Non-equilibrium Renormalization Group Fixed-Points of Quantum Spin Chains in Critical Dynamical Quantum Phase Transitions

Yantao Wu

The Department of Physics, Princeton University

(Dated: December 11, 2019)

We describe a new universality class of dynamical quantum phase transitions of the Loschmidt amplitude of quantum spin chains off equilibrium criticality. We demonstrate that in many cases it is possible to change the conventional linear singularity of the Loschmidt rate function into a smooth peak by tuning one parameter of the quench protocol. Exactly at the point when this change-over occurs, the singularity of the Loschmidt rate function persists, with a critical exponent equal to \( 1/2 \). The non-equilibrium renormalization group fixed-point controlling this universality class is described. An asymptotically exact renormalization group recursion relation is derived around this fixed-point to obtain the critical exponent.

In recent years, there has been a surge of interest in the post-quench dynamics of a quantum system, due to the rapid development in experimental techniques [1–6] and numerical algorithms [7–11]. In particular, critical phenomena are found to appear in the post-quench out-of-equilibrium dynamics of quantum systems. In the seminal paper [12], a notion of dynamical quantum phase transition (DQPT) is identified in the Loschmidt amplitude \( G(t) \) of a quantum quench of the transverse field Ising model:

\[
G(t) = \langle \psi_0 | e^{-iHt} | \psi_0 \rangle = \langle \psi_0 | \psi(t) \rangle
\]

which measures the return probability of a quantum state \( |\psi_0\rangle \) under the time evolution of Hamiltonian \( \hat{H} \). In general, \( G(t) \) satisfies a large-deviation principle [12, 13] and its rate function \( l(t) \) is intensive in the thermodynamic limit,

\[
l(t) = -\frac{1}{L} \ln |G(t)|^2
\]

where \( L \) is the system size. [12] found \( l(t) \) to be singular at certain critical times. Later on, people have discovered many examples of DQPTs, e.g. [14–32], investigating different aspects of them. Significant progress has also been made on their experimental observation [33, 34].

However, almost all DQPTs discovered in one dimension so far exhibit linear singularities in the Loschmidt rate function, generically due to the crossing of two branches of eigenvalues of the transfer matrix of \( G(t) \) [21, 24]. An important question is whether universality classes of DQPTs exist with critical exponents different from one [14]. In a recently study of a disordered many-body localized chain, a critical exponent of approximately 0.2 was numerically observed [35], but, to our best knowledge, there have been few observations of such cases in one-dimensional pure models. However, it has been observed several times that the singularity in the Loschmidt rate function can be changed into a smooth peak by changing parameters of the quench protocol [12, 16, 17, 19–22]. These observations suggest that there exist critical parameters of the quench protocol at which the linear DQPTs terminate. As we will show, for one class of these DQPTs, the non-equilibrium renormalization group (RG) fixed-point at the termination points of the linear DQPTs is qualitatively different from that controlling the linear DQPTs, giving rise to a new universality class with the critical exponent of the rate function equal to \( 1/2 \). Because this universality class appears at the end of the conventional DQPTs, we call it the critical dynamical quantum phase transition.

We confine our attention to DQPTs off equilibrium criticality, where the Loschmidt amplitude of quantum spin chains can be accurately described by finite-dimensional transfer matrices, \( T(t) \):

\[
G(t) = \text{Tr}(T(t)T(t)\cdots),
\]

where in general [21, 24]

\[
T(t) = \sum_s A^s(t),
\]

with \( s \) indexing the physical degree of freedom at a local lattice site. Here, \( A^s(t) \) and \( A^s(t) \) are respectively the matrix in the matrix product state (MPS) representation of \( |\psi_0\rangle \) and \( |\psi(t)\rangle \). Because the system is off equilibrium criticality, such a representation is possible [7, 36], and is evidenced by the many numerical results obtained from MPS-based time evolutions algorithms [19–23, 25, 32]. Our RG procedure will be performed on \( T \).

