Defect production in non-linear quench across a quantum critical point

Diptiman Sen¹, K. Sengupta², and Shreyoshi Mondal²

¹ Center for High Energy Physics, Indian Institute of Science, Bangalore, 560 012, India

² TCMP division, Saha Institute of Nuclear Physics, 1/AF Bidhannagar, Kolkata 700 064, India

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We show that the defect density n, for a slow non-linear power-law quench with a rate τ^{-1} and an exponent $\alpha > 0$, which takes the system through a critical point characterized by correlation length and dynamical critical exponents ν and z, scales as $n \sim \tau^{-\alpha\nu d/(\alpha z\nu+1)}$ [$n \sim (\alpha g^{(\alpha-1)/\alpha}/\tau)^{\nu d/(z\nu+1)}$] if the quench takes the system across the critical point at time t = 0 [$t = t_0 \neq 0$], where g is a non-universal constant and d is the system dimension. These scaling laws constitute the first theoretical results for defect production in non-linear quenches across quantum critical points and reproduce their well-known counterpart for a linear quench ($\alpha = 1$) as a special case. We supplement our results with numerical studies of well-known models and suggest experiments to test our theory.

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Quantum phase transitions have been studied extensively for several years [1]. Such transitions are accompanied by diverging length and time scales [1] leading to the absence of adiabaticity close to the quantum critical point (QCP). Thus a time evolution of a parameter $\lambda(t) = \lambda_0 |t/\tau|^{\alpha} \operatorname{sign}(t)$ in the system Hamiltonian, characterized by a rate $1/\tau$ and an exponent $\alpha > 0$, which takes such a system across a QCP located at $\lambda = \lambda_c$, leads to a failure of the system to follow the instantaneous ground state and hence to the production of defects [2, 3]. All the previous studies on such systems have been restricted to linear quenches ($\alpha = 1$) [4, 5, 6, 7, 8, 9, 10, 11, 12]. For such quenches, the density of these defects $n \sim \tau^{-\nu d/(z\nu+1)}$, where ν and z are the correlation length and the dynamical critical exponents characterizing the critical point, and d is the system dimension [13, 14]. On the experimental side, trapped ultracold atoms in optical lattices provide possibilities of realization of several model quantum spin systems and are particularly suitable for studying their non-equilibrium dynamics [15, 16]. Experimental studies of defect production have indeed been undertaken for a spin-one Bose condensate [17]. Although these experiments can easily investigate non-linear quenches, there have been no theoretical studies of such quench phenomena so far.

In this letter, we show that a slow non-linear powerlaw quench, as discussed above, through a QCP leads to a density of defects which scales either as $n \sim \tau^{-\alpha\nu d/(\alpha z\nu+1)}$ or as $n \sim (\alpha g^{(\alpha-1)/\alpha}/\tau)^{\nu d/(z\nu+1)}$ (where g is a non-universal model dependent constant), depending on whether the quench parameter λ vanishes or stays finite at the critical point. Such a scaling law for the defect density generalizes its earlier known counterpart for linear quenches [13] and thus constitutes a significant extension of our understanding of quench dynamics across a QCP. Our results, to the best of our knowledge, also constitute the first theoretical investigation of defect production due to non-linear power-law quenches. We supplement our theoretical results with numerical studies of the one-dimensional Ising and Kitaev models, and also suggest realistic experiments to test our theory.

We begin our analysis with a study of a model Hamiltonian in d dimensions of the form

$$\begin{split} H &= \sum_{k} \psi^{\dagger}(\vec{k}) \ H(\vec{k};t) \ \psi(\vec{k}), \\ H(\vec{k};t) &= [\lambda(t) + b(\vec{k})]\tau_{3} + \Delta(\vec{k})\tau_{+} + \Delta^{*}(\vec{k})\tau_{-}, \ (1) \end{split}$$

