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Detailed Calculation of the Average Work Done in a Ground State Quench of the Quantum Ising Model

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ABSTRACT

A detailed derivation of the exact expression for the average work done in a transverse field quench of the quantum Ising model ground state is presented. In the thermodynamic limit, it is proved that the average work done generally has inflection points at the critical field for the pre-quench quantum phase transition. The first divergent field derivative is calculated and is shown to diverge logarithmically. We also demonstrate that the average work done is equal to the product of the transverse magnetization of the pre-quench ground state and the change in the magnetic field.

Keywords: Quantum quench, quantum Ising model, quantum phase transition

INTRODUCTION

An initially prepared quantum state evolves unitarily after a rapid change in the Hamiltonian in a quantum quench. The system is isolated from heat and particle baths, and its response time is much longer than the time scale of the Hamiltonian change, so that no adiabatic approximation can be made. Quenches like these generally lead to excited (non-stationary) states, and the resulting non-equilibrium dynamics has been the subject of several investigations on quantum many-body physics in the absence of decohering environmental effects (Polkovnikov et al. 2011; Eisert et al. 2015). Preparing sufficiently isolated states under controllable

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conditions is a technical challenge but experimental progress in the last two decades has allowed quench dynamics to be observed in, for example, ultracold gases in optical lattices (Greiner et al. 2002; Cheneau et al. 2012). Because these isolated quantum systems evolve in time without exchanging matter and heat with a reservoir, conventional statistical mechanical notions, such as temperature, entropy, and equilibriation, are not directly applicable to them. Thus, new theoretical frameworks have been developed to investigate quantum quenches and the novel phenomena that are associated with them. Some recent new discoveries include the emergence of persistent fluctuations despite the absence of energy and matter exchanges with a bath (Rossini et al. 2009; Häppölä et al. 2012; Cosme and Fialko 2014), universal scaling behavior in the vicinity of quantum critical points (Silva 2008; Jacobson et al. 2011; Gambassi and Silva 2012), and the generation of quantum entanglement entropy (Fagotti and Calabrese 2008; Cardy 2011; Daley et al. 2012; Schachenmayer et al. 2013; Alba and Heidrich-Meisner 2014; Alkurtass et al. 2014; Torlai et al. 2014).

In this manuscript we consider the case of a zero temperature instantaneous quench of the transverse magnetic field h in a quantum Ising model. The Hamiltonian is

$$H(h) = -\frac{1}{2}\sum_{j=1}^{N} \sigma_j^x \sigma_{j+1}^x + h\sigma_j^z \qquad (1),$$

where σ_j^a is the a-Pauli operator on site j. There are N spins in the chain and periodic boundary conditions are imposed. The system is thermally isolated and prepared in the ground state $|\varphi(0)\rangle$ of the pre-quench Hamiltonian $H_0 = H(h_0)$ with field h_0. At time $t = 0^+$ the field is suddenly changed to h_1, and the system subsequently evolves according to the post-quench Hamiltonian $H_1 = H(h_1)$. Throughout this work, the subscript index $i = 0$ $(i = 1)$ will refer to pre-quench (post-quench) quantities.

The quantity of interest in this study is the average work done (or quantum work) in these quenches under the formalism developed by Talkner et al. (2007, 2016). This quantum work W is defined as the difference between a projective measurement of the system energy at some time τ after the quench and the initial ground state energy at time $t \leq 0$. That is, if $|\varphi(\tau)\rangle$ is the state vector of the system at time τ, the work done is

$$W = \langle\varphi(\tau)|H_1|\varphi(\tau)\rangle - \langle\varphi(0)|H_0|\varphi(0)\rangle \qquad (2).$$

For a given measurement of quantum work in this quench protocol, one gets the result $W_m = E_1(m) - E_0$, where E_0 is the pre-quench ground state energy and $E_1(m)$ is the m^{th} energy eigenvalue of the post-quench Hamiltonian. This result occurs with total probability $p(m|0) = |\langle E_1(m)|\varphi(0)\rangle|^2$ so that the quantum work distribution $p(W)$ is equal to

$$p(W) = \frac{1}{2\pi}\int \langle\varphi(0)|e^{itH_1}e^{-itH_0}|\varphi(0)\rangle\, e^{-iWt}\, dt \qquad (3).$$

