critical points in time for $b>1$. Incidentally, Eq. (4c) also ensures that any point on the unit circle, $y=e^{i\theta}$, under iteration, first flows to the real axis to $\cos\theta$ and then remains real afterwards. Consequently, complex RG fixed points for $b>1$ are not important.

DQPT has been studied for $b=1$ under periodic BC [1]. The surprising result we find here is that, unlike the thermal case, boundary conditions may even suppress the bulk transition. The transfer matrix solution of the 1D Ising model describes the partition function by the two eigenvalues $\Lambda_\pm = y^{1/2}\pm y^{-1/2}$, with the larger one determining the $N\to\infty$ behavior [17]. For y flowing to $y^*=+1(y^*=-1)$, the larger eigenvalue in magnitude is $\Lambda_+(\Lambda_-)$, so that, with $y=e^{i\theta}$, the rate functions for the two regions ($f_\pm \sim \ln\Lambda_\pm/2$) are (see Supplemental Material [21])

$$f_+(y) = -\frac{1}{2}\ln\cos^2\frac{\theta}{2}, \quad \text{and} \quad f_-(y) = -\frac{1}{2}\ln\sin^2\frac{\theta}{2}, \qquad (5)$$

respectively. As characteristics of the high-temperature phases, $f_\pm$ should be independent of dimensions, remaining valid for all b. Open BC yields only one zero at $y=-1$ [Fig. 2(a)], and therefore no DQPT. On the other hand, periodic and fixed BC give zeros on the imaginary-y axis [Fig. 2(b)]. Two zeros $y=\pm i$ on the unit circle, demarcating the RG flows of the points on the unit circle to $y=\pm1$, are the known transition points [1,2]. The transitions are from a paramagnetic (described by FP at $y=1$, and f_+) to another paramagnetic phase, which we call para′, described by FP $y=-1$ and rate function f_- [Fig. 4(a)].

Now consider an open chain with the boundary term $H_B=-h(\sigma_1^z+\sigma_N^z)$. For a finite chain, there will be contributions from both the FPs $y=\pm1$, so that for an N-site chain (see Supplemental Material [21])

$$L(t,h) = (\cos Jt)^{N-1}\cos^2 ht + (i\sin Jt)^{N-1}\sin^2 ht. \qquad (6)$$

DQPT with $f_\pm(t)$ is recovered in the $N\to\infty$ limit *only if* $h\neq0$. See Fig. 4(a). For an open chain, $L(t)\equiv L(t,h=0)=(\cos Jt)^{N-1}$. Hence, there is no transition [Fig. 4(b)], consistent with one single zero [Fig. 2(a)]. There are four sectors of possible configurations of the two boundary spins, viz., $(\pm,\pm)$. Each of these four sectors individually shows DQPT. However, for the zero-field open chain, requiring superposition of the four sectors, there is a perfect cancellation of the $y=-1$ contributions. Thus, only f_+ survives [Fig. 4(b)]. When the subtle cancellation of the four sectors is disturbed by the small boundary fields, the transitions appear, as shown in Fig. 4(a). We see that boundary conditions (like open-chain) become relevant only at the unphysical fixed point.

For any odd $b>1$, there are four critical points on the unit circle, Figs. 2 and 3. These are A_1, $\theta_A=2J\tau_1=\arccos y_c{}^{-1/b}$, and A_2, $2J\tau_2=2\pi-\theta_A$, on the right half-plane, flowing to $y_c>0$, and K_1, $2J\kappa_1=\pi-\theta_A=\arccos(-y_c)^{-1/b}$, and K_2, $2J\kappa_2=\pi+\theta_A$, on the left half-plane, flowing to the unphysical FP at $-y_c<0$, via $y=-1/y_c$. These transition points ($l\pi\pm\theta_A$, for any integer l) are determined exactly. In this particular case, the nature of the singularity happens to be the same for all, as for the thermal case [a diverging third derivative of f,

