Appendix A

Chapter 2

A-I Supplemental material to “Topological dynamical quantum phase transition in a quantum skyrmion phase"

A-II Calculation of critical exponent α

We adopted a method discussed by Trapin *et al* [A163] to calculate the critical exponent of DQPT. For a one dimensional system Trapin *et al* report $\alpha = 0.1264(2)$ which is less than the value defined by universality class of the problem. They call it as an unconventional critical exponent.

It is a well known fact that the critical exponents depend on factors like dimension of the system, range of the interaction and spin dimension.

Contrary to the system we have in this manuscript, Trapin *et al* only consider a one dimensional chain with nearest-neighbour interaction, this can cause a difference in the value of α that we calculate. Attempts were made to find universality and scaling for DQPTs for one and two dimensional systems [A164]. For 1d system the exponent α is reported to be 1. A recent work by Bandyopadhyay *et al.* [A165] outlines a protocol based on out of time order correlations(OTOC) and string-like observables to experimentally determine the critical exponents of DQPT. Using the method they show a universal scaling critical exponent for one dimensional systems to be $\alpha = 1$. But for 2D systems the analysis in [A164] could not find a conclusive value for α in general.Nonetheless we may still calculate α for our system using the method discussed by Trapin *et al.*. Let $t - t_c$ denote a nonanalytic point. We can approximate the rate function $\mathscr{L}(t)$ around the nonanalyticity as follows,

$$|\mathscr{L}(t) - \mathscr{L}_c| \sim |t - t_c|^{\alpha}. \tag{A.1}$$

Taking logarithm on both sides of Eq. (A.1) gives us the equation of a straight line with slope α.

Consider $\Delta t = t - t_c$ and $\Delta\mathscr{L} = \mathscr{L}(t) - \mathscr{L}_c$. We plot $\ln(|\Delta\mathscr{L}|)$ versus $\ln(|\Delta t|)$ and fit it to a straight line that best fits. The slope of the straight line is the exponent α. Let us consider the nonanalytic point in Fig. A.1(A) which is around $t_c = 43.24$. This region is highlighted in Fig. A.1(B). Now if we plot $\ln(|\Delta\mathscr{L}|)$ versus $\ln(|\Delta t|)$ and fit a straight line as shown in Fig. A.1(C), the exponent α at $t_c = 43.24$ is determined to be 0.4883 ± 0.0218 with this method. The critical exponent α turned out to be similar for other t_c values as well, *e. g.,* $\alpha = 0.7020 \pm 0.0233$ for $t_c = 9.66$.

Since we have computational limitations in our model to look for different system sizes, to accommodate for the finite size effect we consider the skyrmion model proposed by Siegl *et.al* [A144].

Consider an $n \times n$ lattice of quantum spin-1/2's coupled to classical ferromagnetic control fields at its boundary. The Hamiltonian of the system is given as,

$$\begin{aligned}\hat{H} = \; & -J \sum_{\langle i,j\rangle} (S_i^x S_j^x + S_i^y S_j^y) - \Delta \sum_{\langle i,j\rangle} S_i^z S_j^z \\ & -D \sum_{\langle i,j\rangle} (\mathbf{u_{ij}} \times \hat{z}).\left(\mathbf{S}_i \times \mathbf{S}_j\right), \end{aligned} \tag{A.2}$$

with ferromagnetic exchange constant $J > 0$, axial Heisenberg anisotropy $\Delta > 0$, and the strength of DMI interaction D. $\mathbf{u_{ij}}$ is a vector pointing from $\mathbf{S_i}$ to $\mathbf{S_j}$. $\hat{\mathbf{S}}_\mathbf{i} = (S_i^x, S_i^y, S_i^z)$ is a vector of spin operators for spins within the $n \times n$ lattice. A layer of classical ferromagnetic spins $S_i = \frac{\hbar}{2}\hat{z}$ resides outside the lattice.