RG has proved a powerful tool to analyze equilibrium phase transitions [37]. Its utility in DQPTs was first demonstrated by Heyl in [38] which re-explained the linear DQPT in the transverse-field Ising chain through coarse-graining the system Hamiltonian by the decimation rule. We recently generalized Heyl’s RG procedure to the coarse-graining of the transfer matrix of \( G(t) \), which avoided a lot of the mathematical complication of the complex logarithmic function [39]. We review the RG procedure here. To analyze \( l(t) \), we perform the decimation coarse-graining [40], i.e. every other spin is summed away. The decimation coarse-graining is equivalent to
multiplying two neighboring transfer matrices into one. The renormalized transfer matrix \( T^{(n+1)} \) at the \((n+1)\)th RG iteration is thus given by

\[
\begin{align*}
\text{step 1: } T^{(n+1)}_{\text{tmp}} &= T^{(n)} T^{(n)} \\
\text{step 2: } T^{(n+1)} &= T^{(n+1)}_{\text{tmp}} / (T^{(n+1)}_{\text{tmp}})_{11}
\end{align*}
\]  

(5)

where step 2 isolates out the overall multiplicative growth of \( T^{(n)} \) and is necessary for the RG fixed-points to exist.

We assume that the matrix element \((T^{(n+1)}_{\text{tmp}})_{11}\) never becomes zero. If it does, we can divide by \((T^{(n+1)}_{\text{tmp}}))_{12}\), and so on. However, when \( T^{(n+1)} \) becomes a zero matrix, the RG procedure fails, and as we will see, this is exactly what happens at the RG fixed-point of the critical DQPT.

For concreteness, let us first consider the Ising chain with the Hamiltonian,

\[
\hat{H}_{\text{Ising}} = -\sum_{i=1}^{L} \sigma_i^x \sigma_{i+1}^x - \Gamma \sum_{i=1}^{L} \sigma_i^\theta
\]  

(6)

where \( \sigma_i^x \) and \( \sigma_i^z \) are the Pauli matrices at site \( i \), and \( \sigma_i^\theta = \sin \theta \sigma_i^x + \cos \theta \sigma_i^z \) is a magnetic field at site \( i \) pointing at a direction in the \( x \)z plane with angle \( \theta \) clockwise from the \( z \)-axis. Before the time evolution, the system is quenched into the ground state of \( \hat{H}_{\text{Ising}} \) with infinite \( \Gamma \), making the initial state

\[
|\psi_0\rangle = \otimes_i (\cos \theta/2 \uparrow_i \downarrow_i).
\]  

(7)

Following [38], we evolve \( |\psi_0\rangle \) under the \( \hat{H}_{\text{Ising}} \) with \( \Gamma = 0 \). The transfer matrix of \( G(t) \) under this quench protocol is then particularly simple:

\[
T_{\text{Ising}}(t) = \begin{pmatrix}
\frac{1}{2} e^{it} \cos^2(\theta/2) & \frac{1}{2} e^{-it} \sin(\theta) \\
\frac{1}{2} e^{-it} \sin(\theta) & \frac{1}{2} e^{it} \cos^2(\theta/2)
\end{pmatrix}.
\]  

(8)

Its eigenvalues determine the value of \( l(t) \) in the thermodynamic limit and can be found by the root formula of quadratic equations:

\[
\lambda_{\pm} = \frac{1}{2} e^{-it} (e^{2it} \pm \sqrt{e^{4it} \cos^2(\theta) + \sin^2(\theta)}).
\]  

(9)

Confining our attention to \( \theta \in [0, \frac{\pi}{2}] \), we find that when \( \theta > \frac{\pi}{2} \), the two eigenvalues intersect at \( t_c = \frac{\pi}{2} \), giving a linear DQPT. When \( \theta < \frac{\pi}{2} \), there is no DQPT. When \( \theta = \theta_c = \frac{\pi}{2} \), the DQPT persists with a critical exponent \( \frac{1}{2} \). This is our first example of a critical DQPT. The analytic computation of the eigenvalues of \( T \), however, immediately becomes impossible when the dimension of \( T, D \), is larger than 2. We thus resort to an RG analysis of \( l(t) \), which works for arbitrary \( D \), and gives a deeper understanding of the nature of the critical DQPTs.