where $\tau_{i=1,2,3}$ are the usual Pauli matrices with τ_{\pm} = $(\tau_1 \pm i\tau_2)/2$, $b(\vec{k})$ and $\Delta(\vec{k})$ are model dependent functions, and $\psi(\vec{k}) = (c'_1(\vec{k}), c'_2(\vec{k}))$ represents fermionic operators. Many of the model systems with a QCP characterized by $\nu = z = 1$, such as the Ising and XY models [5, 8] in d = 1 and the extended Kitaev models [18, 19, 20]in d = 2, can be mapped onto such a fermionic Hamiltonian via standard Jordan-Wigner transformation. We first consider the case where the system passes through a gapless point at t = 0 and $\vec{k} = \vec{k}_0$. Note that in this case both $b(\vec{k})$ and $\Delta(\vec{k})$ must vanish at $\vec{k} = \vec{k}_0$. In what follows, we shall also assume that $|\Delta(\vec{k})| \sim |\vec{k} - \vec{k}_0|$ and $b(\vec{k}) \sim |\vec{k} - \vec{k}_0|^{z_1}$ at the critical point, where $z_1 \geq 1$ so that $E \sim |\vec{k} - \vec{k}_0|$ and z = 1. In the rest of the analysis, we set $\hbar = 1$, and scale $t \to t\lambda_0, \tau \to \tau\lambda_0, \Delta(\vec{k}) \to \Delta(\vec{k})/\lambda_0$, and $b(\vec{k}) \rightarrow b(\vec{k})/\lambda_0$.

The dynamics of the such a system is governed by the Schrodinger equation given by $i\partial_t\psi(\vec{k}) = H(\vec{k};t)\psi(\vec{k})$ which leads to the equation governing the time evolution of $c_1(\vec{k}) = c'_1(\vec{k})e^{i\int^t dt'[|t'/\tau|^{\alpha}\operatorname{sign}(t')+b(\vec{k})]}$,

$$\left(\frac{d^2}{dt^2} + 2i\left[\left|\frac{t}{\tau}\right|^{\alpha}\operatorname{sign}(t) + b(\vec{k})\right]\frac{d}{dt} + |\Delta(\vec{k})|^2\right)c_1(\vec{k}) = 0.(2)$$

Now we scale $t \to t \tau^{\alpha/(\alpha+1)}$ so that Eq. (2) becomes

$$\left(\frac{d^2}{dt^2} + 2i\left[|t|^{\alpha}\operatorname{sign}(t) + b(\vec{k})\tau^{\frac{\alpha}{\alpha+1}}\right]\frac{d}{dt} + |\Delta(\vec{k})|^2\tau^{\frac{2\alpha}{\alpha+1}}\right)c_1(\vec{k}) = 0.$$
(3)

Noting that the system was in the ground state $(c_1(\vec{k}), c_2(\vec{k})) = (1, 0)$ at the beginning of the quench at $t = -\infty$, we find, using Eq. (3), that the defect probability $p(\vec{k})$ must be given by

$$p(\vec{k}) = \lim_{t \to \infty} |c_1(\vec{k}, t)|^2 = f\left[b(\vec{k})\tau^{\frac{\alpha}{\alpha+1}}; |\Delta(\vec{k})|^2 \tau^{\frac{2\alpha}{\alpha+1}}\right],$$
(4)

where f is a function whose analytical form is not known for $\alpha \neq 1$. Nevertheless, we note that for a slow quench (large τ), $p(\vec{k})$ becomes appreciable only when the instantaneous energy gap $\delta E = 2[(\lambda(t) + b(\vec{k}))^2 + |\Delta(\vec{k})|^2]^{1/2}$ becomes small at some point of time during the quench. Consequently, f must vanish when either of its arguments are large. Thus for a slow quench (large τ), the defect density $n = \int_{\text{BZ}} d^d k / d f \left[b(\vec{k}) \tau^{\frac{\alpha}{\alpha+1}}; |\Delta(\vec{k})|^2 \tau^{\frac{2\alpha}{\alpha+1}} \right]$ (where BZ denotes the Brillouin zone) receives its main contribution from values of f near $\vec{k} = \vec{k}_0$ where both $b(\vec{k})$ and $\Delta(\vec{k})$ vanish and can be written as (extending the range of momentum integration to ∞) $n \simeq$ $\int d^d k / (2\pi)^d f \left[|\vec{k} - \vec{k}_0|^{z_1} \tau^{\frac{\alpha}{\alpha+1}}; |\vec{k} - \vec{k}_0|^2 \tau^{\frac{2\alpha}{\alpha+1}} \right]$. Now scaling $\vec{k} \to (\vec{k} - \vec{k}_0) \tau^{\alpha/(\alpha+1)}$, we find that

