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WORK FLUCTUATION AND IRREVERSIBLE ENTROPY IN
A QUENCHED XY HEISENBERG MAGNET

by

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CERTIFICATION

This is to certify that this master's thesis entitled, “***WORK FLUCTUATION AND IRREVERSIBLE ENTROPY IN A QUENCHED XY HEISENBERG MAGNET***” and submitted by **Francis A. Bayocboc, Jr.** to fulfill part of the requirements for the degree of Master of Science in Physics was successfully defended and approved on 23 May 2015.

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ABSTRACT

WORK FLUCTUATION AND IRREVERSIBLE ENTROPY IN A QUENCHED XY HEISENBERG MAGNET

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In this thesis, we study the emergent thermodynamics associated with an arbitrary quench in the Heisenberg XY model by calculating the work fluctuation and the irreversible entropy produced. For the fluctuation in the work done, an exact expression is obtained and is shown to exhibit non-analytic behavior as the pre-quench transverse field and anisotropy parameter cross quantum critical points. On the other hand, the irreversible entropy is obtained by calculating the difference between the average work done and an effective free energy change. We emphasize on the effect of the anisotropy parameter on the irreversible entropy, adding to previous works done on the Transverse Field Ising Model.

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Chapter 1

Introduction

In this thesis, we study the emergent thermodynamics associated with an instantaneous changing of a parameter of a many-body system referred to as a quantum quench. The term "quantum quench" was coined by Calabrese and Cardy [2] in 2006 to describe an instantaneous change of a system's Hamiltonian parameters, such as magnetic field, and was first studied theoretically by Altman and Auerbach in 2002 [3] and by Sengupta et al. in 2004 [4]. A many-body system is prepared in an eigenstate (usually the groundstate) of the initial Hamiltonian $H(\lambda_0)$ with parameter λ_0 . The Hamiltonian parameter is then changed from λ_0 to λ_1 in a time scale much smaller than the response time of the system to the variation. This quenching of parameters takes the system out of equilibrium and the evolution of the system is dictated by the new Hamiltonian $H(\lambda_1)$. Interesting situations are encountered when the parameter quench are done across critical points, when universal phenomena [5–7], quantum revivals [8–10], and singular behavior may be observed [11–14].

These quantum quenches may also be interpreted as an irreversible thermodynamic process for a many-body quantum system. It is then natural to characterize quench protocols by thermodynamic quantities such as the work done on the system after an instantaneous change of parameters. In general, the state of an isolated system immediately after a quench is an excited state

of the post-quench Hamiltonian and unlike in quasistatic processes, measurements of the system energy after a quench may not be the same. This results in a work done that has statistical fluctuation over different measurements and is described by a probability distribution function $p(W)$. In this thesis, the more accessible characteristic function of the probability density which takes the form of a two-time correlator [15, 16] will be calculated. The statistics of work done, i.e. average work done and fluctuations in the work done, is given by the cumulants of the probability density function. For quench protocols that are done at finite temperatures, the average work done can be related to a dissipated work or an irreversible entropy by using the Jarzynski equality [17]. This irreversible entropy is a measure of the irreversibility of the protocol. Calculations of the emergent thermodynamics after a quantum quench has been studied before such as the work statistics [11] and the irreversible entropy [12] after a field quench in the quantum Ising model, the statistics of work done in quenches in the normal phase Dicke model [18], universal scaling after quenches near a quantum critical point in the sine-Gordon model [19, 20], and the work statistics across quantum critical points in the Heisenberg XYZ model [21].

Recently, an experimental measurement of the irreversible entropy was done for an isolated spin system. This was proposed as a physical quantity that may be used to establish the thermodynamic arrow of time in quantum systems [22]. This measurement is based on interferometric measurements proposed and implemented in quantum systems by the groups of Dorner and Batalhão [23, 24]. Using ^{13}C atoms in a chloroform molecule liquid sample, Batalhão et al. realized a nuclear spin-1/2 system that is initially prepared in a thermal state at inverse temperature β . For the forward process, the system is quenched by a transverse time-modulated radio-frequency field from an initial state of the initial Hamiltonian H_0 . On the other hand, for the backward process, the system is driven by a time reversed Hamiltonian from an equilibrium state of the final Hamiltonian H_1 . The work probability distri-

bution for the forward and backward processes were measured by employing NMR spectroscopy and Ramsey-like interferometric scheme [23, 24]. The irreversibility of the process is then calculated by the using the Tasaki-Crooks fluctuation relation [16, 25, 26]

The specific physical system that will be studied in this thesis is described by the Heisenberg XY model in a transverse magnetic field h with anisotropy parameter γ . This anisotropy parameter is a measure of the difference in the spins states' interactions in the x - and y -directions. The transverse field and anisotropy parameters are the quenching parameters. The XY model was first introduced by Lieb, Schultz, and Mattis [27] to describe antiferromagnetism for linear spin chains with nearest-neighbor interactions. Aside from Lieb et al., the model was also solved extensively by Barouch et al. in [28, 29] where the Liouville equation was solved exactly and the spin correlators were studied. The eigenstate, partition function, specific heat, and susceptibility was also solved by Katsura [30]. The Heisenberg XY model is a quantum critical model which also contains the quantum Ising model. The phase diagram of this model is characterized by two Quantum Phase Transitions (QPT): the QPT that belongs to the universality class of the One-Dimensional Quantum Ising Model and that of the universality class of the critical Heisenberg spin (XX model) [31].

Although many studies have been done regarding quantum quenches in the full Heisenberg XY model, none of these works have considered an extensive analysis of the statistics of work done. These works have focused on the dynamics of the correlation functions [2, 32], Loschmidt echo [6, 9], defect production [33, 34], and entanglement measures [9, 35] after a quench in the XY model. Also, previous works on the statistics of work done have been performed only for field quenches along the Ising line of the XY model [11, 12]. This thesis aims to calculate an exact expression for the work statistics in a quantum critical model. Specifically, this work investigates the effects of the anisotropy parameter on the fluctuation of work done and on the irre-

versible entropy produced. Accordingly, this work completes the study of the statistics of work done of quenches in the full parameter space of the XY model.

This thesis is divided into chapters. An outline of the diagonalization of the XY Hamiltonian by three consecutive transformations: Jordan-Wigner, Fourier, and Bogolyubov, together with the calculation of the characteristic function from the probability distribution is presented in Chapter 2. The analysis of the quantum quench in the XY model is presented in Chapter 3 where calculation of the statistics of work done, i.e. average work done and work fluctuations, from the characteristic function $G(u)$ of the probability distribution function $p(W)$ of the work is done. Calculation of the average work done for an arbitrary quench at finite temperature is presented in Chapter 4 together with analyses of the irreversible entropy ΔS_{irr} produced during specific quench protocols. A summary of major results ends this thesis.

Chapter 2

Theoretical Background

2.1 The XY model

The spin- $\frac{1}{2}$ XY model was proposed by Lieb, Schultz, and Mattis in 1961 [27] to describe antiferromagnetism for linear spin chains, with each spin interacting only with its nearest neighbor. For a chain of N spin- $\frac{1}{2}$ particles in a transverse magnetic field h , the quantum mechanical Hamiltonian of the XY model is given by

$$H = -\frac{J}{2} \sum_{j=1}^N \left[\left(\frac{1+\gamma}{2} \right) \sigma_j^x \sigma_{j+1}^x + \left(\frac{1-\gamma}{2} \right) \sigma_j^y \sigma_{j+1}^y + h \sigma_j^z \right]. \quad (2.1)$$

Here J is the energy-scale parameter, σ_j^α , with $\alpha = x, y, z$, are the spin Pauli matrices describing the spin operators at site j of the one-dimensional spin lattice, and γ is the parameter characterizing the difference in spin interactions along the x and the y axes. For positive values of J , the system is ferromagnetic; otherwise, the system is antiferromagnetic. Periodicity is imposed to the model: $\sigma_{N+1}^\alpha = \sigma_1^\alpha$. For $\gamma = 0$, the XY model reduces to the isotropic XX model; while for $\gamma = 1$, the one-dimensional Transverse Field Ising model is recovered.

The phase diagram of the XY model is parametrized by the anisotropy strength γ and the transverse magnetic field strength h , with symmetries $\gamma \rightarrow -\gamma$ and $h \rightarrow -h$. At zero temperature, the phase diagram is characterized by

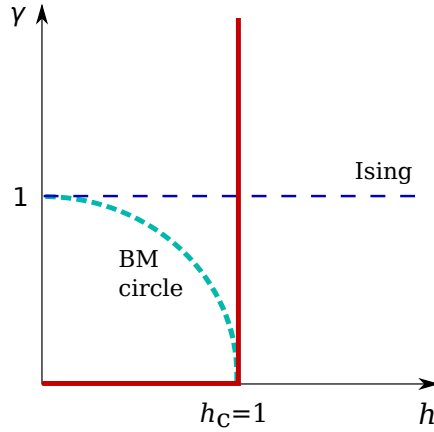


Figure 2.1: Phase diagram of the XY model. Red solid lines are critical lines, γ is the anisotropy parameter, and h is the transverse magnetic field. The horizontal dashed line corresponds to the quantum Ising model and the dashed circular curve is the Barouch-McCoy circle where the ground state is a product state of localized spin states [1].

two Quantum Phase Transitions. The first one belongs to the universality class of the isotropic XX model at anisotropy $\gamma = 0$ and magnetic field $|h| < 1$. This is a line that separates strong ferromagnetic order in the x -direction ($\gamma > 0$) and in the y -direction ($\gamma < 0$). The other one belongs to the universality class of the one-dimensional Transverse Ising model at magnetic field $|h| = 1$. This is a transition from a region of ferromagnetic order ($|h| < 1$) to a region of paramagnetic order ($|h| > 1$). At these two phase transitions, the energy spectrum of the XY model is gapless [31, 36].