Consider transfer matrices \( T(t) \) of dimension \( D \times D \) which depend smoothly on time. Let a transfer matrix be written as

\[
T = \begin{pmatrix}
1 & v^T \\
\mathbf{u} & \mathbf{X}
\end{pmatrix}
\]  

(10)

where \( \mathbf{u} \) and \( v \) are column vectors of dimension \( D-1 \) and \( \mathbf{X} \) is a \((D-1) \times (D-1)\) matrix. To look for the fixed-point transfer matrix \( T^* \), we note that the fixed-point equation of Eq. 5 is

\[
T^* T^* = (1 + v^T u^*) T^*.
\]  

(11)

This matrix equation is redundant and only imposes \((D-1)^2\) number of independent constraints on \( T^* \):

\[
u^* v^T = \mathbf{X}^*.
\]  

(12)

Nonetheless, \( T^* \) is still greatly simplified from \( T \). In particular, one learns from Eq. 11 that \( T^* \) has only one non-zero eigenvalue equal to \((1 + v^T u^*)\), with the corresponding eigenvector \((1, u^*)^T \). Because the RG procedure preserves the leading eigenvector which is given directly by the matrix elements of \( T^* \), the matrix elements of \( T^* \) will experience a discontinuous jump when the leading eigenvector of \( T(t) \) changes discontinuously crossing a critical time. This is exactly what happens at a linear DQPT. In addition, one expects \( T^*(t) \) to depend smoothly on \( t \) for \( t \) not experiencing a DQPT. Indeed these behaviors are seen for \( T^*_{\text{Ising}}(t) \), and also for the Potts chain studied later [Fig. 2, left panel].

At the critical parameter, however, as the smooth time dependence of \( T^*(t) \) changes into a discontinuity, a singularity could develop in this time dependence, suggesting that the RG procedure itself become non-analytic. As mentioned, the non-analyticity of the RG procedure occurs when \( T^* T^* \) becomes the zero matrix. That is, in addition to Eq. 12, the \( \mathbf{u}_c \) and \( v_c \) of \( T_c \) must be such that (hereinafter, we write \( T_c \) as \( T_c \))

\[
1 + v_c^T \mathbf{u}_c = 0.
\]  

(13)

As one varies the quench parameters to approach \( T_c \), from the side with no DQPTs, it is reasonable to assume that \(|1 + v^T u^*| \) depends continuously on the quench parameters. Thus, in general, only one parameter needs to be varied to push \(|1 + v^T u^*| \) to zero to experience a critical DQPT and eventually a linear DQPT. In the Ising example, Eq. 12, 13, and the symmetry of \( T_c \) determine the \( T_c \) uniquely:

\[
T_{c,\text{Ising}} = \begin{pmatrix}
1 & i \\
i & -1
\end{pmatrix}.
\]  

(14)

Simulating the RG flow from \( T_{\text{Ising}}(t_c) \) at \( t_c \), one discovers that the RG iteration indeed tends to \( T_{c,\text{Ising}} \)

When \( t \) is close to \( t_c \), a finite number of RG iterations will take the transfer matrix to the vicinity of \( T_c \). Thus,
to determine the universal behavior of the critical DQPT, one needs to study the RG flow around $T_c$. In a conventional RG analysis, one assumes that the RG equation is analytic at the critical fixed-point and linearizes the RG flow around it [40]. However, in our case, the RG procedure becomes non-analytic precisely at $T_c$. As a result, the naive expansion $u = u_c + \delta u, v = v_c + \delta v,$ and $X = X_c + \delta X$ fails at producing a recursion relation of $\delta u, \delta v$, and $\delta X$ to the leading order. The trick, inspired by Eq. 12, is to do the small-parameter expansion in the following way:

$$T^{(n)} = \left(1_{\delta u^{(n)}} + v_{\delta u^{(n)}} + \delta X^{(n)})^T u_c + \frac{\delta X^{(n)}}{v_{\delta u^{(n)}}} v_c + \delta V^{(n)})^T + \delta X^{(n)}\right) \tag{15}$$