Further in order to define a skyrmion we utilize the following quantities.

$$\left.\begin{matrix} Q \\ \\ C \end{matrix}\right\} = \frac{1}{2\pi} \sum_{\sigma} \tan^{-1}\left(\frac{\mathbf{n}_i(\mathbf{n}_j \times \mathbf{n}_k)}{1 + \mathbf{n}_i\mathbf{n}_j + \mathbf{n}_i\mathbf{n}_k\mathbf{n}_k\mathbf{n}_j}\right), \tag{A.3}$$

where the sum runs over all the elementary triangles formed by nearest-neighbour lattice sites i, j, k which include the classical ferromagnetic boundary sites as well and no two triangles overlap. The magnitude of the winding parameter Q quantifies the stability of the skyrmion. It is computed with $\mathbf{n_i} = 2\langle \mathbf{S}_i \rangle \hbar$, where $\langle \mathbf{S}_i \rangle = (\langle S_i^x \rangle, \langle S_i^y \rangle, \langle S_i^z \rangle)$ is the classical magnetic moment or spin expectation value. The topological index C takes $\mathbf{n_i} = \langle \mathbf{S_i} \rangle / |\langle \mathbf{S_i} \rangle|$. $C = \pm 1$ for quantum skyrmions.

For a 3×3 lattice when $\Delta = 0.5J$ and $D = 2J$ we identified a quantum skyrmion phase with $C = -1$ and $Q = -0.981$. We note that parameters $\Delta = 0.5J$ and $D = 0$ give a quantum ferromagnet with $C = 0$ and $Q = 0$. Fig. A.2(A) shows the rate function and the calculation of critical exponent for this case. The critical exponent in this case is calculated to be 0.5020 ± 0.0240. Similar observations were done with 4×4 lattice case also, where parameters $\Delta = 0.5J$ and $D = 2J$ get a skyrmion phase with $C = -1$ and $Q = -0.981$. $D = 0$ gives a ferromagnetic ground state with $C = 0$ and $Q = 0$. We initiate the system from the skyrmion phase and at $t = 0$ we quench the system by setting $D = 0$. The results are summarised in Fig. A.2(B). The critical exponent in this case is found to be 0.5667 ± 0.02878.

Next, we investigate DQPT on another 2d model considering a triangular lattice within a circle with ferromagnetic classical boundaries having the following Hamiltonian,

$$\begin{aligned}\hat{H} = \quad & -J_1 \sum_{\langle i,j \rangle} (S_i^x S_j^x + S_i^y S_j^y) - K \sum_{\langle i,j \rangle} S_i^z S_j^z \\ & +\mathbf{D_1} \sum_{\langle i,j \rangle} \left(\mathbf{S}_i \times \mathbf{S}_j\right),\end{aligned} \tag{A.4}$$

Here $J_1 > 0$ is the nearest-neighbour ferromagnetic coupling constant, $K > 0$ is the axial Heisenberg anisotropy coefficient and $D_1 > 0$ is the strength of the DMI vector $\mathbf{D_1}$. The direction of DMI is the same as the one shown in Fig. 2.1 . $\hat{\mathbf{S}}_\mathbf{i} = (S_i^x, S_i^y, S_i^z)$ is a vector of spin operators for spins within the circular triangular lattice. A layer of classical ferromagnetic spins $S_i = \frac{\hbar}{2}\hat{z}$ resides outside the lattice. We make use of the quantities Q and C to identify quantum skyrmions here also.

In a 7-spin triangular lattice case with circular boundary for $J_1 = 1$, $K = 0.61 J_1$ and $D_1 = 2J_1$ we see a skyrmion phase with $C = 1$ and $Q = 0.993$. In the same configuration $D_1 = 0$ gives a ferromagnetic phase with $C = 0$ and $Q = 0$. We initiated the system at the skyrmion phase and quenched it to a ferromagnetic phase by setting $D_1 = 0$ at $t = 0$. The resulting rate function is shown in Fig. A.3. The critical exponent calculated is 0.6130 ± 0.0191 at $t_c = 43.58$.