2.1.1 Diagonalization of the Hamiltonian

Diagonalization of the ferromagnetic XY Hamiltonian was first carried out by Lieb et al. in 1961 [27] for the case of zero magnetic field and by Niemeijer in 1967 [37] for the case where a magnetic field along the z axis is present. The diagonalization involves a succession of transformations of the Hamiltonian in Eq. (2.1) to spinless fermionic operators, to momentum space operators, and to quasi-particle fermionic operators. We shall consider the ferromagnetic

case and set $J = 1$:

$$H = -\frac{1}{2} \sum_{j=1}^N \left[\left(\frac{1+\gamma}{2} \right) \sigma_j^x \sigma_{j+1}^x + \left(\frac{1-\gamma}{2} \right) \sigma_j^y \sigma_{j+1}^y + h \sigma_j^z \right]. \quad (2.2)$$

The first transformation involves a mapping from spin operators σ_j to spinless fermionic operators ψ_l by means of a Jordan-Wigner transformation given by

$$\sigma_j^+ = \prod_{l=1}^{j-1} (1 - 2\psi_l^\dagger \psi_l) \psi_j \quad \sigma_j^- = \prod_{l=1}^{j-1} (1 - 2\psi_l^\dagger \psi_l) \psi_j^\dagger. \quad (2.3)$$

The spin operators σ_j^\pm are called the raising (lowering) operators and the spinless fermionic operator ψ_l follows the usual anti-commutation rule

$$\begin{aligned} \{\psi_\alpha, \psi_\beta^\dagger\} &= \delta_{\alpha\beta} \\ \{\psi_\alpha, \psi_\beta\} &= \{\psi_\alpha^\dagger, \psi_\beta^\dagger\} = 0, \end{aligned}$$

where anti-commutation is given by $\{A, B\} = AB + BA$. In terms of the raising and lowering operators σ^\pm , the x -, y -, and z -Pauli spin matrices at site j are given by

$$\sigma_j^x = \sigma_j^+ + \sigma_j^- \quad i\sigma_j^y = \sigma_j^+ - \sigma_j^- \quad \sigma_j^z = [\sigma_j^+, \sigma_j^-], \quad (2.4)$$

where the commutation is defined as $[A, B] = AB - BA$. The Hamiltonian in terms of the raising and lowering operators is

$$H = -\frac{1}{2} \sum_{j=1}^N \left[\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+ + \gamma (\sigma_j^+ \sigma_{j+1}^+ + \sigma_j^- \sigma_{j+1}^-) + h [\sigma_j^+, \sigma_j^-] \right]. \quad (2.5)$$

Substituting the Jordan-Wigner transforms in Eq. (2.3) reformulates the Hamiltonian in terms of the spinless fermion operators ψ_j

$$\begin{aligned} H = & -\frac{1}{2} \sum_{j=1}^{N-1} \left(\psi_j^\dagger \psi_{j+1} + \psi_{j+1}^\dagger \psi_j + \gamma \psi_j^\dagger \psi_{j+1}^\dagger + \gamma \psi_{j+1} \psi_j \right) + h \sum_{j=1}^N \psi_j^\dagger \psi_j - \frac{hN}{2} \\ & + \prod_{j=1}^N \frac{(1 - 2\psi_j^\dagger \psi_j)}{2} \left(\psi_N^\dagger \psi_1 + \psi_1^\dagger \psi_N + \gamma \psi_N^\dagger \psi_1^\dagger + \gamma \psi_1 \psi_N \right). \quad (2.6) \end{aligned}$$

The Hamiltonian in equation (2.6) is quadratic in operators ψ_j . The coefficient $\prod_{j=1}^N (1 - 2\psi_j^\dagger \psi_j)/2$ in the second line of the Hamiltonian in equation (2.6) distinguishes the two sectors of the theory, namely, the model with even and odd number of particles N . For even N , the value of the coefficient is $+1$, while -1 for odd N . With this configuration, the appropriate boundary condition for an even numbered model is antiperiodic while periodic for odd numbered model:

$$\begin{aligned}\psi_{j+N} &= -\psi_j && \text{if } N = \text{even} \\ \psi_{j+N} &= \psi_j && \text{if } N = \text{odd},\end{aligned}$$

We should note that the effect of the boundary terms (second line of equation (2.6)) or the effect of the parity of the number of particles in the model is negligible when we consider calculations in the thermodynamic limit in the next chapter. The Hamiltonian can be written as

$$H = -\frac{1}{2} \sum_{j=1}^N \left(\psi_j^\dagger \psi_{j+1} + \psi_{j+1}^\dagger \psi_j + \gamma \psi_j^\dagger \psi_{j+1}^\dagger + \gamma \psi_{j+1} \psi_j - 2h \psi_j^\dagger \psi_j \right) - \frac{hN}{2} \quad (2.7)$$

while taking note of the parity of N and the appropriate boundary conditions. From this point forward, we shall consider the case of odd numbered model.

We will now perform a mapping of the model from real space to momentum space by means of a symmetric Fourier transform given by

$$\psi_j = \frac{e^{i\pi/4}}{\sqrt{N}} \sum_{q=0}^{N-1} e^{i\frac{2\pi}{N}qj} \phi_q \quad j = 1, \dots, N, \quad (2.8)$$

$$\phi_q = \frac{e^{-i\pi/4}}{\sqrt{N}} \sum_{j=1}^N e^{-i\frac{2\pi}{N}qj} \psi_j \quad q = 1, \dots, N-1, \quad (2.9)$$

where q is the momentum associated with the particle at site j . Note that the operators ϕ_q follow the anticommutation relation

$$\{\phi_q^\dagger, \phi_{q'}\} = \delta_{qq'}, \quad (2.10)$$

and it can be easily seen that $\phi_q^\dagger \phi_q = \phi_{-q}^\dagger \phi_{-q}$. The products of the real space operators ψ_j are given in terms of the momentum space operators ϕ_q by

$$\sum_{j=1}^N \psi_j^\dagger \psi_{j+1} = \sum_{q=0}^{N-1} e^{i\frac{2\pi}{N}q} \phi_q^\dagger \phi_q, \quad \sum_{j=1}^N \psi_{j+1}^\dagger \psi_j = \sum_{q=0}^{N-1} e^{-i\frac{2\pi}{N}q} \phi_q^\dagger \phi_q, \quad (2.11)$$

$$\sum_{j=1}^N \psi_j^\dagger \psi_{j+1}^\dagger = -i \sum_{q=0}^{N-1} e^{-i\frac{2\pi}{N}q} \phi_{-q}^\dagger \phi_q^\dagger, \quad \sum_{j=1}^N \psi_{j+1} \psi_j = i \sum_{q=0}^{N-1} e^{i\frac{2\pi}{N}q} \phi_q \phi_{-q}, \quad (2.12)$$

and $\sum_j \psi_j^\dagger \psi_j = \sum_q \phi_q^\dagger \phi_q$. Note that we have used the identity

$$\sum_{j=0}^N e^{i\frac{2\pi}{N}j(q-q')} = N\delta_{q,q'}. \quad (2.13)$$

The Hamiltonian in momentum space is

$$H = \frac{1}{N} \sum_{q=0}^{N-1} \left\{ \phi_q^\dagger \phi_q \left[h - \cos\left(\frac{2\pi}{N}q\right) \right] + \frac{\gamma}{2} \sin\left(\frac{2\pi}{N}q\right) [\phi_q \phi_{-q} + \phi_{-q}^\dagger \phi_q^\dagger] \right\} - \frac{hN}{2}. \quad (2.14)$$

The mapping from an interacting theory to a non-interacting one will be done by means of a Bogolyubov transformation given by

$$\phi_q = \chi_q \cos \theta_q + \chi_{-q}^\dagger \sin \theta_q, \quad (2.15a)$$

$$\phi_{-q}^\dagger = -\chi_q \sin \theta_q + \chi_{-q}^\dagger \cos \theta_q, \quad (2.15b)$$

where $\chi_{\pm q}$ are fermionic quasi-particle operators. We can think of the transformation given by equations (2.15) as just a rotation of the operators $\phi_{\pm q}$ by an angle θ_q given by

$$\tan(2\theta_q) = \frac{\gamma \sin(\frac{2\pi}{N}q)}{h - \cos(\frac{2\pi}{N}q)}. \quad (2.16)$$

Substituting equations (2.15) to the Hamiltonian in equation (2.14) and using the Bogolyubov angle expression in equation (2.16) to remove the off-diagonal terms gives us the final form of the Hamiltonian in terms of the quasi-particle fermionic operators $\chi_{\pm q}$:

$$H = \sum_{q=0}^{N-1} \epsilon(q) \left\{ \chi_q^\dagger \chi_q - \frac{1}{2} \right\}. \quad (2.17)$$

$\epsilon(q)$ is the energy spectrum of the XY model given by

$$\epsilon(q) = \sqrt{\left[h - \cos\left(\frac{2\pi q}{N}\right)\right]^2 + \gamma^2 \sin^2\left(\frac{2\pi q}{N}\right)}. \quad (2.18)$$

The energy spectrum $\epsilon(q)$ of the model becomes gapless at the phase transition given by the critical magnetic field line at $|h| = 1$ and by the XX line at $\gamma = 0$ and $|h| < 1$.

2.1.2 Ground state and Partition function

The lowest energy state of the model is a state with no quasi-particle:

$$\chi_q |\Psi_0\rangle = 0, \quad (2.19)$$

when we let an annihilation operator act on the state $|\Psi_0\rangle$, the product would be zero since there is no quasi-particle to annihilate to begin with. Thus, the ground state energy is given by

$$E_{\text{GS}} = -\frac{1}{2} \sum_{q=0}^{N-1} \epsilon(q). \quad (2.20)$$

In terms of the spinless fermions, the ground state $|\Psi_0\rangle$ is given by

$$|\Psi_0\rangle = \prod_{q=0}^{N-1} (\cos \theta_q + \sin \theta_q \phi_q^\dagger \phi_{-q}^\dagger) |0_q, 0_{-q}\rangle, \quad (2.21)$$

where $|0_q, 0_{-q}\rangle$ is a state with no physical fermions.

For a system with fixed number of particles and is at thermal equilibrium with a heat bath of temperature T , the canonical partition function is given by

$$\mathcal{Z} = \text{Tr} e^{-\beta H} = \sum_n e^{-\beta E_n}, \quad (2.22)$$

where $\beta = 1/k_B T$ is the inverse temperature, k_B is the Boltzmann constant, and H is the Hamiltonian of the system. The sum in the second equality is a sum over all eigenstates n with corresponding energy E_n .

The eigenstates of the Hamiltonian in equation (2.17) are $|0_q\rangle$ which corresponds to unoccupied state q and $|1_q\rangle$ which corresponds to an occupied state q in momentum space. Thus, the partition function becomes

$$\begin{aligned}\mathcal{Z} &= \sum_{n=0,1} \langle n_q | \exp \left\{ -\beta \sum_{q=0}^{N-1} \epsilon(q) \left[\chi_q^\dagger \chi_q - \frac{1}{2} \right] \right\} | n_q \rangle \\ &= \prod_{q=0}^{N-1} \sum_{n=0,1} \exp \left\{ -\beta \epsilon(q) \left[n - \frac{1}{2} \right] \right\}.\end{aligned}$$

The summation over n becomes a hyperbolic cosine and the final form of the partition function is

$$\mathcal{Z} = 2^N \prod_{q=0}^{N-1} \cosh \left[\frac{\beta \epsilon(q)}{2} \right]. \quad (2.23)$$

2.2 Probability distribution function

In this section, we shall consider the probability distribution function of the work done by a time-dependent Hamiltonian. We shall follow a derivation due to Talker et al. [15].