Then assuming Eq. 13, one obtains to the leading order (see the SM [41] for the derivation),

$$\delta u^{(n+1)} = \delta u^{(n)} + \frac{\delta X^{(n)}}{v_{\delta u^{(n)}}} v_c u_c + \frac{\delta X^{(n)}}{v_{\delta u^{(n)}}} v_c \delta X^{(n)}$$

$$\left(\delta V^{(n+1)})^T = \left(\delta V^{(n)})^T + \delta X^{(n)} v_c \delta X^{(n)}\right) \tag{16}$$

$$\delta X^{(n+1)} = -\frac{\delta X^{(n)}}{v_{\delta u^{(n)}}} v_c \delta X^{(n)}$$

This recursion relation is asymptotically exact in the sense that as $t \to t_c$ and $n \to \infty$, $\delta u, \delta v, \delta X$ become progressively smaller, making the expansion more and more accurate near criticality.

To connect the recursion relation with the rate function, note that [42]:

$$l(t) = -\sum_{n=0}^{n_0} \frac{1}{2n} \ln |T^{(n)}(t)| - \sum_{n=n_0+1}^{\infty} \frac{1}{2n} \ln |T^{(n)}(t)| \tag{17}$$

Here $T^{(0)}$ is the unrenormalized transfer matrix. $n_0$ is a finite, but otherwise arbitrary, positive integer. $n_0$ number of RG iterations would need to be carried out to reach the vicinity of $T_c$ so that $\|\delta u\|, \|\delta v\|$, and $\|\delta X\|$ are all much less than one and Eq. 16 can be applicable for $n > n_0$. Because $n_0$ is finite, $-\sum_{n=0}^{n_0} \frac{1}{2n} \ln |T^{(n)}(t)|$ is an analytic function of $t$ and will be dropped from the singular part of the rate function, $l_s(t)$. Thus, to the leading order of $\delta u$ and $\delta v$,

$$l_s(t) = \frac{\infty}{n=n_0} \frac{1}{2n+1} \ln |V^{(n)}(t)| + \left(\delta V^{(n)}(t)\right)^T u_c \tag{18}$$

This prompts us to simplify Eq. 16 by defining $\delta w = \frac{1}{2}(\delta V^{(n)}(t) + \delta V^{(n)}(t))^T u_c$, which have the following recursion relation

$$\delta w^{(n+1)} = \delta w^{(n)} + \frac{\delta X^{(n)}}{2\delta w^{(n)}}$$

$$\delta X^{(n+1)} = -\frac{\delta X^{(n)}}{2\delta w^{(n)}} \tag{19}$$

Quite remarkably, Eq. 19 has a conservative quantity:

$$\Delta x \equiv \delta x^{(n+1)} + (\delta w^{(n+1)})^2 = \delta x^{(n)} + (\delta w^{(n)})^2 \tag{20}$$

Because $\Delta x$ depends only on $T$ at the starting point of the RG flow, it is an analytic function of $t$. At criticality, in addition, because $\delta x^{(n)}$ and $\delta w^{(n)}$ both tend to zero as $n \to \infty$, $\Delta x$ must be zero to start with. One can thus write to the leading order of $\delta t = t - t_c$,

$$\Delta x(t) = a \delta t \tag{21}$$

where $a$ is a non-universal constant. When $t \neq t_c$, while $\delta w^{(n)}$ does not tend to zero as $n \to \infty$, $\delta x^{(n)}$ still does. This means that $\delta w^{(n)}$ tends to $\sqrt{\Delta x(t)} \sim \sqrt{T-T_c}$, which explains the square root non-analytic time-dependence of $T^{(n)}(t)$ near criticality in Fig. 2.