Fig. 4(c)]. The flows of the four arcs of the unit circle are shown in Fig. 2(d). K_1K_2, being characterized by FP $y=-1$, is expected to be sensitive to any constraint on the boundary spins. For, say, fixed boundary spins, a sequence of phases occurs in time, para-ferro-para′-ferro-para, separated by the four critical points. The two para phases with FP $y=\pm1$ have ferromagnetic phases in between. However, in the unbiased case, the algebraic sum of the contributions of the four boundary sectors may lead to cancellation as in the $b=1$ case. A signature of the cancellation in the K_1K_2 region is the failure of Eq. (4b) for f as $y\to-1$ on renormalization. This stability problem is also seen in the one-dimensional case, Fig. 4(a) *vis-à-vis* Fig. 4(b) [the recursion relation, Eq. (4b), fails for $\pi/2<2Jt<3\pi/2$]. We, therefore, conjecture that for the open BC case (free boundary spins) there is no intermediate para′ phase, but instead the whole arc $A_1K_1K_2A_2$ represents the ferro phase—a major boundary effect on bulk DQPT.

For even b, there are again four points on the unit circle [Figs. 2(c) and 3(a)], A_i, ($i=1$, 4), which have identical angular relations as the four points for odd b, except that here all flow to y_c in two steps via $y=1/y_c$. All points in arcs A_1A_4 and A_2A_3 flow to ∞ implying an ordered state, while the remaining two arcs, A_1A_2 and A_3A_4, flow to 1, the disordered phase. Therefore, there is an oscillation between ordered (broken-symmetry) phase and the standard disordered phase with critical points at four different times. The nonanalytic features at the four critical times are the same as for the temperature-driven critical point at y_c. In essence, DQPT here follows closely the thermal transition.

To show the generality of the boundary effect, let us consider the three state Potts chain of N sites (3QPC) involving 3×3 matrices [7]. The interaction term is

$$H=-J\sum_j(\Omega_j^\dagger\Omega_{j+1}+\text{H.c.}), \tag{7}$$

where $\Omega=\text{diag}(1,e^{i2\pi/3},e^{i4\pi/3})$. Analogous to the transverse field of Eq. (2), the spin flipping term for Potts spin is $H_\Gamma=-\Gamma\sum_j T_j$, where the elements of the 3×3 matrix T are given by $T^{\alpha\beta}=1-\delta_{\alpha\beta}$, ($\alpha,\beta=1$, 2, 3). Γ can be used to prepare the chain in a product state of equal-amplitude superpositions of the three states of each spin. The chain evolves in time with H of Eq. (7), once Γ is switched off. Two boundary conditions are considered here, viz., periodic and open BCs. These two differ by an interaction term connecting the first and the Nth sites. (See Supplemental Material [21].)

In the Potts model the basic energy scale for a bond is the gap $3J$, and so define $y=\exp(3\beta J)$. The RG equation for y is [20,22]

$$y_1=R(y)\equiv(y^2+2)/(2y+1), \tag{8}$$

whose fixed points are $y_p=1$, $y_u=-2$ ("unphysical"), and $y=\pm\infty$. The DQPT involves the transition between the two stable phases described by y_p and y_u, [analogous to Fig. 2(d)], with the critical times at the points of intersection of the unit circle and the line of zeros of $L(y)=0$. These intersections are A_1, $y_{A1}=e^{i2\pi/3}$, and A_2, $y_{A2}=e^{i4\pi/3}$, which flow into each other under the RG transformation. In other words, A_1 and A_2 are period-2 FPs of RG, i.e., the fixed points of $R^{(2)}=R(R(y))$. By linearizing $R^{(2)}$ around A_1 or A_2, the thermal eigenvalue is found to be 1, which leads to a kink in Ref at the transition points [7]. The emergence of these novel unphysical fixed points *distinguishes* the DQPT from thermal transitions in general, and, in particular, the 3-state Potts chain from TFIM, though both show similar nonanalyticity [23].

Now consider a free (i.e., open) chain. There is only one zero at $y=-2$ outside the unit circle [compare with Fig. 2(a)]. There cannot be any DQPT. A direct computation of the rate function $f(y)$ by the transfer matrix method [7,17] shows that $f(y)\sim-\ln[(y+2)/3]$, ($y=e^{i\theta}$), and no DQPT, in agreement with the zeros. From the RG point of view, we see that the phase described by the unphysical fixed point at $y=-2$ does not occur for the open chain case, though it exists for the periodic case. This exact result provides yet another example of boundary conditions affecting the bulk transition in the quantum case, when an unphysical FP is involved.