Calculation of the work done by an external force involves two measurements of the system energy: the energy of the initial state at $t = 0$ and the energy after some time t_f . A system is prepared in a thermal state described by a density matrix

$$\rho(0) = \frac{e^{-\beta H(0)}}{\mathcal{Z}(0)}, \quad (2.24)$$

where $H(0)$ is the Hamiltonian at $t = 0$, β is the reciprocal temperature, and $\mathcal{Z}(0) = \text{Tr} \exp[-\beta H(0)]$. A measurement of the energy of the initial state would give the eigenvalue E_n of $H(0)$. The probability of getting E_n is given by

$$p_n = \frac{e^{-\beta E_n}}{\mathcal{Z}(0)}. \quad (2.25)$$

After this measurement, the state is now found at the corresponding eigenstate $|\varphi_n\rangle$ of $H(0)$ satisfying $H(0)|\varphi_n\rangle = E_n|\varphi_n\rangle$. The state $|\varphi_n\rangle$ would

then evolve according to

$$|\tilde{\varphi}(t)\rangle = U(t)|\varphi_n\rangle \quad (2.26)$$

where the evolution operator $U(t)$ is due to the Hamiltonian $H(t)$. A second measurement at time t_f would then yield an eigenvalue $|\tilde{E}_m\rangle$ with corresponding eigenstate $|\tilde{\varphi}_m\rangle$ of $H(t_f)$. The probability of measuring $|\tilde{E}_m\rangle$ is given by

$$\begin{aligned} p_{m|n} &= |\langle \tilde{\varphi}_m | \varphi(t_f) \rangle|^2 \\ &= |\langle \tilde{\varphi}_m | [U(t_f)|\varphi_n\rangle]|^2. \end{aligned} \quad (2.27)$$

Thus, the probability of measuring both E_n and \tilde{E}_m is given by

$$p_{m|n}p_n = |\langle \tilde{\varphi}_m | U(t_f)|\varphi_n\rangle|^2 \frac{e^{-\beta E_n}}{\mathcal{Z}(0)} \quad (2.28)$$

and the probability distribution function of the work done W is given by

$$\begin{aligned} p(W) &= \sum_{m,n} \delta(W - [\tilde{E}_m - E_n]) p_{mn} p_n \\ &= \sum_{m,n} \delta(W - (\tilde{E}_m - E_n)) |\langle \tilde{\varphi}_m | U(t_f)|\varphi_n\rangle|^2 \frac{e^{-\beta E_n}}{\mathcal{Z}(0)} \end{aligned} \quad (2.29)$$

where $\delta(W - (\tilde{E}_m - E_n))$ is the Dirac delta function. The characteristic function $G(u)$ is obtained by taking the Fourier transform of the probability distribution function (2.29):

$$\begin{aligned} G(u) &= \int dW e^{iuW} p(W) \\ &= \int dW e^{iuW} \sum_{m,n} \delta(W - (\tilde{E}_m - E_n)) |\langle \tilde{\varphi}_m | U(t_f)|\varphi_n\rangle|^2 \frac{e^{-\beta E_n}}{\mathcal{Z}(0)}. \end{aligned} \quad (2.30)$$

Using the property of dirac delta functions $\int f(x)\delta(x-a)dx = f(a)$, the

integral becomes

$$\begin{aligned}
G(u) &= \sum_{m,n} e^{iu(\tilde{E}_m - E_n)} |\langle \tilde{\varphi}_m | U(t_f) | \varphi_n \rangle|^2 \frac{e^{-\beta E_n}}{\mathcal{Z}(0)} \\
&= \sum_{m,n} e^{iu(\tilde{E}_m - E_n)} \langle \varphi_n | U^\dagger(t_f) | \tilde{\varphi}_m \rangle \langle \tilde{\varphi}_m | U(t_f) | \varphi_n \rangle \frac{e^{-\beta E_n}}{\mathcal{Z}(0)} \\
&= \sum_{m,n} \langle \varphi_n | U^\dagger(t_f) e^{iu\tilde{E}_m} | \tilde{\varphi}_m \rangle \langle \tilde{\varphi}_m | U(t_f) e^{-iuE_n} \frac{e^{-\beta E_n}}{\mathcal{Z}(0)} | \varphi_n \rangle. \quad (2.31)
\end{aligned}$$

By noting that $\exp(-iuH(0))|\varphi_n\rangle = \exp(-iuE_n)|\varphi_n\rangle$, $\exp(-iuH(t_f))|\tilde{\varphi}_m\rangle = \exp(-iu\tilde{E}_m)|\tilde{\varphi}_m\rangle$, and $\exp(-\beta H(0))|\varphi_n\rangle = \exp(-\beta E_n)|\varphi_n\rangle$, we can rewrite (2.31) in terms of the Hamiltonians $H(0)$ and $H(t_f)$:

$$\begin{aligned}
G(u) &= \sum_{m,n} \langle \varphi_n | U^\dagger(t_f) e^{iuH(t_f)} | \tilde{\varphi}_m \rangle \langle \tilde{\varphi}_m | U(t_f) e^{-iuH(0)} \frac{e^{-\beta H(0)}}{\mathcal{Z}(0)} | \varphi_n \rangle \\
&= \sum_n \langle \varphi_n | U^\dagger(t_f) e^{iuH(t_f)} \sum_m | \tilde{\varphi}_m \rangle \langle \tilde{\varphi}_m | U(t_f) e^{-iuH(0)} \rho(0) | \varphi_n \rangle,
\end{aligned}$$

where $\rho = \exp(-\beta H(0))/\mathcal{Z}(0)$ is the density matrix of the initial state. Because of the completeness of the eigenstates $|\tilde{\varphi}_m\rangle$'s, the summation over m becomes $\sum_m |\tilde{\varphi}_m\rangle \langle \tilde{\varphi}_m| = \mathbf{I}$. Thus, the characteristic function is given by

$$\begin{aligned}
G(u) &= \sum_n \langle \varphi_n | U^\dagger(t_f) e^{iuH(t_f)} U(t_f) e^{-iuH(0)} \rho(0) | \varphi_n \rangle \\
&= \text{Tr} \{ U^\dagger(t_f) e^{iuH(t_f)} U(t_f) e^{-iuH(0)} \rho(0) \}, \quad (2.32)
\end{aligned}$$

where the trace Tr is over the eigenstates $|\varphi_n\rangle$. Equation (2.32) can be written as

$$G(u) = \langle e^{iuH_H(t_f)} e^{-iuH(0)} \rangle, \quad (2.33)$$

where $\exp(iuH_H(t_f)) = U^\dagger(t_f) \exp(iuH(t_f)) U(t_f)$ is the operator $\exp(iuH(t_f))$ in the Heisenberg representation.

The logarithm of the characteristic function $G(u)$ is known as the cumulant generating function. This cumulant generating function $\ln G(u)$ can be expanded in terms of the cumulants κ_n :

$$\ln G(u) = \frac{iu}{1!} \kappa_1 + \frac{(iu)^2}{2!} \kappa_2 + \frac{(iu)^3}{3!} \kappa_3 + \cdots = \sum_{n=1}^{\infty} \frac{(iu)^n}{n!} \kappa_n. \quad (2.34)$$

The n^{th} cumulant of the probability distribution function $p(W)$ are calculated by repeated differentiation of the cumulant generating function:

$$\kappa_n = \frac{1}{i^n} \frac{\partial^n}{\partial u^n} \ln G(u) \Big|_{u=0}. \quad (2.35)$$

Chapter 3

Work Statistics

We will now consider the non-equilibrium process where the system is prepared in the ground state $|\Psi_0\rangle$ of the XY model Hamiltonian H_0 with transverse magnetic field strength h_0 and anisotropy strength γ_0 . The parameters h_0 and γ_0 are then suddenly changed to values h_1 and γ_1 , respectively, such that the time interval of the parameter switch is much smaller than the response time of the system. This process is called a quantum quench. This process takes the system out of equilibrium and the work done W after the quench is characterized by a probability distribution function (PDF) $p(W)$ because measurements of the system energy after the quench may not yield the same value [11, 18]. With $\rho(0) = 1$ for the ground state at zero temperature, the work probability distribution function $p(W)$ in equation (2.29) becomes

$$p(W) = \sum_n \delta(W - (\tilde{E}_n - E_0)) |\langle \tilde{\Psi}_n | \Psi_0 \rangle|^2, \quad (3.1)$$

where E_0 is the energy of the initial (ground) state $|\Psi_0\rangle$ and \tilde{E}_n 's are the eigenenergies of the eigenstates $|\tilde{\Psi}_n\rangle$ of the final Hamiltonian H_1 with post-quench transverse field h_1 and post-quench anisotropy parameter γ_1 .

3.1 Characteristic function

For a quantum system with a sudden switch of Hamiltonian from H_0 to H_1 , the evolution operator $U(t)$ in equation (2.33) becomes $U(t) = 1$ [15]. Thus, the associated characteristic function $G(u)$ of the work PDF (3.1) for an arbitrary quench in the XY model is given by

$$G(u) = \langle e^{iuH_1} e^{-iuH_0} \rangle. \quad (3.2)$$

The quantum average appearing in equation (3.2) is evaluated with respect to the ground state $|\Psi_0\rangle \equiv |\Psi_{0,q}, \Psi_{0,-q}\rangle$ of the initial Hamiltonian H_0 at zero temperature:

$$G(u) = \langle \Psi_0 | e^{iuH_1} e^{-iuH_0} | \Psi_0 \rangle. \quad (3.3)$$

Since $|\Psi_0\rangle$ is an eigenstate of the initial Hamiltonian

$$H_0 = \frac{1}{2} \sum_{q=0}^{N-1} \epsilon_0(q) [\chi_q^\dagger \chi_q + \chi_{-q}^\dagger \chi_{-q} - 1], \quad (3.4)$$

then the exponential e^{-iuH_0} acting on it becomes

$$e^{-iuH_0} |\Psi_0\rangle = e^{-iuE_0} |\Psi_0\rangle.$$

$E_0 = -\frac{1}{2} \sum_{q=0}^{N-1} \epsilon_0(q)$ is the ground state energy of the initial state where $\epsilon_0(q)$ is given in term of the initial field and anisotropy parameters as

$$\epsilon_0(q) = \left[\left(h_0 - \cos \frac{2\pi q}{N} \right)^2 + \gamma_0^2 \sin^2 \frac{2\pi q}{N} \right]^{1/2}.$$

The characteristic function simplifies into

$$G(u) = e^{iuE_0} \langle \Psi_0 | e^{iuH_1} | \Psi_0 \rangle. \quad (3.5)$$

Since the ground state $|\Psi_0\rangle$ is not an eigenstate of the post-quench Hamiltonian

$$H_1 = \frac{1}{2} \sum_{q=0}^{N-1} \epsilon_1(q) [\tilde{\chi}_q^\dagger \tilde{\chi}_q + \tilde{\chi}_{-q}^\dagger \tilde{\chi}_{-q} - 1], \quad (3.6)$$

with

$$\epsilon_1(q) = \left[\left(h_1 - \cos \frac{2\pi q}{N} \right)^2 + \gamma_1^2 \sin^2 \frac{2\pi q}{N} \right]^{1/2},$$

the average over $|\Psi_0\rangle$ cannot be evaluated straightforwardly. In order for us to evaluate the quantum average in equation (3.5), the ground state of the pre-quench Hamiltonian $|\Psi_0\rangle$ must be written in terms of the eigenstates of the post-quench Hamiltonian $|\tilde{\Psi}_n\rangle \equiv |\tilde{\Psi}_{n,q}, \tilde{\Psi}_{n,-q}\rangle$ (with $n = 0, 1$). This relationship is obtained by using the Bogolyubov transformation (equations (2.15)) for H_0 :

$$\psi_q = \chi_q \cos \theta_q + \chi_{-q}^\dagger \sin \theta_q, \quad \psi_{-q}^\dagger = -\chi_q \sin \theta_q + \chi_{-q}^\dagger \cos \theta_q, \quad (3.7)$$

and H_1 :

$$\psi_q = \tilde{\chi}_q \cos \tilde{\theta}_q + \tilde{\chi}_{-q}^\dagger \sin \tilde{\theta}_q, \quad \psi_{-q}^\dagger = -\tilde{\chi}_q \sin \tilde{\theta}_q + \tilde{\chi}_{-q}^\dagger \cos \tilde{\theta}_q. \quad (3.8)$$