Taking the Fourier transform of this distribution gives the characteristic function

$$G(u) = \langle\varphi(0)|e^{iuH_1}e^{-iuH_0}|\varphi(0)\rangle \qquad (4),$$

whose logarithm in $G(u)$ is the generating function for the cumulants of $p(W)$. From the known properties of this cumulant generating function, the average work done is $\langle W\rangle = -i\lim_{u\to 0}\partial \ln G(u)/\partial u$ and the variance in the work done is $\Sigma^2 = -\lim_{u\to 0} \partial^2 \ln G(u)/\partial u^2$. These statistical measures of the work done in a quenched quantum Ising model have been investigated at zero initial temperature (Silva 2008), non-zero temperatures (Dorner et al. 2012), and the more general anisotropic XY model (Bayocboc Jr. and Paraan 2015). These studies have shown that signatures of the quantum phase transition of the model, such as the vanishing excitation gap, can be revealed through an analysis of the work statistics. In this paper, we focus on providing a detailed derivation of the exact solution for the average work done along the quantum Ising line to complement the previous work of Silva (2008) and Bayocboc Jr. and Paraan (2015). In particular, we will prove that the average work done is not an analytic function of the pre-quench field h_0 when the excitation gap closes at the quantum critical point.

The characteristic function $G(u)$ is given as an expectation value (4) with respect to the pre-quench ground state $|\varphi(0)\rangle$. It is convenient to calculate this quantum average in the basis of single-particle fermionic Jordan-Wigner Fock states. The result is (Silva 2008; Dorner et al. 2012):

$$G(u) = e^{iu\Delta \mathrm{E}}\prod_{n=0}^{N-1}[\cos^2\Delta_n + e^{iu\epsilon_1(q_n)}\sin^2\Delta_n] \qquad (5).$$

In the previous equation, $\Delta E = E_1 - E_0$ is the difference between the ground state energies of the post-quench and pre-quench Hamiltonians. Additionally, the angle $\Delta_n = \theta_1(q_n) - \theta_0(q_n)$ is the difference between the post-quench and pre-quench Bogolyubov angles. These Bogolyubov angles satisfy

$$\tan[2\theta_i(q_n)] = \frac{\sin q_n}{h_i - \cos q_n} \quad (6).$$

Finally, the energy spectrum of elementary excitations is

$$\epsilon_i(q_n) = \sqrt{(h_i - \cos q_n)^2 + \sin^2 q_n} \quad (7),$$

where $q_n = 2\pi n/N$ for odd N or $q_n = 2\pi(n + ½)/N$ for even N. The effect of N being odd or even is negligible in the thermodynamic limit $N \to \infty$. The excitation gap closes at the critical field value $h_i = \pm 1$, which signals a quantum phase transition between a ferromagnetic ($|h_i| < 1$) and paramagnetic ($|h_i| > 1$) ground state.

The average work done can be calculated from the first derivative of ln G, which yields

$$\langle W \rangle = \frac{1}{2} \sum_{n=0}^{N-1} [\epsilon_0(q_n) - \epsilon_1(q_n) \cos 2\Delta_n] \quad (8).$$

We now take the thermodynamic limit $N \to \infty$, and find that the average work per spin $\langle w \rangle \equiv \lim_{N\to\infty} \langle W \rangle / N$ becomes the definite integral

$$\langle w \rangle = \frac{h_0 - h_1}{4\pi} \int_0^{2\pi} \frac{h_0 - \cos k}{\sqrt{(h_0 - \cos k)^2 + \sin^2 k}}\, dk \quad (9).$$

The average work per spin is singular when the pre-quench Hamiltonian is quantum critical ($h_0 = \pm 1$). In the following section we prove that $\langle w \rangle$ is indeed non-analytic (not infinitely differentiable) at these quantum critical points.