$$n = \tau^{-\frac{\alpha d}{\alpha+1}} \int \frac{d^d k}{(2\pi)^d} f(|\vec{k}|^{z_1} \tau^{\alpha(1-z_1)/(\alpha+1)}; |\vec{k}|)$$

$$\simeq \tau^{-\frac{\alpha d}{\alpha+1}} \int \frac{d^d k}{(2\pi)^d} f(0; |\vec{k}|) \sim \tau^{-\frac{\alpha d}{\alpha+1}},$$
(5)

where in arriving at the last line, we have used $z_1 > 1$ and $\tau \to \infty$. (If $z_1 = 1$, the integral in the first line is independent of τ , so the scaling argument still holds). Note that for $\alpha = 1$, Eq. (5) reduces to its counterpart for a linear quench [13].

Next we generalize our results for a critical point with arbitrary ν and z. To this end, we consider a generic time dependent Hamiltonian $H_1[t] \equiv H_1[\lambda(t)]$, whose states are labeled by $|\vec{k}\rangle$ and $|0\rangle$ denotes the ground state. If there is a second order phase transition, the basis states change continuously with time during this evolution and can be written as $|\psi(t)\rangle = \sum_{\vec{k}} a_{\vec{k}}(t) |\vec{k}[\lambda(t)]\rangle$ and the defect density can be obtained in terms of the coefficients $a_{\vec{k}}(t)$ as $n = \sum_{\vec{k} \neq 0} |a_{\vec{k}}(t \to \infty)|^2$ so that one gets [13]

$$n \simeq \int \frac{d^d k}{(2\pi)^d} \Big| \int_{-\infty}^{\infty} d\lambda \langle \vec{k} | \frac{d}{d\lambda} | 0 \rangle e^{i\tau \int^{\lambda} d\lambda' \delta \omega_{\vec{k}}(\lambda')} \Big|^2, \quad (6)$$

where $\delta \omega_{\vec{k}}(\lambda) = \omega_{\vec{k}}(\lambda) - \omega_0(\lambda)$ are the instantaneous excitation energies, and we have replaced the sum over \vec{k} by a *d*-dimensional momentum integral. We note, following Ref. 13, that near a critical point, $\delta \omega_{\vec{k}}(\lambda) = \Delta F(\Delta/|\vec{k}|^z)$, where Δ is the energy gap, z is the dynamical critical exponent and $F(x) \sim 1/x$ for large x. Also, since the quench term vanishes at the critical point, $\Delta \sim |\lambda|^{\alpha z \nu}$ for a non-linear quench, one can write $\delta \omega_{\vec{k}}(\lambda) = |\lambda|^{\alpha z \nu} F'(|\lambda|^{\alpha z \nu}/|\vec{k}|^z)$ where $F'(x) \sim 1/x$ for

large x. Further, one has $\langle \vec{k} | \frac{d}{d\Delta} | 0 \rangle = |\vec{k}|^{-z} G(\Delta/|\vec{k}|^z)$ near a critical point where G(0) is a constant. This allows us to write $\langle \vec{k} | \frac{d}{d\lambda} | 0 \rangle = \frac{\lambda^{\alpha z \nu - 1}}{|\vec{k}|^z} G'(\lambda^{\alpha z \nu}/|\vec{k}|^z)$ where G'(0) is a constant [1, 13]. Putting these in Eq. (6) and changing the integration variables to $\eta = \tau^{\alpha \nu/(\alpha z \nu + 1)} |\vec{k}|$ and $\xi = |\vec{k}|^{-1/(\alpha \nu)} \lambda$, we find that

$$n \simeq C \tau^{-\alpha\nu d/(\alpha z\nu+1)},\tag{7}$$

where C is a non-universal number independent of τ .