Inversion of equations (3.7) will give

$$\chi_q = \psi_q \cos \theta - \psi_{-q}^\dagger \sin \theta \quad \chi_{-q}^\dagger = \psi_q \sin \theta + \psi_{-q}^\dagger \cos \theta. \quad (3.9)$$

Substitution of equations (3.8) to equations (3.9) gives the relation of the pre- and post-quench Bogolyubov operators:

$$\chi_q = \tilde{\chi}_q \cos \Delta_q - \tilde{\chi}_{-q}^\dagger \sin \Delta_q, \quad (3.10a)$$

$$\chi_{-q} = \tilde{\chi}_{-q} \cos \Delta_q + \tilde{\chi}_q^\dagger \sin \Delta_q, \quad (3.10b)$$

where $\Delta_q = \theta_1(q) - \theta_0(q)$ is the difference between the post- and pre-quench Bogolyubov angles and $\theta_0(q)$ and $\theta_1(q)$ given by equation (2.16) with $h, \gamma = h_0, \gamma_0$ and h_1, γ_1 , respectively. Equations (3.10) will enable us to write the ground state of H_0 in terms of the ground state of H_1 . Let us define

$$|\Psi_0\rangle = \mathcal{A}_{\chi_q \chi_{-q}} |\tilde{\Psi}_0\rangle,$$

where \mathcal{A} is a normalization factor. Expanding χ_q and χ_{-q} using equations (3.10) and noting that $\tilde{\chi}_{\pm q}|\tilde{\Psi}_0\rangle = 0$, we have

$$\begin{aligned} |\Psi_0\rangle &= \mathcal{A}(\tilde{\chi}_q \cos \Delta_q - \tilde{\chi}_{-q}^\dagger \sin \Delta_q)(\tilde{\chi}_{-q} \cos \Delta_q + \tilde{\chi}_q^\dagger \sin \Delta_q)|\tilde{\Psi}_0\rangle \\ &= \mathcal{A}(\cos \Delta_q \sin \Delta_q \tilde{\chi}_q \tilde{\chi}_q^\dagger + \sin^2 \Delta_q \tilde{\chi}_q^\dagger \tilde{\chi}_{-q}^\dagger)|\tilde{\Psi}_0\rangle \\ &= \mathcal{A}(\cos \Delta_q \sin \Delta_q |\tilde{\Psi}_0\rangle + \sin^2 \Delta_q |\tilde{\Psi}_1\rangle). \end{aligned}$$

The normalization constant \mathcal{A} is calculated by imposing $\langle \Psi_0 | \Psi_0 \rangle = 1$:

$$\begin{aligned} \langle \Psi_0 | \Psi_0 \rangle &= |\mathcal{A}|^2 (\cos \Delta_q \sin \Delta_q \langle \tilde{\Psi}_0 | + \sin^2 \Delta_q \langle \tilde{\Psi}_1 |) \\ &\quad \times (\cos \Delta_q \sin \Delta_q |\tilde{\Psi}_0\rangle + \sin^2 \Delta_q |\tilde{\Psi}_1\rangle) \\ &= |\mathcal{A}|^2 (\cos^2 \Delta_q \sin^2 \Delta_q \langle \tilde{\Psi}_0 | \tilde{\Psi}_0 \rangle + \sin^4 \Delta_q \langle \tilde{\Psi}_1 | \tilde{\Psi}_1 \rangle) = 1 \end{aligned}$$

where it can be easily seen that $|\mathcal{A}|^2 = \frac{1}{\sin^2 \Delta}$ or $\mathcal{A} = \frac{1}{\sin \Delta}$. Thus, the relation of the pre-quench and the post-quench grounds states is given by

$$|\Psi_0\rangle = (\cos \Delta_q + \sin \Delta_q \tilde{\chi}_q^\dagger \tilde{\chi}_{-q}^\dagger) |\tilde{\Psi}_0\rangle. \quad (3.11)$$

We can use equation (3.11) to rewrite equation (3.5) in terms of the post-quench ground state $|\tilde{\Psi}_0\rangle$:

$$\begin{aligned} G(u) &= e^{\frac{i u}{2} \sum_{q=0}^{N-1} \epsilon_0(q)} \langle \tilde{\Psi}_0 | (\cos \Delta_q + \sin \Delta_q \tilde{\chi}_{-q} \tilde{\chi}_q) \\ &\quad e^{\frac{i u}{2} \sum_{q=0}^{N-1} \epsilon_1(q) (\tilde{\chi}_q^\dagger \tilde{\chi}_q + \tilde{\chi}_{-q}^\dagger \tilde{\chi}_{-q-1})} (\cos \Delta_q + \sin \Delta_q \tilde{\chi}_q^\dagger \tilde{\chi}_{-q}^\dagger) | \tilde{\Psi}_0 \rangle \end{aligned}$$

After operating the post-quench operators to the ground state of H_1 , the zero temperature characteristic function $G(u)$ is written in its final form as a product over the pseudomomentum q given by

$$G(u) = e^{i u \delta} \prod_{q=0}^{N-1} \left\{ \cos^2 \Delta_q + e^{i u \epsilon_1(q)} \sin^2 \Delta_q \right\}, \quad (3.12)$$

where

$$\delta = E_1 - E_0 = \frac{1}{2} \sum_{q=0}^{N-1} [\epsilon_0(q) - \epsilon_1(q)]$$

is the difference between the post- and pre-quench ground state energies.

3.2 Cumulants of $p(W)$

Now that the characteristic function of the probability density function of the work done for an arbitrary quantum quench in the XY model is calculated (equation (3.12)), let us turn our attention to the cumulants of the work PDF.

3.2.1 Average work and fluctuation in work done

Let us use equation (2.35) to compute for the average work done $\langle W \rangle = \kappa_1$ for an arbitrary quench of the field strength and the anisotropy parameter in the XY model. The cumulant generating function $\ln G(u)$ is given by

$$\begin{aligned} \ln G(u) &= \ln \left\{ e^{iu\delta} \prod_{q=0}^{N-1} [\cos^2 \Delta_q + e^{iu\epsilon_1(q)} \sin^2 \Delta_q] \right\} \\ &= iu\delta + \sum_{q=0}^{N-1} \ln [\cos^2 \Delta_q + e^{iu\epsilon_1(q)} \sin^2 \Delta_q]. \end{aligned} \quad (3.13)$$

where $\delta = -\frac{1}{2} \sum_q [\epsilon_1(q) - \epsilon_0(q)]$. Since

$$\frac{\partial}{\partial u} \left[\sum_{q=0}^{N-1} \ln [\cos^2 \Delta_q + e^{iu\epsilon_1(q)} \sin^2 \Delta_q] \right] = \sum_{q=0}^{N-1} \frac{i\epsilon_1(q) e^{iu\epsilon_1(q)} \sin^2 \Delta_q}{\cos^2 \Delta_q + e^{iu\epsilon_1(q)} \sin^2 \Delta_q}, \quad (3.14)$$

then the average work done is

$$\langle W \rangle = \sum_{q=0}^{N-1} \left\{ \frac{1}{2} \epsilon_0(q) - \frac{1}{2} \epsilon_1(q) + \epsilon_1(q) \sin^2 \Delta_q \right\}. \quad (3.15)$$

Simplifying the terms with $\epsilon_1(2)$ (trigonometric double-angle identity) will lead to the result

$$\langle W \rangle = \frac{1}{2} \sum_{q=0}^{N-1} [\epsilon_0(q) - \epsilon_1(q) \cos 2\Delta_q]. \quad (3.16)$$

We can express the average work in terms of the quench parameters h and γ by using equation (2.16) and the trigonometric identity $\cos 2\Delta_q =$

$\cos 2\theta_0 \cos 2\theta_1 + \sin 2\theta_0 \sin 2\theta_1$. Doing so will give

$$\langle W \rangle = \frac{1}{2} \sum_{q=0}^{N-1} \frac{1}{\epsilon_0(q)} \left\{ (h_0 - h_1) \left[h_0 - \cos\left(\frac{2\pi q}{N}\right) \right] + \gamma_0(\gamma_0 - \gamma_1) \sin^2\left(\frac{2\pi q}{N}\right) \right\}. \quad (3.17)$$

On the other hand, the fluctuations in measurements of the work done on the system $\sigma_W^2 = \langle W^2 \rangle - \langle W \rangle^2$ are measured by the second cumulant κ_2 . Taking the derivative of equation (3.14) and using trigonometric identity $\sin 2\Delta = 2 \sin \Delta \cos \Delta$ yields

$$\sigma_W^2 = \langle W^2 \rangle - \langle W \rangle^2 = \frac{1}{4} \sum_{q=0}^{N-1} \epsilon_1^2(q) \sin^2 2\Delta_q. \quad (3.18)$$

By using equation (2.16) and the trigonometric identity $\sin 2\Delta = \sin \theta_1 \cos \theta_0 - \cos \theta_1 \sin \theta_0$, the work fluctuation is given in terms of the quench parameters h and γ as

$$\sigma_W^2 = \frac{1}{4} \sum_{q=0}^{N-1} \frac{1}{\epsilon_0^2(q)} \left\{ \gamma_1 \sin(2\pi q/N) [h_0 - \cos(2\pi q/N)] - \gamma_0 \sin(2\pi q/N) [h_1 - \cos(2\pi q/N)] \right\}^2. \quad (3.19)$$

For the thermodynamic limit ($N \rightarrow \infty$), the argument $2\pi q/N$ of the trigonometric functions becomes infinitesimal and the summation over q becomes an integral over $k = 2\pi q/N$. Thus, the fluctuations in the measured work done per spin in the thermodynamic limit is

$$\lim_{N \rightarrow \infty} \frac{\sigma_W^2}{N} = \frac{1}{8\pi} \int_0^{2\pi} \sin^2 k \frac{[\gamma_1(h_0 - \cos k) - \gamma_0(h_1 - \cos k)]^2}{(h_0 - \cos k)^2 + \gamma_0^2 \sin^2 k} dk. \quad (3.20)$$

3.2.2 Contour integral representation of σ_W^2/N

Let us now consider the contour integral representation of the work fluctuation. Let z be a complex number within a unit circle centered at the origin of the complex plane. z is given by

$$z = e^{ik} \Rightarrow dz = iz dk. \quad (3.21)$$

The trigonometric functions sine and cosine are given in terms of z by

$$\sin k = \frac{1}{2i}(z - z^*) \quad \cos k = \frac{1}{2}(z + z^*),$$

where z^* is the complex conjugate of z . Thus, the contour integral representation of the work fluctuation per spin is

$$\frac{\sigma_W^2}{N} = -\frac{1}{32\pi i} \oint_{\mathcal{C}} \frac{(z^2 - 1)^2 [(z^2 + 1)(\gamma_1 - \gamma_0) - 2z(\gamma_1 h_0 - \gamma_0 h_1)]^2}{z^3 [(2h_0 z - z^2 - 1)^2 - \gamma_0^2 (z^2 - 1)^2]} dz, \quad (3.22)$$

where the contour \mathcal{C} is a unit circle located at the origin of the complex plane.