AVERAGE WORK DONE

The symmetry and periodicity of the trigonometric functions allow us to put the integral (9) in the form

$$\langle w \rangle = \frac{h_0 - h_1}{\pi} \int_0^{\pi/2} \frac{h_0 + 1 - 2\sin^2 u}{\sqrt{(h_0+1)^2 - 4h_0 \sin^2 u}}\, du. \qquad (10).$$

After factoring and rearranging terms, the resulting integrals are recognized as the complete elliptic integrals

$$K(\kappa) = \int_0^{\pi/2} (1 - \kappa^2 \sin^2\theta)^{-1/2} d\theta \qquad (11),$$

$$E(\kappa) = \int_0^{\pi/2} (1 - \kappa^2 \sin^2\theta)^{1/2}\, d\theta \qquad (12),$$

with modulus κ. We find that

$$\langle w \rangle = \frac{h_0 - h_1}{2\pi h_0} |h_0 + 1| \left[\frac{h_0 - 1}{h_0 + 1} K(\alpha) + E(\alpha)\right] \qquad (13),$$

where $\alpha^2 = 4h_0/(h_0+1)^2 \le 1$. Also, from the known connection formulas for the complete elliptic integrals (Gradshteyn and Ryzhik 2007; Olver et al. 2010)

$$K(\alpha) = (1 + h_0)K(h_0), \qquad (14),$$

$$E(\alpha) = \frac{1}{1+h_0}[2E(h_0) - (1 - h_0^2)K(h_0)], \qquad (15),$$

$$\Re[E(\kappa^{-1})] = \frac{1}{\kappa}[E(\kappa) - (1-\kappa^2)K(\kappa)] \qquad (16),$$

we can simplify our result to

$$\langle w \rangle = \frac{\operatorname{sgn} h_0}{\pi}(h_0 - h_1)\Re[E(h_0^{-1})] \qquad (17).$$

A similar result for this compact formula (17) has been reported without derivation by Bayocboc Jr. and Paraan (2015).

SINGULARITIES AT CRITICALITY

The exact expression (17) for $\langle w\rangle$ reveals that the average work per spin is not analytic at ($|h_0|=1$), since $E(\kappa)$ is not infinitely differentiable at $|\kappa|=1$. As seen in graphs of $\langle w\rangle$ at different pre-quench and post-quench fields (Figure 1), quantum criticality is manifested as a sudden change of curvature of the average work done at the pre-quench critical fields $h_0=\pm1$. In fact, we now prove that these points are actually inflection points by explicitly calculating the needed derivatives.

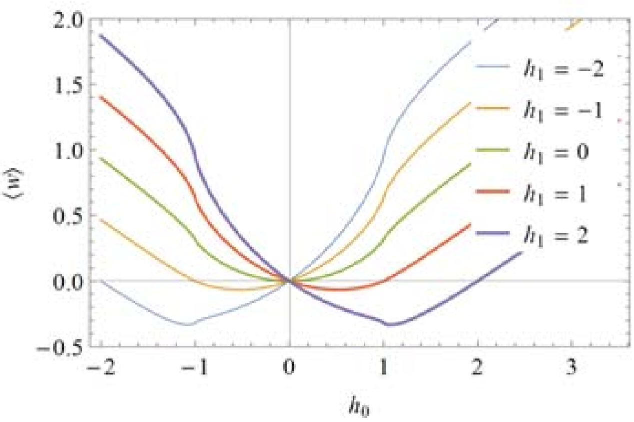

Figure 1. The average work done per spin $\langle w\rangle$ for different post-quench fields h_1 generally have inflection points at the pre-quench critical fields $h_0=\pm1$.

The first derivative of $\langle w\rangle$ with respect to h_0 is exactly

$$\frac{\partial\langle w\rangle}{\partial h_0}=\frac{\mathrm{sgn}\, h_0}{\pi h_0}\Re[h_1E(h_0^{-1})+(h_0-h_1)K(h_0^{-1})] \qquad (18).$$

This derivative is graphed in Figure 2 for several field quenches and we verify that it generally diverges at the critical points $h_0=\pm1$. The only exceptions are when the post-quench field is also at the same critical value as the post-quench field $h_0=h_1=\pm1$.