Our results are summarized at the beginning, and, to that, we add the following details. The four transition points (critical times) for dynamical quantum phase transitions are determined exactly for the Ising model on hierarchical lattices of any $b>1$. The ordered (broken-symmetry) state appears as a phase only in higher dimensions ($b>1$). For all odd b, the phase transitions involve one phase characterized by a stable, but unphysical, fixed point. There are no such unphysical fixed points for even b, and, therefore, no sensitivity to boundary conditions. We anticipate that our results would lead to explorations of other unphysical fixed points in various quantum systems to look for new phases, criticality, and boundary effects not found in thermal phase transitions [24].

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Note added.—Recently, Ref. [24] appeared, which discussed the role of complex fixed points for Potts chains.

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[1] M. Heyl, A. Polkovnikov, and S. Kehrein, Phys. Rev. Lett. **110**, 135704 (2013).
[2] M. Heyl, Phys. Rev. Lett. **115**, 140602 (2015).

[3] The periodic nature, when it happens, is one of the dramatic aspects of the transition. It should be mentioned that DQPT is not necessarily periodic in every situation.

[4] DQPT is different from dynamical transitions or dynamics of usual phase transitions, which are all bereft of any special time [5].

[5] J. Cardy, *Scaling and Renormalization in Statistical Physics* (Cambridge University Press, Cambridge, England, 2015).

[6] F. Andraschko and J. Sirker, Phys. Rev. B **89**, 125120 (2014).

[7] C. Karrasch and D. Schuricht, Phys. Rev. B **95**, 075143 (2017).

[8] A. A. Zvyagin, Low Temp. Phys. **42**, 971 (2016), and references therein.

[9] B. Pozsgay, J. Stat. Mech. (2013) P10028.

[10] M. Heyl, Rep. Prog. Phys. **81**, 054001 (2018), and references therein.

[11] P. Jurcevic, H. Shen, P. Hauke, C. Maier, T. Brydges, C. Hempel, B. P. Lanyon, M. Heyl, R. Blatt, and C. F. Roos, Phys. Rev. Lett. **119**, 080501 (2017).

[12] N. Fläschner, D. Vogel, M. Tarnowski, B. S. Rem, D.-S. Lühmann, M. Heyl, J. C. Budich, L. Mathey, K. Sengstock, and C. Weitenberg, Nat. Phys. **14**, 265 (2018).

[13] H. Touchette, Phys. Rep. **478**, 1 (2009).

[14] S. Suzuki, J.-I. Inoue, and B. K. Chakrabarti, *Quantum Ising Phases and Transitions in Transverse Ising Models* (Springer, Heidelberg, 2013).

[15] For a lattice of N sites, the complete spectrum, $H|\phi_C\rangle = E_C|\phi_C\rangle$, is given by $|\phi_C\rangle = \bigotimes_{j=1,N}|\bullet\rangle_j$, and $E_C = -J\sum_{\langle jk\rangle} s_j s_k$, where $|\bullet\rangle_j$ is either $|\uparrow\rangle$ or $|\downarrow\rangle$ eigenstate of σ_j^z with $s_j = \pm 1$ in configuration C (there are 2^N states).

[16] The initial state is $|\psi_0\rangle = \bigotimes_j|\rightarrow\rangle_j$, where $|\rightarrow\rangle$ is an eigenstate of σ^x. For TFIM, the paramagnetic and the ferromagnetic states are defined with respect to the net orientation in the z direction. The state with all spins in the x direction, by this definition, is a para state.

[17] K. Huang, *Statistical Mechanics*, 2nd ed. (Wiley, New York, 1987).

[18] R. B. Griffiths and M. Kaufman, Phys. Rev. B **26**, 5022 (1982).

[19] S. M. Bhattacharjee, What is dimension?, in *Topology and Condensed Matter Physics*, edited by S. M. Bhattacharjee, M. Mj, and A. Bandyopadhyay (Springer, Singapore, 2017).

[20] B. Derrida, L. De Seze, and C. Itzykson, J. Stat. Phys. **33**, 559 (1983).

[21] See Supplemental Material at http://link.aps.org/supplemental/10.1103/PhysRevLett.123.160603 for details.

[22] The RG equation can be obtained by comparing M^2 with M where M is the transfer matrix of Ref. [7].

[23] More details on the Potts model for different b will be reported elsewhere.

[24] Y. Wu, arXiv:1906.07945.