The contour integral is evaluated by the residue theorem. Thus, by letting

$$f(z) = \frac{(z^2 - 1)^2 [(z^2 + 1)(\gamma_1 - \gamma_0) - 2z(\gamma_1 h_0 - \gamma_0 h_1)]^2}{z^3 [(2h_0 z - z^2 - 1)^2 - \gamma_0^2 (z^2 - 1)^2]}, \quad (3.23)$$

the contour integral representation of the work fluctuation in equation (3.22) is evaluated as

$$\frac{\sigma_W^2}{N} = -\frac{1}{32\pi i} \oint_{\mathcal{C}} f(z) dz = -\frac{1}{32\pi i} \left[2\pi i \sum_{z=z_i} \text{Res} f(z) \right], \quad (3.24)$$

where the sum is over all poles of $f(z)$ inside the unit circle \mathcal{C} . The poles of $f(z)$ consist of zero and generally non-zero poles given by

$$z_{\pm}^{(1)} = \frac{h_0 \pm \sqrt{h_0^2 + \gamma_0^2 - 1}}{\gamma_0 + 1} \quad (3.25a)$$

$$z_{\pm}^{(2)} = \frac{-h_0 \pm \sqrt{h_0^2 + \gamma_0^2 - 1}}{\gamma_0 - 1}. \quad (3.25b)$$

Equation (3.24) is an exact analytic expression for the work fluctuation per spin for an arbitrary quench in the XY model. The poles of $f(z)$ (equations (3.25)) depend only on the parameters of initial Hamiltonian H_0 . For non-critical pre-quench Hamiltonian, the poles may be located inside or outside of the unit circle \mathcal{C} . In fact, only two of the four non-zero poles are inside the contour \mathcal{C} for values of the transverse field h_0 and anisotropy parameter

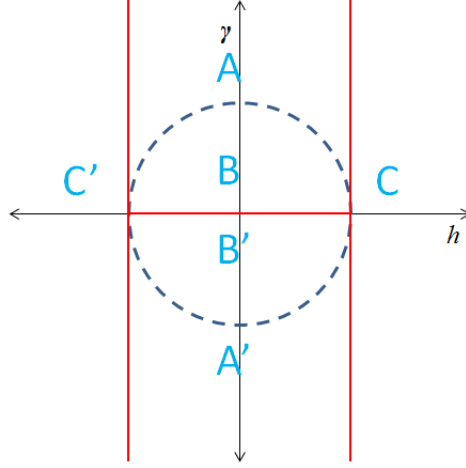


Figure 3.1: Regions in the phase diagram of the Heisenberg XY model.

γ_0 that are not critical. Table 3.1 gives the position of the poles for the different region of the XY model phase diagram (see figure 3.1). Thus, equation (3.24) becomes a sum of only three residues (including $z = 0$) for non-critical H_0 . However, for critical pre-quench Hamiltonian H_0 , some of the poles fall along the contour \mathcal{C} (See table 3.2). As the transverse field h_0 and anisotropy γ_0 cross the quantum critical points, these poles move from inside to outside of the unit circle or vice versa. This results to non-analyticity in the work fluctuation.

Table 3.1: Position of the poles for noncritical h_0 and γ_0

Region	Inside \mathcal{C}	Outside \mathcal{C}	Real poles	Imaginary poles
A	$z_+^{(1)}$ and $z_-^{(1)}$	$z_+^{(2)}$ and $z_-^{(2)}$	all	none
B	$z_+^{(1)}$ and $z_-^{(1)}$	$z_+^{(2)}$ and $z_-^{(2)}$	none	all
C	$z_-^{(1)}$ and $z_+^{(2)}$	$z_+^{(1)}$ and $z_-^{(2)}$	all	none
A'	$z_+^{(2)}$ and $z_-^{(2)}$	$z_+^{(1)}$ and $z_-^{(1)}$	all	none
B'	$z_+^{(2)}$ and $z_-^{(2)}$	$z_+^{(1)}$ and $z_-^{(1)}$	none	all
C'	$z_+^{(1)}$ and $z_-^{(2)}$	$z_-^{(1)}$ and $z_+^{(2)}$	all	none

Table 3.2: Position of the poles for critical h_0 and γ_0

Critical line	Poles on \mathcal{C}
Isotropic XX line ($\gamma_0 = 0, h_0 < 1$)	$z_-^{(1)} = z_+^{(2)}$ and $z_+^{(1)} = z_-^{(2)}$
$h_0 = 1, \gamma > 0$	$z_+^{(1)} = z_+^{(2)}$
$h_0 = 1, \gamma < 0$	$z_-^{(1)}$ and $z_-^{(2)}$
$h_0 = -1, \gamma > 0$	$z_-^{(1)}$ and $z_-^{(2)}$
$h_0 = -1, \gamma < 0$	$z_+^{(1)}$ and $z_+^{(2)}$
Multicritical points ($\gamma = 0, h_0 = 1$)	$z_+^{(1)} = z_-^{(1)} = z_+^{(2)} = z_-^{(2)}$

3.3 Examples of quenches in the XY model

Let us now consider some examples of transverse field and anisotropy quenches in the Heisenberg XY model. First, the case of field quenches for different fixed values of anisotropy $\gamma_0 = \gamma_1$. Figure 3.2 shows the fluctuation in measured work done per spin in the thermodynamic limit ($N \rightarrow \infty$). The fluctuation is non-analytic when the pre-quench transverse field is tuned to $|h_0| = 1$. These non-analyticities take the form of cusps along the line $|h_0| = 1$. Fluctuations suddenly change along these lines due to the quantum phase transition of the Transverse Ising model. It is also observed that when the anisotropy between interactions in the x - and y -directions is increased, the cusps are smoothened but the value of the fluctuations also increase. Larger γ lessen the effect of the critical field but increases the range of possible measured work done. However, for the case of field quenches along the XX line ($\gamma_0 = \gamma_1 = 0$), there is no fluctuation in measurements of the work done per spin for any quench $h_0 \rightarrow h_1$ as seen in the top left plot of figure 3.2. This means that the average work (equation (3.17)) reduces to a delta-peaked work done that only depends on the difference between the pre- and post-quench transverse fields

$$\langle W \rangle = -\frac{N}{2}(h_1 - h_0). \quad (3.26)$$

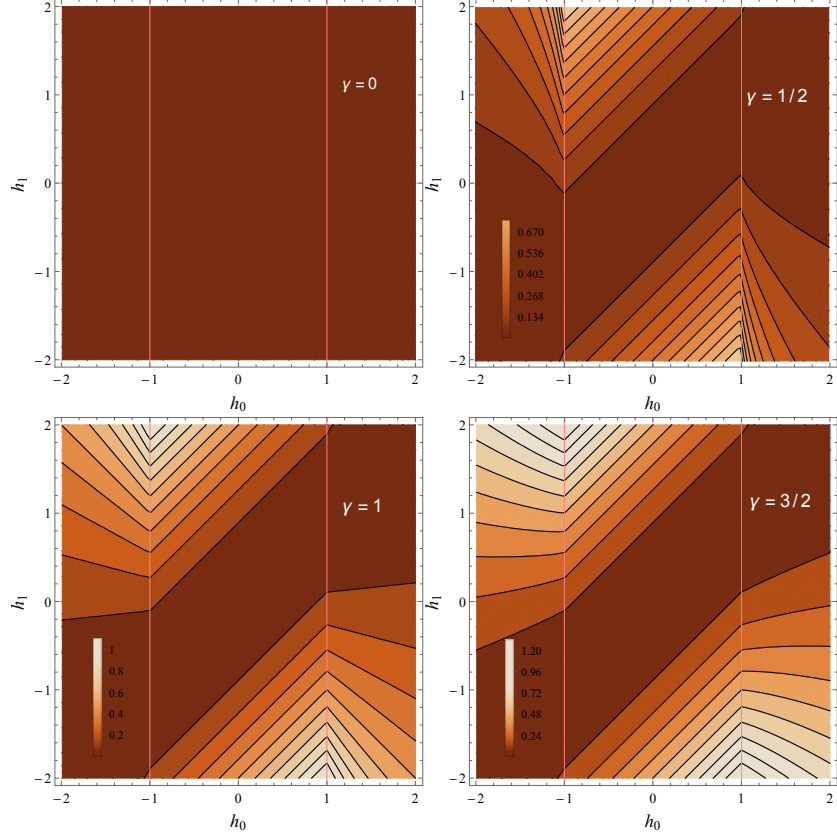


Figure 3.2: The work fluctuation per spin at different fixed anisotropy strength ($\gamma = 0, \frac{1}{2}, 1, \frac{3}{2}$ from left to right). Except for the field quenches along the XX line ($\gamma = 0$), σ_W^2/N ($N \rightarrow \infty$) is not analytic when the pre-quench transverse magnetic field is $|h_0| = 1$. This behavior is due to the quantum phase transition of the Ising universality class. Along the XX line, $p(W)$ is a delta-peaked function with $\sigma_W^2/N = 0$.

In the XX line, the transverse field acts as chemical potential $\mu = \frac{h}{2}$ which is the amount of energy added to the system's ground state energy for every particle at site j (see equation (2.7) with $\gamma = 0$). The set of eigenstates of the pre-quench Hamiltonian $H_0(h_0, \gamma_0 = 0)$ is also the set of eigenstates of the post-quench Hamiltonian $H_1(h_1, \gamma_1 = 0)$. Hence, the probability distribution function of the work done for any field quenches along the XX line is delta-peaked with no work fluctuation.

Secondly, let us take the case of anisotropy quenches at fixed $h_0 = h_1$.