We now investigate the divergence at critical h_0 using the asymptotic formulas for the elliptic integrals at unit modulus (Olver et al. 2010). The leading term of the asymptotic expansion of the exact derivative (18) about the critical field $h_0=1$ is

$$\frac{\partial\langle w\rangle}{\partial h_0}\approx\frac{h_1}{\pi}+\frac{(h_1-1)}{2\pi}\ln\left|\frac{h_0-1}{8}\right|,\qquad h_0\approx1 \qquad (19).$$

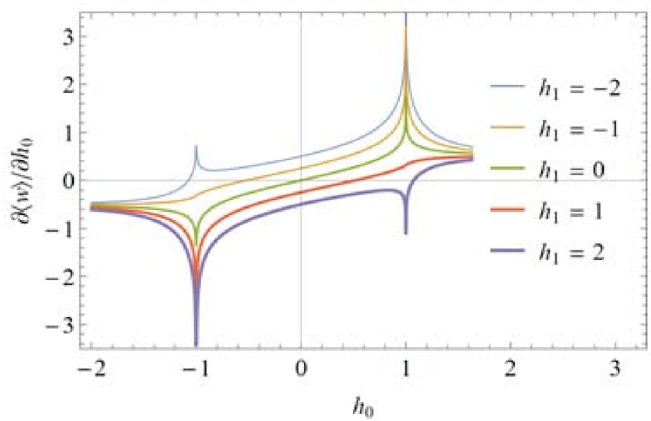

Figure 2. The derivative $\partial\langle w\rangle/\partial h_0$ diverges at the pre-quench critical fields $h_0 = \pm 1$, except when $h_1 = h_0$.

This result shows that the leading divergence in the derivative $\partial\langle w\rangle/\partial h_0$ is logarithmic in $|h_0 - 1|$. This divergence vanishes when $h_0 = h_1 = 1$. Similarly, an expansion about $h_0 = -1$ yields

$$\frac{\partial\langle w\rangle}{\partial h_0} \approx \frac{h_1}{\pi} + \frac{(h_1+1)}{2\pi}\ln\left|\frac{h_0+1}{8}\right|, \quad h_0 \approx -1 \tag{20}$$

These approximations about $h_0 = \pm 1$ are compared with the exact results in Figure 3 for the case when the post-quench Hamiltonian is also critical ($h_1 = \pm 1$). The logarithmic divergence is seen to be captured by the approximate expansions about $h_0 = \pm 1$ (dashed lines), and we find that the derivative remains continuous when $h_0 = h_1 = \pm 1$:

$$\left.\frac{\partial\langle w\rangle}{\partial h_0}\right|_{h_0=h_1=\pm 1} = \pm\frac{1}{\pi} \tag{21}$$

To finally prove that the average work per spin has inflection points at critical pre-quench fields, we need to verify that the second derivative $\partial^2\langle w\rangle/\partial h_0^2$ changes sign at $h_0 = \pm 1$, as depicted in Figure 4. Let us define the complement $h_0'^2 \equiv 1 - h_0^2$. The second derivative becomes

$$\frac{\partial^2\langle w\rangle}{\partial h_0^2} = \frac{\operatorname{sgn} h_0}{\pi h_0^2 h_0'^2}\Re[(h_0^3 + h_0^2 h_1 - 2h_1)E(h_0^{-1}) + h_0'^2(h_0 + h_1)K(h_0^{-1})] \tag{22}$$

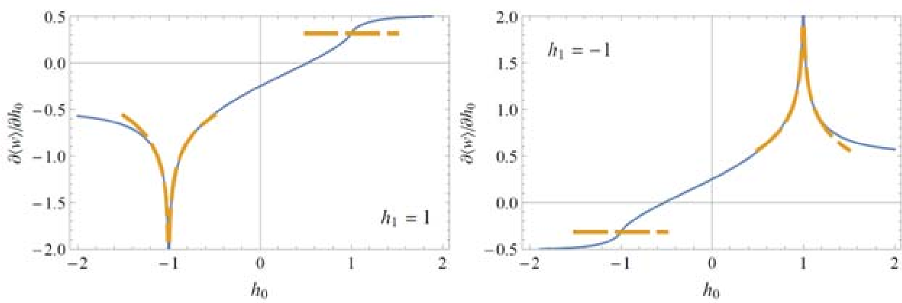

Figure 3. The derivative $\partial\langle w\rangle/\partial h_0$ (solid line) diverges logarithmically at the critical fields except at $h_0 = h_1 = \pm 1$. The approximate expansions about $h_0 = \pm 1$ are also shown (dashed lines).