Next we focus on the case where the quench term does not vanish at the QCP for $\vec{k} = \vec{k}_0$. We again consider the Hamiltonian $H(\vec{k})$ in Eq. (1), but now assume that the critical point is reached at $t = t_0 \neq 0$. This renders our previous scaling argument invalid since $\Delta(\vec{k}_0) = 0$ but $b(\vec{k}_0) \neq 0$. In this situation, $|t_0/\tau| = g^{1/\alpha}$, where $g = |b(\vec{k}_0)|$ is a non-universal model dependent constant, so that the energy gap δE may vanish at the critical point for $\vec{k} = \vec{k}_0$. We now note that the most important contribution to the defect production comes from times near t_0 and from momenta near k_0 . Therefore, we expand the diagonal terms in $H(\vec{k})$ about $t = t_0$ and $\vec{k} = \vec{k}_0$ to obtain

$$H' = \sum_{\vec{k}} \psi^{\dagger}(\vec{k}) \left[\left\{ \alpha g^{(\alpha-1)/\alpha} \left(\frac{t-t_0}{\tau} \right) + b'(\delta \vec{k}) \right\} \tau_3 + \Delta(\vec{k})\tau_+ + \Delta^*(\vec{k})\tau_- \right] \psi(\vec{k}), \quad (8)$$

where $b'(\delta \vec{k})$ represents all terms in the expansion of $b(\vec{k})$ about $\vec{k} = \vec{k}_0$ and we have neglected all terms $R_n = (\alpha - n+1)(\alpha - n+2)...(\alpha - 1)g^{(\alpha - n+1)/\alpha}|(t-t_0)/\tau|^n \operatorname{sign}(t)/n!$ for n > 1 in the expansion of t/τ about t_0 . We shall justify neglecting these higher order terms shortly.

Eq. (8) describes a linear quench of the system with $\tau_{\rm eff}(\alpha) = \tau/(\alpha g^{(\alpha-1)/\alpha})$. Hence one can use the wellknown results of Landau-Zener dynamics [21] to write an expression for the defect density $n = \int_{\rm BZ} d^d k \ p(\vec{k}) = \int_{\rm BZ} d^d k \exp[-\pi |\Delta(\vec{k})|^2 \tau_{\rm eff}(\alpha)]$. For a slow quench, the contribution to n comes from \vec{k} near \vec{k}_0 so that

$$n \sim \tau_{\text{eff}}(\alpha)^{-d/2} = \left(\alpha g^{(\alpha-1)/\alpha}/\tau\right)^{d/2}.$$
 (9)

Note that for $\alpha = 1$, we get back the familiar result $n \sim \tau^{-d/2}$ as a special case and the dependence of n on the non-universal constant g vanishes. Also, since the quench is effectively linear, one can use the results of Ref. [13] to find the scaling of the defect density when the critical point at $t = t_0$ is characterized by arbitrary ν and z,

$$n \sim \left(\alpha g^{(\alpha-1)/\alpha}/\tau\right)^{\nu d/(z\nu+1)}$$
. (10)

Next we justify neglecting higher order terms R_n . We note that the significant contribution to n comes at times



FIG. 1: Variation of the defect density n with the quench exponent α for representative values of $\tau = 10$ (black solid line), $\tau = 15$ (red dashed line) and $\tau = 20$ (blue dotted line). A polynomial fit of the form $n = a\alpha^b$ yields exponents which are very close to the theoretical result 1/2 for all values of τ .

t when the energy levels of $H'(\vec{k};t)$ (Eq. (8)) for a given \vec{k} are close to each other: $(t - t_0)/\tau \sim \Delta(\vec{k})$. Also, for a slow quench, the contribution to the defect density is significant only when $p(\vec{k})$ is significant, *ie.*, when $|\Delta(\vec{k})|^2 \sim 1/\tau_{\rm eff}(\alpha)$. Using these arguments, it is easy to see that $R_n/R_{n-1} = (\alpha - n + 1)g^{-1/\alpha}(t - t_0)/(n\tau) \sim (\alpha - n + 1)/(n\sqrt{\tau})$. Thus we find that all higher order terms $R_{n>1}$, which were neglected in arriving at Eq. (9), are unimportant in the limit of slow quench (large τ).