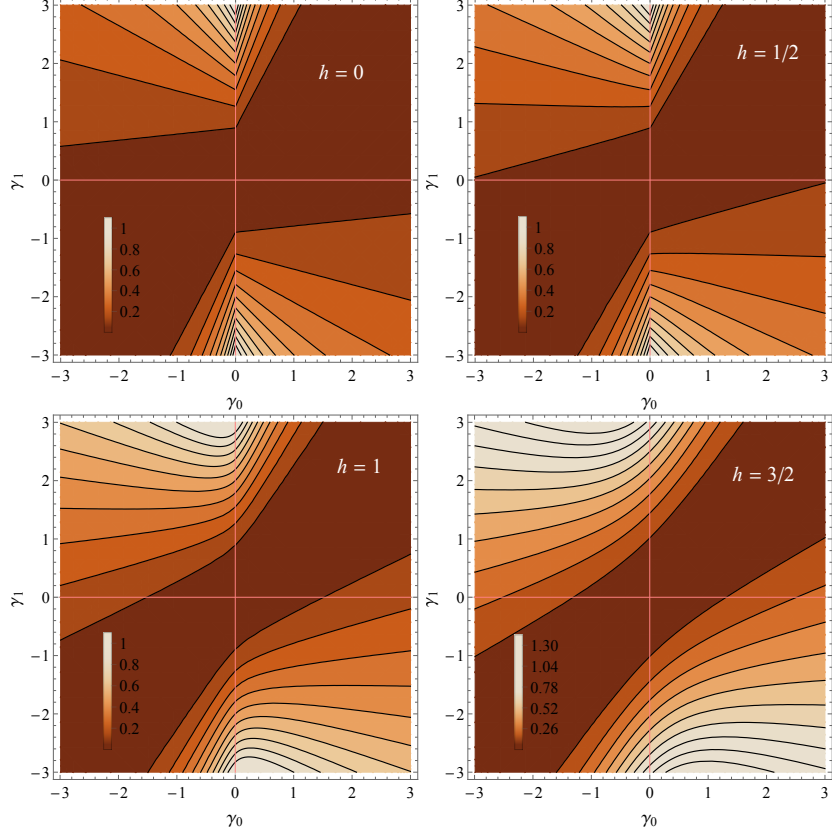


Figure 3.3: The work fluctuation per spin at different fixed transverse field strength ($h = 0, 1/2, 1, 3/2$ from left to right) is not analytic when the pre-quench anisotropy parameter is $\gamma_0 = 0$ for $|h| < 1$.

Work fluctuation per spin ($N \rightarrow \infty$) for this case is shown in figure 3.3. Cusps show when the initial anisotropy parameter is critical for quenches inside the ferromagnetic phase as seen in the top two contour plots in figure 3.3. As with the field quenches at fixed γ , this non-analyticity is due to a quantum phase transition. This transition line separates strong ordering of the spins in the x - and the y -directions (XX line in figure 2.1). The work fluctuation is analytic when the anisotropy quench does not cross the XX critical line ($\gamma = 0$ for $|h| > 1$).

Lastly, we consider the case of quenches where the post-quench parameters are tuned to fixed values. Figure 3.4 shows contour plots for quenches

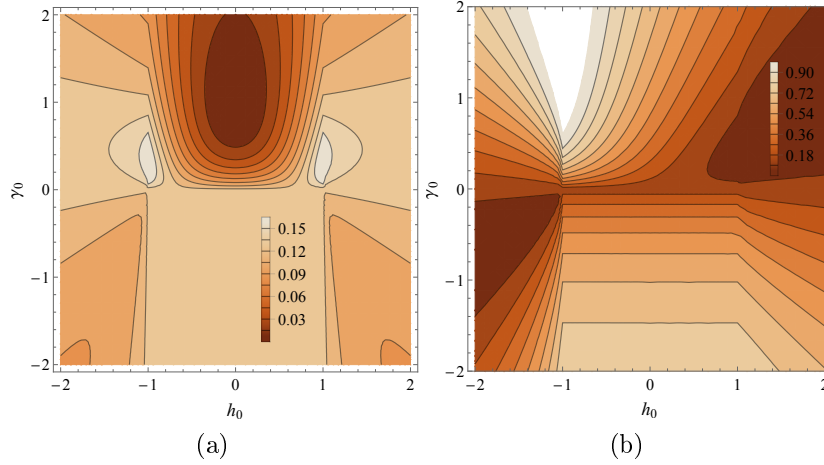


Figure 3.4: Work fluctuation per spin ($N \rightarrow \infty$) that end at fixed post-quench parameters. (a) Quenches that end at $(h_1 = 0, \gamma_1 = 1)$. (b) Quenches that end at $(h_1 = 2, \gamma_1 = 1)$.

that end at the zero-field transverse Ising model (Figure 3.4a) and at a high-field ($h = 2$) Ising model (Figure 3.4b). These plots show the non-analyticity of the work fluctuation per spin at the critical field lines $h_0 = \pm 1$. It can be observed in figure 3.4a that quenches that began near the same point as the post-quench parameters have the minimum fluctuation in work done and increases as the pre-quench parameters go out of the region of high ferromagnetic order in the x -direction ($\gamma > 0$ and $|h| < 1$). On the other hand, quenches that began in the region of high ferromagnetic order in the y -direction ($\gamma < 0$ and $|h| < 1$) have constant work fluctuations per spin. Figure 3.4b also shows that quenches starting near the same point as the post-quench parameters have minimum fluctuations in the work done.

Figure 3.5 shows work fluctuation per spin for quenches that end at a point on the isotropic XX line. Figure 3.5a shows work fluctuation that end at the zero-field XX line ($h_1 = 0, \gamma_1 = 0$). Non-analyticity of the work fluctuation per spin also manifests as cusps at the critical field lines. An addition to this, it is observed that the work fluctuation per spin is zero at the line $\gamma_0 = 0$. This adds to the earlier observation that the work done for

quantum quenches along the XX line is delta-peaked. The probability density of the work done after the quench is delta-peaked at $W = -\frac{1}{2}N(h_1 - h_0)$. On the other hand, Figure 3.5b shows the work fluctuation per spin for quenches that end at the multicritical point $(h_1 = 1, \gamma_1 = 0)$. The work fluctuation is only non-analytic at the field line $h = -1$. The work fluctuation per spin appears to be analytic when the pre- and post-quench Hamiltonians are on the same critical line ($h_0 = h_1 = 1$).

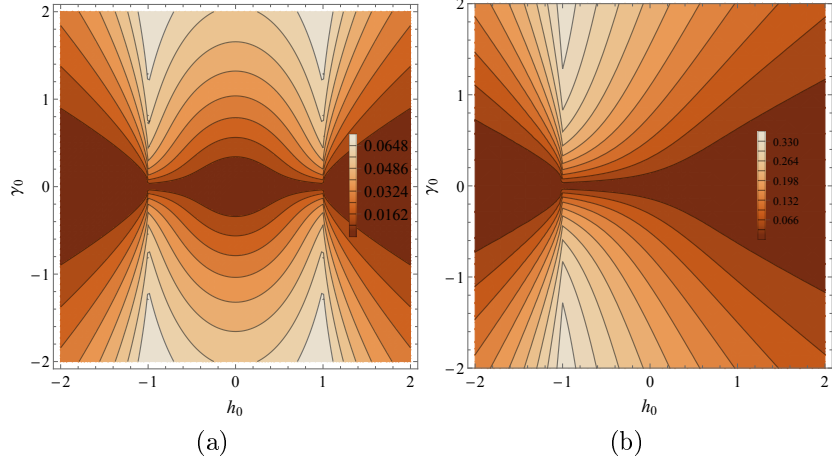


Figure 3.5: Work fluctuation per spin ($N \rightarrow \infty$) that end at fixed post-quench parameters. (a) Quenches that end at $(h_1 = 0, \gamma_1 = 0)$. (b) Quenches that end at $(h_1 = 1, \gamma_1 = 0)$.

Chapter 4

Irreversible Entropy

In this chapter, we shall compute for the irreversible entropy produced during an arbitrary quench in the XY model. This irreversible entropy ΔS_{irr} is a measure of the irreversibility of a protocol done on a quantum system. We will consider the case where the system is initially prepared in a thermal state of H_0 at reciprocal temperature β and described by a density matrix

$$\rho(H_0) = \frac{e^{-\beta H_0}}{\mathcal{Z}_0} \quad (4.1)$$

with partition function

$$\mathcal{Z}_0 = \text{Tr}[e^{-\beta H_0}]. \quad (4.2)$$

After some time, the coupling with the heat bath is removed and the quench protocol is performed.

4.1 Fluctuation relations

For finite systems, the average work done $\langle W \rangle$ and the free energy difference ΔF is related by the Jensen's inequality

$$\langle W \rangle \geq \Delta F \quad (4.3)$$

in accordance with the second law of thermodynamics [12, 38]. The equality is reached for quasistatic processes. $\Delta F = F_1 - F_0$ is the difference between

the free energies of the two equilibrium configurations corresponding to the post- and pre-quench Hamiltonians H_1 and H_0 , respectively. The difference between the average work done $\langle W \rangle$ and the change in free energy ΔF is supplied by introducing an irreversible/dissipated work:

$$\langle W \rangle_{\text{irr}} = \langle W \rangle - \Delta F. \quad (4.4)$$

For isolated systems where heat transfer is zero, the irreversible work is due to the irreversible entropy produced during the quench [12]

$$\Delta S_{\text{irr}} = \beta \langle W \rangle_{\text{irr}} = \beta [\langle W \rangle - \Delta F]. \quad (4.5)$$

The free energy change ΔF is obtained using the known Jarzynski equality [17]

$$\langle e^{-\beta W} \rangle = e^{-\beta \Delta F},$$

or, equivalently,

$$\Delta F = -\frac{1}{\beta} \ln \langle e^{-\beta W} \rangle. \quad (4.6)$$

The quantum average of the exponential $\exp(-\beta W)$ in equation (4.6) is similar to the characteristic function of the work PDF in equation (3.2) by noting that the work done is equal to the difference of the final and the initial energies of the system and by introducing $u = i\beta$

$$\langle e^{-\beta W} \rangle = G(i\beta) = \text{Tr}[e^{-\beta H_1} e^{\beta H_0} \rho(H_0)]. \quad (4.7)$$

The second equality in equation (4.7) then becomes

$$\langle e^{-\beta W} \rangle = \frac{1}{\mathcal{Z}_0} \text{Tr}[e^{-\beta H_1}]. \quad (4.8)$$

By noting that the post-quench partition function is given by

$$\mathcal{Z}_1 = \text{Tr}[e^{-\beta H_1}], \quad (4.9)$$

it is shown that the quantum average in equation (4.6) is equivalent to the ratio of the system's post-quench partition function to the pre-quench partition function as in [17]

$$\langle e^{-\beta W} \rangle = \frac{\mathcal{Z}_1}{\mathcal{Z}_0}. \quad (4.10)$$