We observed DQPT in various systems with different geometry and interactions around the same time domain $43.24 < t_c < 45.44$ with system sizes 7, 9, 16, 19 and the critical exponents for respective sizes are 0.6130 ± 0.0191, 0.5020 ± 0.0240, 0.5667 ± 0.02878

and 0.4883 ± 0.0218. This is shown in Fig. A.4. In the all cases we find the exponents around 0.5, which hints a universality in skyrmion to ferromagnetic state DQPT.

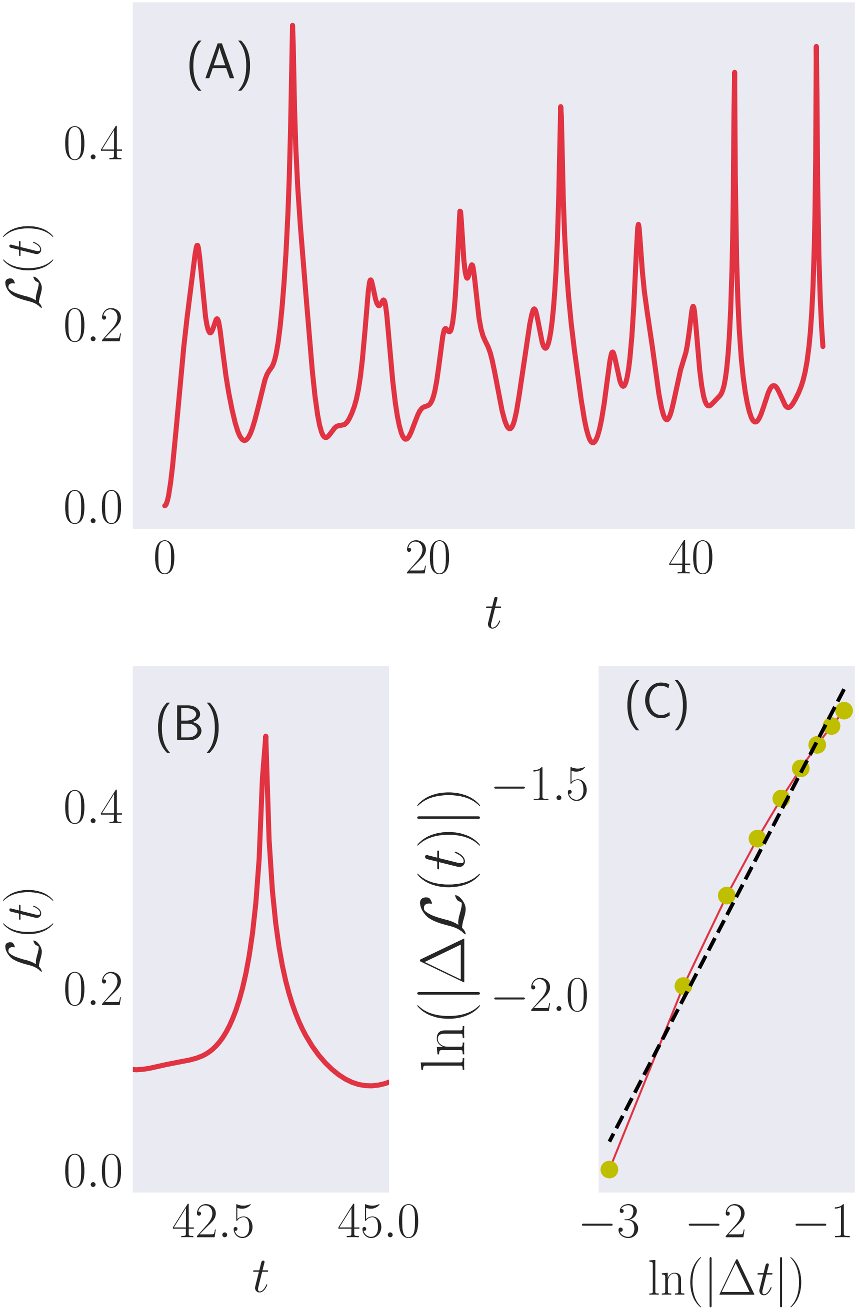
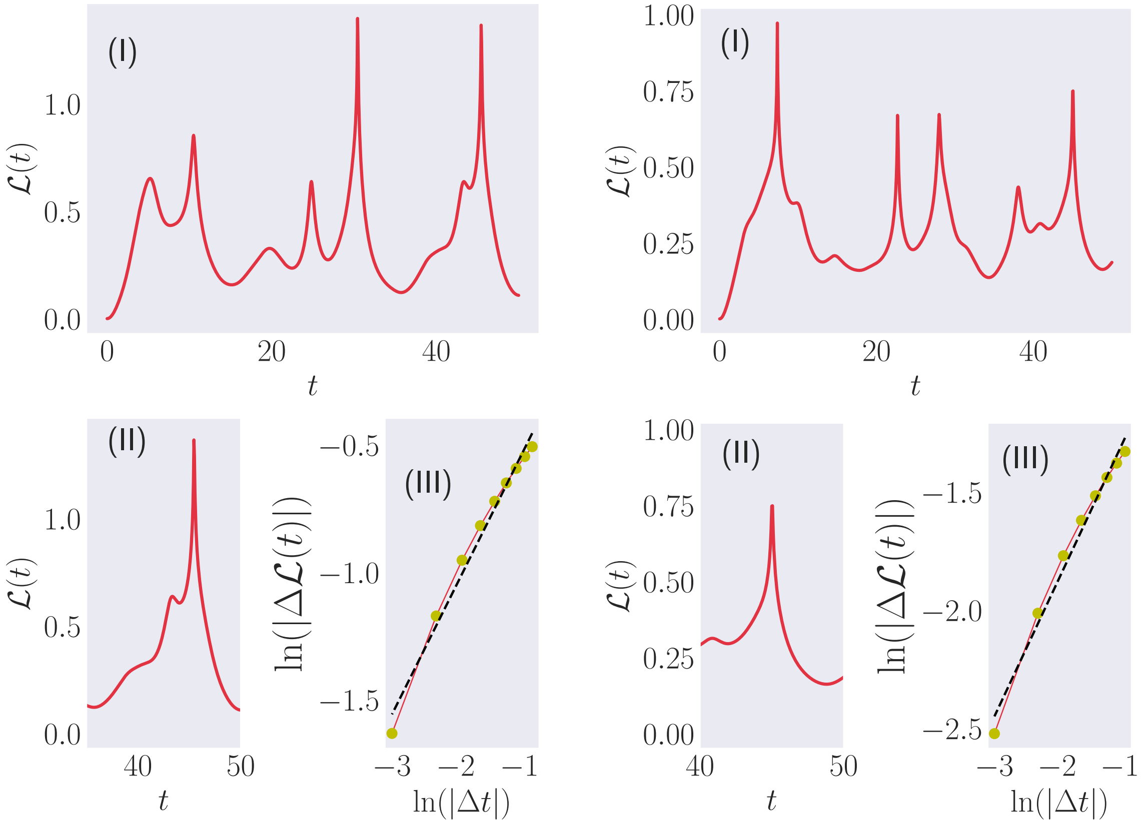