The scaling relations for the defect density n given by Eqs. (7) and (10) represent the central results of this letter. For such power-law quenches, unlike their linear counterpart, n depends crucially on whether the quench term vanishes at the critical point. For quenches which do not vanish at the critical point, n scales with the same exponent as that of a linear quench, but is characterized by a modified non-universal effective rate $\tau_{\rm eff}(\alpha)$. If, however, the quench term itself vanishes at the critical point, we find that n scales with a novel α dependent exponent $\alpha \nu d/(\alpha z\nu + 1)$. For $\alpha = 1$, $\tau_{\text{eff}}(\alpha) = \tau$ and $\alpha\nu d/(\alpha z\nu + 1) = \nu d/(z\nu + 1)$; hence both Eqs. (7) and (10) reproduce the well-known defect production law for linear quenches as a special case [13]. We note that the scaling of n will show a cross-over between the expressions given in Eqs. (7) and (10) near some value of $\tau = \tau_0$ which can be found by equating these two expressions; this yields $\tau_0 \sim |b(\vec{k}_0)|^{-z\nu-1/\alpha}$. For $\alpha > 1$, the scaling law will thus be given by Eq. 7 (Eq. 10) for $\tau \ll (\gg)\tau_0$. We also note here that our results do not apply to quenches which take a system through a critical line [20, 22].

We now supplement these analytical results with numerical studies of well-known models. The first model



FIG. 2: Plot of $\ln(n)$ vs $\ln(\tau)$ for the 1D Kitaev model for $\alpha = 2$ (black solid line), $\alpha = 4$ (red dotted line), $\alpha = 6$ (blue dashed line) and $\alpha = 8$ (green dash-dotted line). The slopes of these lines agree reasonably with the predicted theoretical values $-\alpha/(\alpha + 1)$ as shown in the table.

that we choose for this purpose is the one-dimensional Ising model in a transverse field with the Hamiltonian $H_{\text{Ising}} = -J(\sum_{\langle ij \rangle} S_i^z S_j^z - g_0 \sum_i S_i^x)$ where J is the nearest neighbor coupling and g_0 is the dimensionless transverse field. A standard Jordan-Wigner transformation [1] then maps H_{Ising} to a free fermionic Hamiltonian $H'_{\text{Ising}}/J = \sum_k \psi_k^{\dagger} [(g_0 - \cos(k))\tau_3 + \sin(k)\tau_1]\psi_k$. Thus a time variation $g_0(t) = |t/\tau|^{\alpha} \text{sign}(t)$ takes the system through two critical points at $t_0 = \tau(-\tau)$ where the energy gap vanishes at $k_0 = 0(\pi)$ so that $g_0 = 1(-1)$ at these points. Thus the defect production around both these critical points have the same $\tau_{\text{eff}}(\alpha) = \tau/\alpha$ and we expect (Eq. (9)) the defect density to go as $n \sim \sqrt{\alpha}$ for a fixed τ . To confirm this expectation, we solve the time-dependent Schrödinger equation $i\partial_t \psi(k,t) =$ $H'_{\text{Ising}}\psi(k,t)$ and compute the defect probability p_k and hence n for fixed τ and for several representative values of $\alpha \geq 1$. These values of α and τ are chosen so that we are in the regime where all $R_{n>1}$ can be safely neglected. The plot of n as a function of α for $\tau = 10, 15, \text{ and } 20$ is shown in Fig. 1. A fit to these curves yields exponents of 0.506 ± 0.006 ($\tau = 10$), 0.504 ± 0.004 ($\tau = 15$), and 0.505 ± 0.002 ($\tau = 20$) which are indeed remarkably close to the theoretical value 1/2 predicted by Eq. (9). The systematic positive deviations in the exponents comes from the neglected terms $R_{n>1}$. We note that the range of α for which such deviation remains small grows with τ , as expected from our theoretical prediction.