4.2 Average work at finite temperature

We shall now calculate the average work done for a quench that is performed on a thermal state. The system is initially prepared in a canonically distributed mixed state of the initial Hamiltonian H_0 in effective thermal equilibrium with a heat bath of temperature $1/\beta$. The system is canonically distributed and its density matrix is given by equation (4.1). The characteristic function of the work PDF for a quench at finite temperature is given by

$$G(u) = \text{Tr}[e^{iuH_1} e^{-iuH_0} \rho(H_0)], \quad (4.11)$$

where the trace is evaluated with respect to the eigenstates $|\Psi_{n,q}, \Psi_{n,-q}\rangle$ of the pre-quench Hamiltonian H_0 . The partition function associated with the Hamiltonian of the XY model (equation (3.4)) is given by

$$\begin{aligned} \mathcal{Z}_0 &= \text{Tr} \exp \left\{ -\frac{\beta}{2} \sum_{q=0}^{N-1} \epsilon_0(q) [\chi_q^\dagger \chi_q + \chi_{-q}^\dagger \chi_{-q} - 1] \right\} \\ &= 2^N \prod_{q=0}^{N-1} \cosh \left[\frac{\beta \epsilon_0(q)}{2} \right]. \end{aligned} \quad (4.12)$$

Thus, with the use of equations (3.4) and (3.6), and tracing over the eigenstates $|\Psi_{n,q}, \Psi_{n,-q}\rangle$, the characteristic function of the work PDF $p(W)$ is

$$\begin{aligned} G(u) &= \frac{1}{\mathcal{Z}_0} \prod_{q=0}^{N-1} \sum_{n_{\pm q}=0,1} e^{-\frac{1}{2}(iu+\beta)\epsilon_0(q)[n_q+n_{-q}-1]} \\ &\quad \times \langle \Psi_{n,q}, \Psi_{n,-q} | e^{\frac{1}{2}iu\epsilon_1(q)[\tilde{\chi}_q^\dagger \tilde{\chi}_q + \tilde{\chi}_{-q}^\dagger \tilde{\chi}_{-q} - 1]} | \Psi_{n,q}, \Psi_{n,-q} \rangle. \end{aligned} \quad (4.13)$$

With the application of appropriate creation operators to equation (3.11), the eigenstates of the pre-quench Hamiltonian is written in terms of the eigenstates of the post-quench Hamiltonian

$$|\Psi_{n,q}, \Psi_{n,-q}\rangle = (\chi_q^\dagger)^n (\chi_{-q}^\dagger)^n (\cos \Delta_q + \sin \Delta_q \tilde{\chi}_q^\dagger \tilde{\chi}_{-q}^\dagger) |\tilde{\Psi}_{n,q}, \tilde{\Psi}_{n,-q}\rangle, \quad (4.14)$$

where the pre-quench Bogolyubov operators $\chi_{q\pm}^\dagger$ are given in terms of the post-quench Bogolyubov operators $\tilde{\chi}_{\pm q}^\dagger$ by equations (3.10). With the use of

equation (4.14), the matrix elements in equation (4.13) can be evaluated and will give

$$G(u) = \frac{1}{\mathcal{Z}_0} \prod_{q=0}^{N-1} \left\{ e^{\frac{1}{2}(iu+\beta)\epsilon_0} \left[e^{-\frac{1}{2}iu\epsilon_1} \cos^2 \Delta_q + e^{\frac{1}{2}iu\epsilon_1} \sin^2 \Delta_q \right] + e^{-\frac{1}{2}(iu+\beta)\epsilon_0} \left[e^{\frac{1}{2}iu\epsilon_1} \cos^2 \Delta_q + e^{-\frac{1}{2}iu\epsilon_1} \sin^2 \Delta_q \right] + 2 \right\}. \quad (4.15)$$

The first and the second cumulants from equation (4.15) via equation (2.35) correspond to the average work done and work fluctuations, respectively, for a quantum quench of the XY model at finite temperature. The first cumulant gives

$$\langle W \rangle = \frac{1}{2} \sum_{q=0}^{N-1} (\epsilon_0 - \epsilon_1 \cos 2\Delta_q) \tanh \left[\frac{\beta \epsilon_0(q)}{2} \right], \quad (4.16)$$

or, equivalently,

$$\begin{aligned} \langle W \rangle = \frac{1}{2} \sum_{q=0}^{N-1} \frac{1}{\epsilon_0(q)} & \left[(h_0 - h_1) \left(h_0 - \cos \frac{2\pi q}{N} \right) \right. \\ & \left. + \gamma_0 (\gamma_0 - \gamma_1) \sin^2 \frac{2\pi q}{N} \right] \tanh \left[\frac{\beta \epsilon_0(q)}{2} \right], \end{aligned} \quad (4.17)$$

for the average work done after an arbitrary quench in the XY model. If we take the zero temperature limit ($\beta \rightarrow \infty$) of equation (4.17), the hyperbolic tangent will approach unity and the finite temperature case will simplify to the zero temperature case (equation (3.16)).

4.3 Irreversible entropy produced

The irreversible entropy produced then is computed as

$$\Delta S_{\text{irr}} = \beta \langle W \rangle + \ln \frac{\mathcal{Z}_1}{\mathcal{Z}_0}. \quad (4.18)$$

where the partition functions \mathcal{Z}_0 and \mathcal{Z}_1 for the XY ferromagnet are given by equation (4.12) with parameters (h_0, γ_0) and (h_1, γ_1) , respectively. The

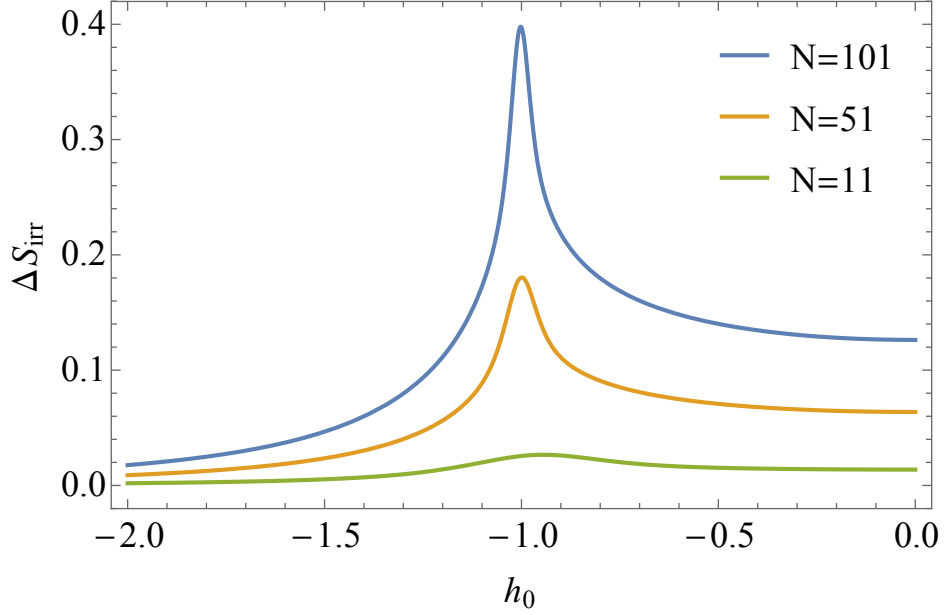


Figure 4.1: Irreversible entropy produced for quenches with magnitude $\delta h = 0.01$ along the Ising line $\gamma = 1$ with different number of particles N at inverse temperature $\beta = 100$.

average work done after a quench in the XY model for finite temperature is given by equation (4.17)). Thus, for an arbitrary quench in the XY model, the irreversible entropy produced is

$$\Delta S_{\text{irr}} = \sum_{q=0}^{N-1} \left\{ \beta (\epsilon_0 - \epsilon_1 \cos 2\Delta_q) \tanh \left[\frac{\beta \epsilon_0(q)}{2} \right] + \ln \frac{\cosh [\beta \epsilon_1(q)/2]}{\cosh [\beta \epsilon_0(q)/2]} \right\}. \quad (4.19)$$

Let us now consider some specific cases of quenches in the XY model and characterize the irreversible entropy produced.

Case 1– First, let us consider a quantum quench of the transverse magnetic field along the Ising Line ($\gamma_0 = \gamma_1 = 1$). Let us set the value of the difference between the post- and pre-quench transverse field to $\delta h = 0.01$.

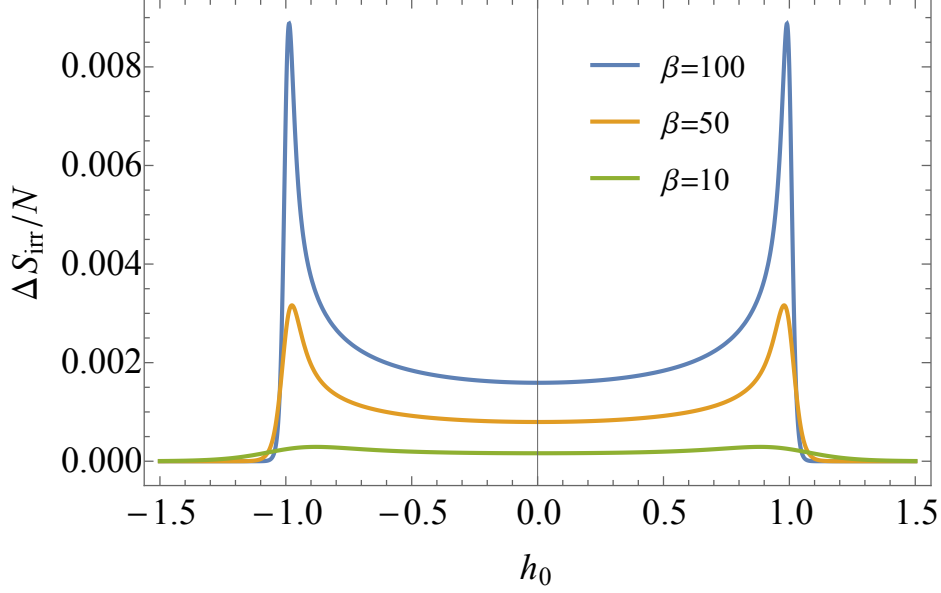


Figure 4.2: Irreversible entropy produced per spin for small field quench along the ising line at different inverse temperature β . There are $N = 1001$ particles.

The irreversible entropy produced will have the form

$$\Delta S_{\text{irr}} = \sum_{q=0}^{N-1} \left\{ \beta(h_0 - h_1) \frac{[h_0 - \cos(2\pi q/N)]}{\epsilon_0(q)} \tanh \left[\frac{\beta}{2} \epsilon_0(q) \right] + \ln \frac{\cosh \left[\frac{\beta \epsilon_1(q)}{2} \right]}{\cosh \left[\frac{\beta \epsilon_0(q)}{2} \right]} \right\}. \quad (4.20)$$

The result for a quench in the XY model along the Ising line (equation (4.20)) reproduces the result in reference [12]. Figure 4.1 shows the irreversible entropy produced for quenches along the Ising line ($\gamma = 1$) in the XY model.¹ The production of irreversible entropy peaks at the critical field $h_0 = 1$. This is due to the quantum phase transition of the Ising universality class. Figure (4.1) shows that the peak in irreversible entropy increases as the number of the particles in the lattice increases at constant temperature ($\beta = 100$). This

¹Figure 4.1 is similar to the result of [12] except for the value of ΔS_{irr} due to the difference in the energy scale used. Reference [12] used an energy scale which is twice of the energy scale used in this thesis.

result implies that the irreversible entropy is an extensive property of the quenched system.