Fig. A.1 **How to calculate critical exponent associated to a nonanalyticity.** (A) Rate function showing nonanalyticity. (B) Zoomed in on the first nonanalytic point at $t \sim 43.24$. (C) $\ln(|\Delta\mathscr{L}|)$ vs. $\ln(|\Delta t|)$: Red line with green dots is observed data, black dashed line is the straight line approximation.



(A) (B)

Fig. A.2 **(A) Critical exponent in DQPT of a** 3×3 **square lattice.** (I) Rate function showing nonanalyticity. (II) Zoomed in on a nonanalytic point at $t \sim 45.44$. (III) $\ln(|\Delta\mathscr{L}|)$ vs. $\ln(|\Delta t|)$: Red line with green dots is observed data, black dashed line is the straight line approximation. **(B) Critical exponent in DQPT of a** 4×4 **square lattice.** (I) Rate function showing nonanalyticity. (II) Zoomed in on a nonanalytic point at $t \sim 45$. (III) $\ln(|\Delta\mathscr{L}|)$ vs. $\ln(|\Delta t|)$: Red line with green dots is observed data, black dashed line is the straight line approximation.

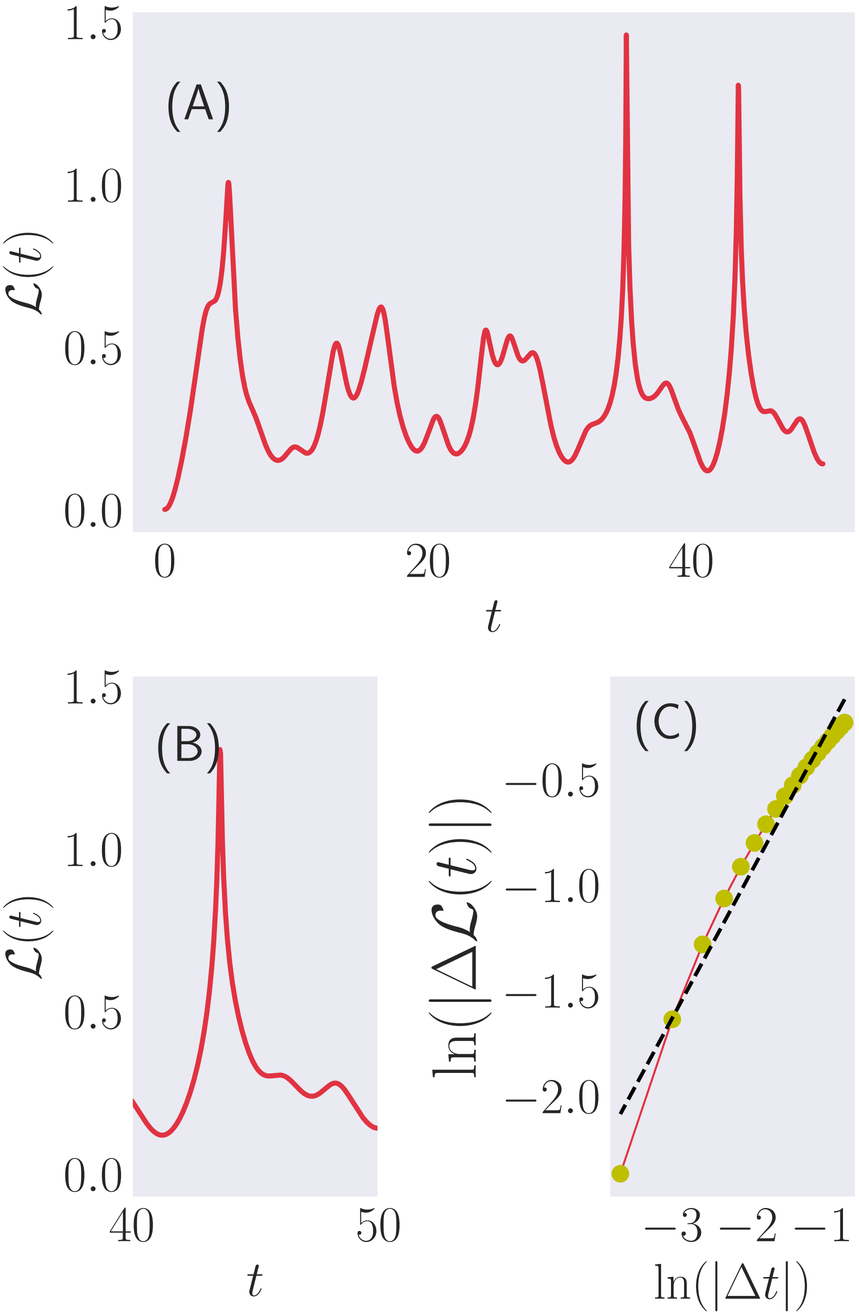


Fig. A.3 **Nonanalytic rate function and the calculation of exponent for a 7-spin triangular lattice.** (A) Rate function is showing nonanalyticity. (B) Zoomed in on nonanalytic point at $t \sim 43.58$. (C) $\ln(|\Delta\mathscr{L}|)$ vs. $\ln(|\Delta t|)$: Red line with green dots is observed data, black dashed line is the straight line approximation.

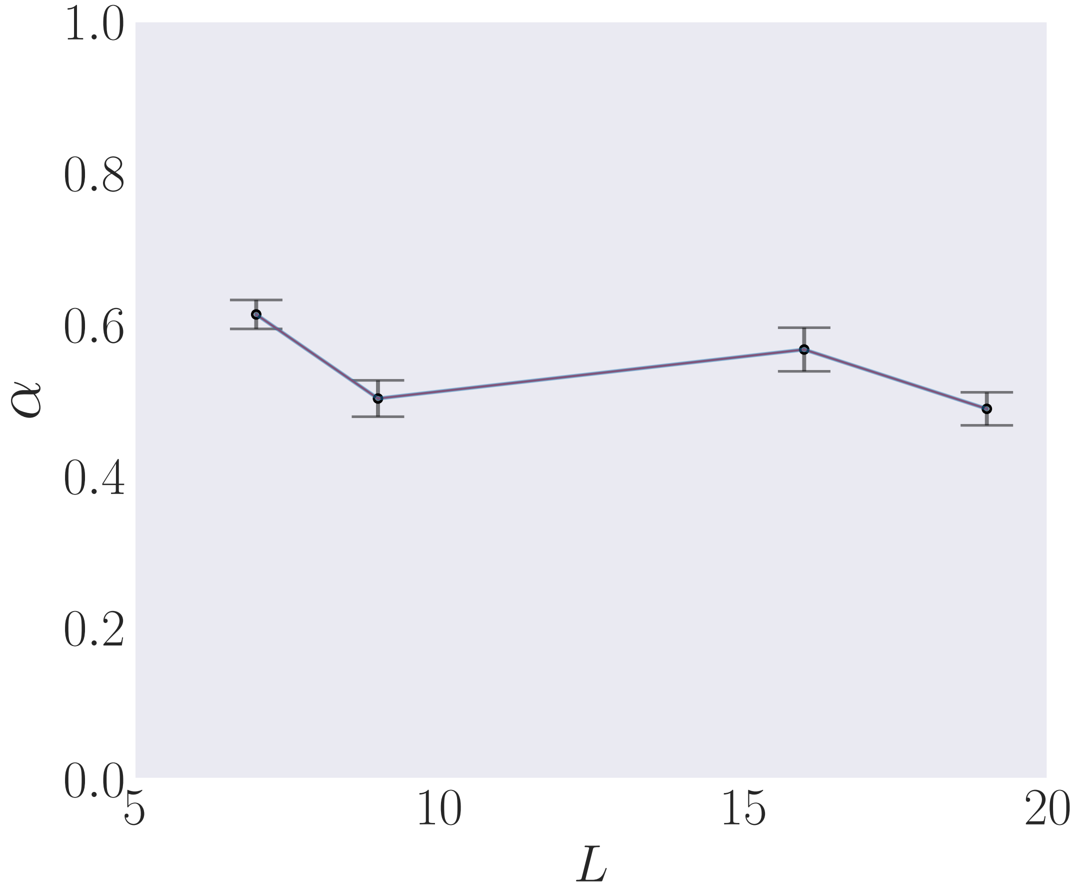


Fig. A.4 Critical exponents α in DQPT of three similar 2d models vs. system size L around the same time domain $43.24 < t_c < 45.44$. All the cases show a universal exponent around 0.5.