Replacing $\delta x^{(n)}$ by $\Delta x$, one obtains:

$$\delta w^{(n+1)} = \frac{1}{2}(\delta w^{(n)} + \frac{a}{2}\delta t) u_c, \delta w^{(n+1)}(t) = \delta w^{(n)} \tag{22}$$

where we have noted that $\delta w^{(n)}$ is an analytic function of $t$ and is a constant $\delta w_0$ to the leading order of $\delta t$. Making one last re-definition $\delta \tilde{w} \equiv \delta w^{(n)}$, and rewriting Eq. 18, one finally obtains a set of equations simple enough to extract the critical behavior of $l_s(t)$:

$$\delta \tilde{w}^{(n+1)} = \frac{1}{2}(\delta \tilde{w}^{(n)} + \frac{a}{2}\delta t), \delta \tilde{w}^{(n+1)}(t) = \delta \tilde{w}^{(n)} \tag{23}$$

where we have again dropped analytic parts from $l_s(t)$. Now look for $t_1$ and $t_2$ such that $\delta \tilde{w}^{(n+1)}(t_1) = \delta \tilde{w}^{(n+1)}(t_2)$ so that the RG flow for $n \geq n_0 + 1$ at $t_1$ and that for $n \geq n_0$ at $t_2$ coincide. This requires $\sqrt{\Delta x(t_1)} = \frac{1}{2}(1 + \frac{a}{2}\delta t)$. Then, one has (see the SM [41] for a derivation)

$$l_s(t_1) = \frac{\infty}{n=n_0} \frac{1}{2n+1} \ln |\sqrt{\Delta x(t_1)} + 1| \frac{1}{2} l_s(t_2) + C \tag{24}$$

where $C$ is a constant. If the critical behavior of $l_s(t)$ is to be $l_s(t) = l_0 - A \delta t^\alpha + o(\delta t^\alpha)$, then to satisfy Eq. 24, $a$ has to be $\frac{1}{2}$.

As mentioned, the hint of the critical DQPT has been noted several times in the literature. Let us consider in detail an example in [20], which studies the three-state Potts chain with the Hamiltonian,

$$\hat{H}_{\text{Potts}} = -J \sum_{i=1}^{L} (\sigma_i \sigma_{i+1}^1 + \sigma_i \sigma_{i+1}^1 \sigma_i) - \sum_{i=1}^{L} (\sigma_i^1 + \sigma_i + \sigma_i) \tag{25}$$
The operators $\hat{\sigma}_i$ and $\hat{\tau}_i$ act on the three states of the local Hilbert space at site $i$, which we label by $|0\rangle_i$, $|1\rangle_i$, and $|2\rangle_i$. In this local basis, $\hat{\sigma}_i$ is a diagonal matrix with diagonal elements $\omega^s$ where $\omega = e^{2i\pi/3}$ and $s = 0, 1, 2$. $\hat{\tau}_i$ permutes $|0\rangle_i \rightarrow |1\rangle_i$, $|1\rangle_i \rightarrow |2\rangle_i$, etc., and together with $\hat{\sigma}_i^\dagger$ acts as a transverse-field. Off equilibrium criticality, this transfer matrix can be efficiently obtained with the time evolution algorithms [8] based on the density matrix renormalization group [43, 44]. In Fig. 3 of [20], its authors studied the Loschmidt rate function of the fully polarized ferromagnetic quenched state:

$$|\psi_0\rangle = \otimes_i |0\rangle_i$$

(26)

They found that as $J$ was varied from 0.03 to 0.1, the first peak of $l(t)$ changed from a smooth peak to a linear cusp. They also studied the rate function in the change-over region, but on a very limited parameter set, and concluded that the singularity seems still linear. Here we do a more refined scan of the parameter $J$ with the infinite-system time evolution block decimation algorithm (iTEBD) [8] implemented in ITensor [45]. A bond dimension of 10 is found to converge the calculation. The time step is set to be $10^{-4}$ before $t = 0.94485$ and $10^{-10}$ afterwards. The result of the calculation is given in Fig. 1.