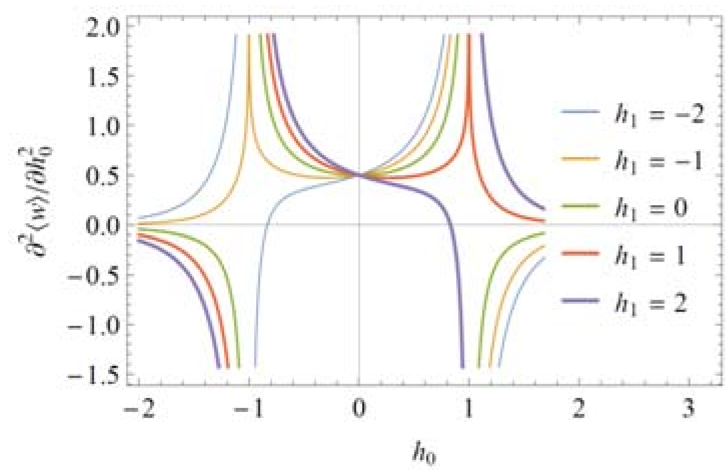

Figure 4. The second derivative $\partial^2\langle w\rangle/\partial h_0^2$ changes sign at the pre-quench critical fields $h_0 = \pm 1$, except when $h_1 = h_0$. In the special case when both Hamiltonians are at the same critical field $h_0 = h_1 = \pm 1$ (black arrows), the second derivative of the average work per spin diverges logarithmically at $h_0 = \pm 1$.

Again, asymptotic expansions about h_0 give the following leading order divergences when $h_0 \neq h_1 \neq 1$:

$$\frac{\partial^2\langle w\rangle}{\partial h_0^2} \sim \frac{1}{2\pi}\frac{h_1 \mp 1}{h_0 \mp 1}, \qquad (h_0 \approx \pm 1) \tag{23}$$

Since this derivative changes sign at $h_0 = \pm 1$, we confirm that the average work per spin indeed has inflection points when the pre-quench field is at its critical value and $h_1 \neq h_0$. This time, in the special case that the post-quench field is critical $h_1 = \pm 1$, the leading divergence of the second derivative at $h_0 = h_1$ is logarithmic:

$$\left.\frac{\partial^2\langle w\rangle}{\partial h_0^2}\right|_{h_1=\pm 1} \sim -\frac{5}{2\pi} - \frac{1}{\pi}\ln\left|\frac{h_0 \mp 1}{8}\right|, \quad (h_0 \approx \pm 1) \qquad (24).$$

DISCUSSION AND CONCLUSION

We have calculated the average work done in a zero temperature field quench of the quantum Ising model. In the thermodynamic limit, we presented an exact expression for the average work per spin $\langle w\rangle$ in terms of complete elliptic integrals. We have shown that the average work per spin is not infinitely differentiable at the pre-quench fields $h_0 = \pm 1$, where a quantum phase transition occurs. When the post-quench field $h_1 \neq \pm 1$, the first derivative $\partial\langle w\rangle/\partial h_0$ does not exist and diverges logarithmically at $h_0 = \pm 1$. In this case, the non-analyticity at the critical point takes the form of an inflection point. When the post-quench Hamiltonian is also critical, the non-analyticity at $h_0 = h_1 = \pm 1$ is weakened. That is, the first derivative $\partial\langle w\rangle/\partial h_0$ at $h_0 = h_1$ exists and the logarithmic divergence first appears in the second derivative $\partial^2\langle w\rangle/\partial h_0^2$.

It is interesting to note that complete elliptic integrals are encountered frequently in the study of the quantum Ising model. In fact, the derived expression for the average work done (10) is similar to that for the transverse magnetization of the quantum Ising model (Niemeijer 1967). Some exact solutions on a chain of spins 1/2. Physica 36:377-419). That is, if $\bar{m}$ is the average magnetization of the ground state of the Ising model with field h_0:

$$\bar{m} = \lim_{N\to\infty}\frac{1}{N}\sum_{i=1}^{N}\langle\varphi(0)|\sigma_i^z|\varphi(0)\rangle \qquad (25),$$

then $\langle w\rangle = (h_0 - h_1)\bar{m}/2$. Thus, the logarithmic divergence (19) of the field derivative $\partial\langle w\rangle/\partial h_0$ at the pre-quench quantum critical point also mirrors the logarithmic divergence of the zero-temperature magnetic susceptibility $\chi_{T\to 0} = \partial\bar{m}/\partial h$ of an unquenched Ising model at the critical field $h = \pm 1$, where the excitation gap vanishes and the quantum phase transition occurs.

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NOTE

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