On the other hand figure 4.2 shows the irreversible entropy produced per spin for small field quench $\delta h = 0.01$ at different value of the inverse temperature β . The peak of $\Delta S_{\text{irr}}/N$ increases as the temperature decreases (β increases). This is a result of the emergence of thermal fluctuation at higher temperature. The signature of quantum criticality decreases at higher temperature with the emergence of these thermal fluctuations [12].

Figure 4.3 shows the same quench protocol at inverse temperature $\beta = 100$ for different value of anisotropy strength γ . The number of particles is kept at $N = 1001$. The irreversible entropy produced has its highest peak when the quench is done across the multicritical point ($|h| = 1, \gamma = 0$). For larger values of the anisotropy parameter, the irreversible entropy per spin decreases for field quench that is done inside the ferromagnetic phase ($|h| < 1$) and increases for field quenches that are done in the paramagnetic phase ($|h| > 1$).

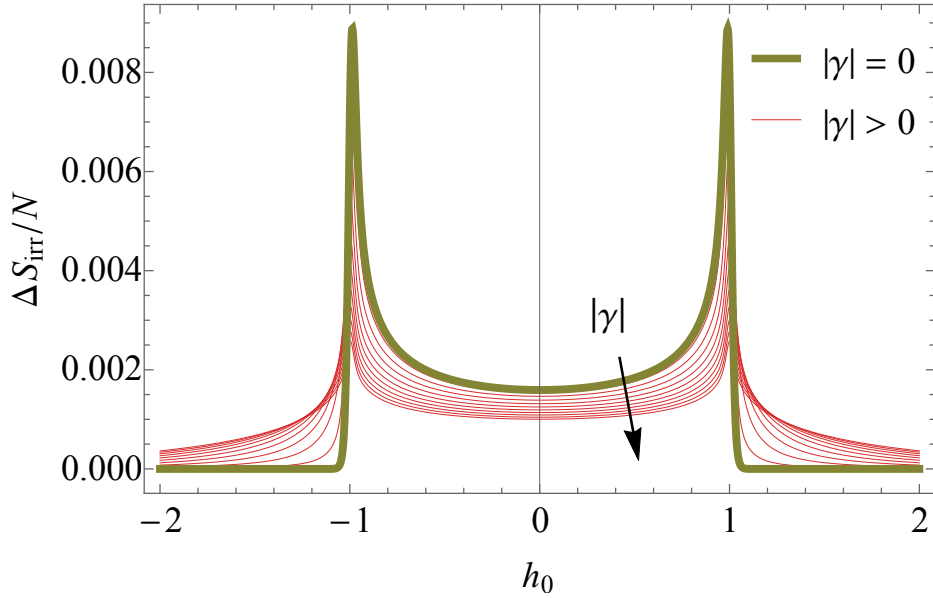


Figure 4.3: Irreversible entropy produced per spin for small field quenches $\delta h = 0.01$. There are $N = 1001$ spins at $\beta = 100$ inverse temperature.

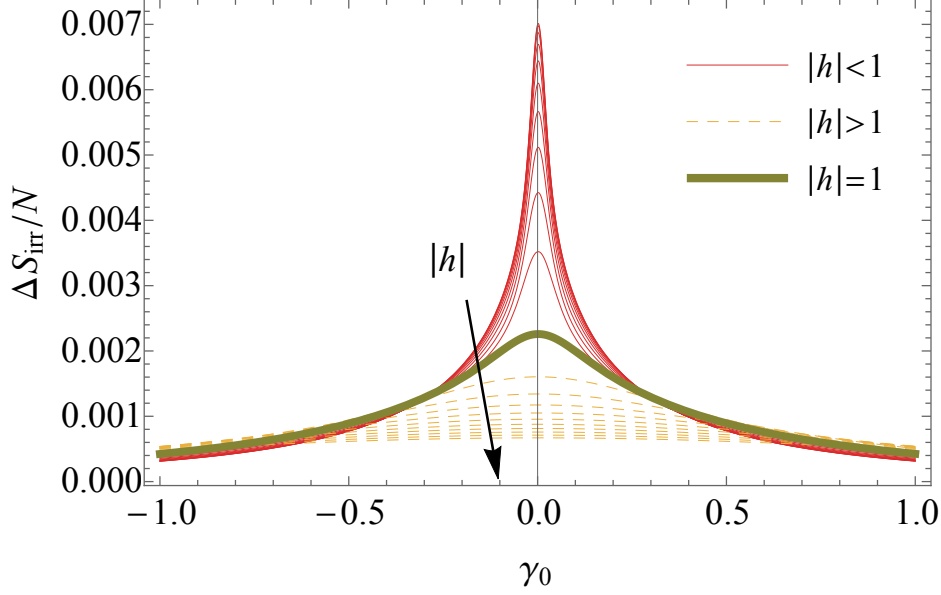


Figure 4.4: Irreversible entropy produced per spin for small anisotropy quenches $\delta\gamma = 0.01$. There are $N = 1001$ spins at $\beta = 100$ inverse temperature.

Case 2– For the case of a quantum quench of the anisotropy parameter γ along a constant magnetic field, $h_0 = h_1 = h$, the irreversible entropy produced is given by

$$\Delta S_{\text{irr}} = \sum_{q=0}^{N-1} \left\{ \beta(\gamma_0 - \gamma_1) \frac{\gamma_0 \sin^2(2\pi q/N)}{\epsilon_0(q)} \tanh \left[\frac{\beta \epsilon_0(q)}{2} \right] + \ln \frac{\cosh^2 \left[\frac{\beta \epsilon_1(q)}{2} \right]}{\cosh^2 \left[\frac{\beta \epsilon_0(q)}{2} \right]} \right\}. \quad (4.21)$$

Figure (4.4) shows the behavior of the irreversible entropy produced per spin for anisotropy quenches $\delta\gamma = 0.01$ with $N = 1001$ particles at $\beta = 100$ inverse temperature. The irreversible entropy production peaks when quench protocol crosses XX line ($\gamma_0 = 0$). It is observed that the peak in the irreversible entropy produced is highest when the magnetic field is $|h| \ll 1$ (deep inside the ferromagnetic phase). As the magnetic field is increased and goes outside of the ferromagnetic phase, the irreversible entropy produced

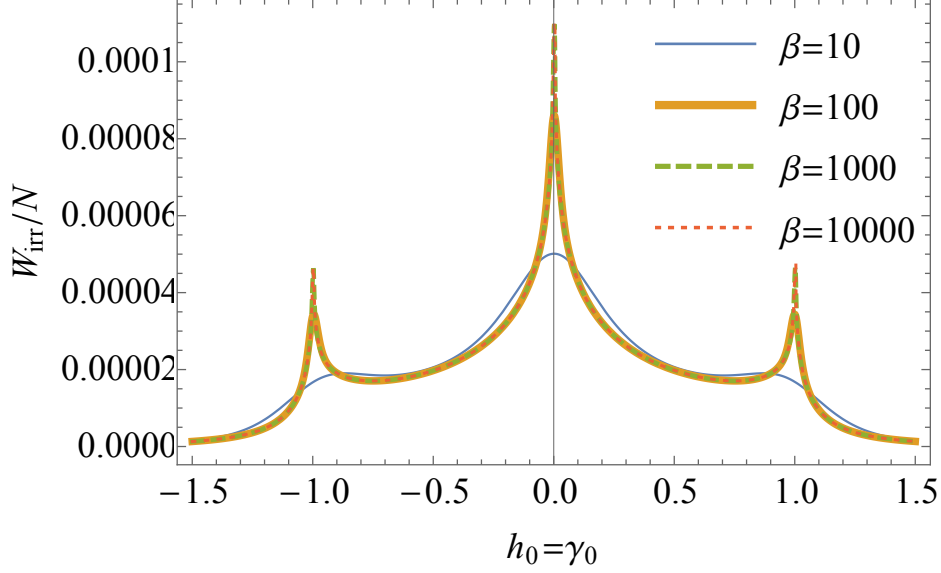


Figure 4.5: Dissipated work for small simultaneous quenches $\delta h = \delta \gamma = 0.01$ along the line $h = \gamma$.

per spin decrease. In contrast with the field quenches along the Ising line, the irreversible entropy for this case is not maximum when the quench is done at the multicritical point (green curve in Fig. (4.4)).

Case 3– Lastly, let us consider the case of a simultaneous quench of the transverse field and the anisotropy parameter in the XY model. This protocol is done along the diagonal line $h = \gamma$ in the phase diagram. For this case, the irreversible entropy produced is given by

$$\Delta S_{\text{irr}} = \sum_{q=0}^{N-1} \left\{ \frac{\beta(h_0 - h_1)}{\epsilon_0(q)} \left[[h_0 - \cos(2\pi q/N)] + h_0 \sin^2(2\pi q/N) \right] \tanh \left[\frac{\beta \epsilon_0(q)}{2} \right] + \ln \frac{\cosh \left[\frac{\beta \epsilon_1(q)}{2} \right]}{\cosh \left[\frac{\beta \epsilon_0(q)}{2} \right]} \right\}. \quad (4.22)$$

The dissipated work per spin $\langle W \rangle_{\text{irr}}/N = \Delta S_{\text{irr}}/(N\beta)$ for small quenches $\delta h = \delta \gamma = 0.01$ is shown in figure (4.5) at different inverse temperature β . The three peaks in the dissipated work $\langle W \rangle_{\text{irr}}$ correspond to the three critical lines that are crossed by this quench. It is observed that for small temperature (large β), the curves of dissipated work coincide except when

the quenches crossed the critical lines. Of the four curves, only $\beta = 10$ has slight difference in the behavior with the other curves. This is due to the decrease in the signature of quantum criticality as thermal fluctuations emerge at higher temperatures.

Chapter 5

Concluding Remarks

In this thesis, we studied the emergent thermodynamics associated with a non-equilibrium protocol done by an arbitrary instantaneous quantum quench of the parameters in the Heisenberg XY model. From the characteristic function of the probability distribution function of the work done, we were able to calculate an exact expression for the work fluctuation per spin. We have shown that the work fluctuation exhibits non-analytic behavior when the pre-quench parameters are tuned across quantum critical points. This is connected to the criticality of the XY model at these points. On the other hand, when the pre- and post-quench parameters are on the same critical line, the work fluctuation is analytic. Furthermore, for quenches along the XX line, the work PDF is delta peaked about one value. Thus, leading to zero work fluctuation. This happens because the isotropic XX model ground state is an eigenstate of both the pre- and post-quench Hamiltonians.

We also investigated the irreversible entropy produced during an arbitrary quench. The irreversible entropy was shown to peak when quantum critical points are crossed by the quench protocol. In general, increasing the number of particles induces a higher irreversible entropy implying that ΔS_{irr} is an extensive property of the quenched system.

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