![Graph](image)

**Fig. 1.** The rate function of the three-state Potts chain. Left: The rate function for $J = 0.9J_c$, $1.1J_c$, and $J_c$, obtained through the iTEBD algorithm. Right: The log-log plot of the rate function at $J_c$, for $t \in [t_c - 4.832 \times 10^{-6}, t_c - 1 \times 10^{-6}]$ and $t \in [t_c + 1 \times 10^{-6}, t_c + 1.88 \times 10^{-5}]$, where $t_c = 0.9449044833$. A linear-fit is performed on this plot to obtain the critical exponents.

We find that the smooth peak changes to the linear cusp at approximately $J_c = 0.0572776316(1)$ with a critical time at $t_c = 0.9449044833(1)$. While the critical parameter and time are non-universal and thus sensitive to the approximations in the numerical calculation, i.e. the finite bond dimension and the non-zero time step, it is clear from the RG argument that the critical exponent is a robust universal value. Indeed, the rate function at $t_c$ shows a singular cusp with a critical exponent which is numerically fitted to be 0.502 and 0.505 for $t < t_c$ and $t > t_c$ respectively (Fig. 1, right panel). Eq. 12 is verified beyond the floating-point accuracy ($10^{-15}$) for $T^{(500)}(t)$ for all $t$ studied. Eq. 13 is also satisfied to very high precision: at the estimated critical parameter and time, $|1 + \mathbf{v}^T \mathbf{u}^\dagger|$ is found to be less than 0.0001 (Fig. 2).

In the end, we note that the critical DQPT discussed above is not the only possible behavior at the change-over between no DQPT and linear DQPT. In particular, consider the exactly soluble XY Ising chain with the Hamiltonian,

$$\hat{H}_{XY} = \sum_{i=1}^N \frac{1}{2} \gamma \hat{\sigma}_i^x \hat{\sigma}_{i+1}^x + \frac{1 - \gamma}{2} \hat{\sigma}_i^y \hat{\sigma}_{i+1}^y - h \hat{\sigma}_i^z$$

(27)

When $\gamma = 1$, the system becomes a transverse field Ising chain and [12] noted that the linear DQPT terminates when the pre-quenched Hamiltonian is at the equilibrium critical point, i.e. $h_0 = 1$. When $\gamma \neq 1$, [16] further noted that linear DQPTs occur and terminate within each gapped phase without crossing any equilibrium phase transition. We did the calculation in more detail and have found that in the former termination point, the singularity of the rate function is given by [41]

$$l_s(t) \sim \int_0^1 d\delta k \ln |(\delta k)^2 + (\delta t)^2 + (\delta k)^2| \sim A_{\pm} |\delta t|$$

(28)

whereas, in the latter case, the singularity is given by [41]

$$l_s(t) \sim \int_{-1}^1 d\delta k \ln |(\delta k + \delta t)^2 + (\delta k)^4|$$

$$\sim \text{smooth but non-analytic in } \delta t.$$

Here the integration limits $\pm 1$ do not play a special role, and any other finite integration limits will give the same singularity. There are therefore at least three kinds of singularities at the boundary between no DQPT and linear DQPT, presumably corresponding to distinct physical mechanisms. A classification of all the possible cases will be left to future work.

The author is grateful to Ling Wang for hosting him at the Beijing Computational Science Research Center, introducing him to DQPTs, and many stimulating discussions. He is also grateful for mentorship from his advisor Roberto Car at Princeton. The author acknowledges support from the DOE Award DE-SC0017865.
[41] Supplementary Material.

[42] M. Nauenberg and B. Nienhuis, Phys. Rev. Lett. 33, 1598 (1974), URL https://link.aps.org/doi/10.1103/PhysRevLett.33.1598.

[43] S. R. White, Phys. Rev. Lett. 69, 2863 (1992), URL https://link.aps.org/doi/10.1103/PhysRevLett.69.2863.

[44] U. Schollwck, Annals of Physics 326, 96 (2011), ISSN 0003-4916, January 2011 Special Issue, URL http://www.sciencedirect.com/science/article/pii/S0003491610001752.

[45] ITensor Library (version 2.0.11), URL http://itensor.org.