Next, we consider the one-dimensional Kitaev model [20, 23, 24] which has the Hamiltonian $H_K = \sum_{i \in \text{even}} (J_1 S_i^x S_{i+1}^x + J_2 S_i^y S_{i-1}^y)$, where the sum extends over even sites *i* on the disconnected chains of the underlying hexagonal lattice, and \mathbf{S}_i denotes the

spin at site i. Such a model can be realized as the $J_3 = 0$ limit of the well-known Kitaev model and can be mapped, via a standard Jordan-Wigner transformation [20, 24], onto the fermionic Hamiltonian $H'_K = 2\sum_k \psi_k^{\dagger} (-J_-\sin(k)\tau_3 + J_+\cos(k)\tau_2) \psi_k =$ $2\sum_k \psi_k^{\dagger} H'(k)\psi_k$ where $\psi(k) = (c_1(k), c_2(k))$ are fermionic operators, $0 \leq k \leq \pi$ extends over half the Brillouin zone, $J_{\pm} = J_1 \pm J_2$, and we have chosen the lattice spacing to be unity. Here the time variation $J_{-}(t) = J |t/\tau|^{\alpha} \operatorname{sign}(t)$, keeping J_{+} fixed, takes the system through a single critical point at t = 0 and $k = k_0 = \pi/2$ which has $\nu = z = 1$. The defect density, according to Eq. (7), is therefore expected to scale as $n \sim \tau^{-\alpha/(\alpha+1)}$. To check this prediction, we numerically solve the Schrödinger equation $i\partial_t \psi(k) = H'_K(k;t)\psi(k,t)$ and compute the defect density $n = \int_0^{\pi} dk / \pi p(k)$ as a function of the quench rate τ for α with fixed $J_+/J = 1$. A plot of $\ln(n)$ as a function of $\ln(\tau)$ for different values of α is shown in Fig. 2. The slope of these lines, as can be seen from Fig. 2, changes from -0.67 towards -1 as α increases from 2 towards larger values. This behavior is consistent with the prediction of Eq. (7). The slopes of these lines also show excellent agreement with Eq. (7)as shown in the inset of Fig. 2.

Experimental verification of our results may be achieved in several possible ways. First, there has been a concrete proposal for the realization of the Kitaev model using an optical lattice^[16]. In such a realization, all the couplings can be independently tuned using separate microwave radiations. In the proposed experiment, one needs to keep $J_3 = 0$ and vary $J_{1(2)} =$ $J(1 \pm |t/\tau|^{\alpha} \operatorname{sign}(t))/2$ so that J_{+} remains constant while J_{-} varies in time. The variation of the defect density, which in the experimental setup would correspond to the bosons being in the wrong spin state, would then show the theoretically predicted power-law behavior (Eq. (7)). Secondly, a similar quench experiment can be carried out with spin one bosons in a magnetic field described by an effective Hamiltonian $H_{\text{eff}} = c_2 n_0 \langle \mathbf{S} \rangle^2 + c_1 B^2 \langle S_z^2 \rangle$ [17] where $c_2 < 0$ and n_0 is the boson density. Such a system undergoes a quantum phase transition from the ferromagnetic to polar condensate at $B^* = \sqrt{|c_2|n_0}/c_1$. A quench of the magnetic field $B^2 = B_0^2 |t/\tau|^{\alpha}$ thus would lead to scaling of defect density with an effective rate $\tau_{\rm eff}(\alpha) = \tau/(\alpha g^{(\alpha-1)/\alpha})$, where $g = |c_2|n_0/c_1$. A measurement of the dependence of the defect density n on α should therefore serve as test of prediction of Eq. (10). Finally, spin gap dimer compounds such as BaCuSi₂O₆ are known to undergo a singlet-triplet quantum phase transition at $B_c \simeq 23.5 \text{T}$ which is known to be very well described by the mean-field exponents z = 2 and $\nu = 2/3$ [25]. Thus a non-linear quench of the magnetic field through its critical value $B = B_c + B_0 |t/\tau|^{\alpha} \operatorname{sign}(t)$ should lead to scaling of defects $n \sim \tau^{-6\alpha/(4\alpha+3)}$ in d = 3. In the experiment, the defect density would correspond to residual singlets in the final state which can be computed by measuring the total magnetization of the system immediately after the quench.

To conclude, we have obtained general scaling laws of the defect density for an arbitrary power-law quench through a QCP which reproduce their linear counterpart as a special case. We have verified our theoretical prediction by numerical simulation of model systems and have suggested several possible experiments to test our results. Our results have been recently used to find the optimal passage through a QCP [26].

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