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Supporting material for “Emergent thermodynamics in a quenched quantum many-body system”

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Appendix A: Diagonalization of the transverse Ising model

The quantum Ising model in a transverse field describes a lattice of spin-1/2 particles that interact with their nearest-neighbours via ferromagnetic coupling along the z -axis and with an external field applied along the x -axis. For a spatially homogeneous one-dimensional lattice of N spins in a uniform field, the Hamiltonian is

$$H = - \sum_{j=1}^N \lambda \sigma_j^x + \sigma_j^z \sigma_{j+1}^z, \quad (\text{S-1})$$

where λ is a dimensionless parameter that measures the strength of the external field and the Pauli spin-1/2 operators are defined with periodic boundary conditions $\sigma_{N+1}^\alpha = \sigma_1^\alpha$ ($\alpha = x, y, z$). Under the canonical transformation $\sigma_j^x \rightarrow \sigma_j^z, \sigma_j^z \rightarrow -\sigma_j^x \forall j$ the Hamiltonian Eq. (S-1) becomes

$$H = - \sum_{j=1}^N \lambda \sigma_j^z + \sigma_j^x \sigma_{j+1}^x, \quad (\text{S-2})$$

The spin operators are mapped to a spinless fermionic operators by a Jordan-Wigner transformation, thus

$$c_j = \frac{1}{2} \prod_{l=1}^{j-1} \sigma_l^z (\sigma_j^x + i \sigma_j^y),$$

$$c_j^\dagger = \frac{1}{2} \prod_{l=1}^{j-1} \sigma_l^z (\sigma_j^x - i \sigma_j^y).$$

Here, the operators c_j (c_j^\dagger) annihilate (create) a Jordan-Wigner fermion at the j^{th} lattice site and obey the usual fermionic anti-commutation relations. This in turn allows the definition of the parity operator

$$\Pi := \prod_{j=1}^N [1 - 2c_j^\dagger c_j],$$

which measures whether the number of fermions in the chain is even ($\Pi = 1$) or odd ($\Pi = -1$). Following the Jordan-Wigner transformation the Hamiltonian Eq. (S-2) factorises

into two orthogonal parity subspaces,

$$H = P^+ H^+ P^+ + P^- H^- P^-.$$

Here, $P^\pm = (1/2)(1 \pm \Pi)$ are the projectors onto the even (+) and odd (-) parity subspaces and

$$H^\pm = -\lambda - \sum_j^N \left(2\lambda c_j^\dagger c_j - (c_j^\dagger c_{j+1} + c_{j+1} c_j + \text{h.c.}) \right), \quad (\text{S-3})$$

are the even and odd parity subspace contributions to the Hamiltonian. The even and odd parity subspace Hamiltonians are identical with the exception that in H^+ we impose the boundary condition $c_{N+1} = -c_1$ and in H^- we impose $c_{N+1} = c_1$. Note that the parity of the chain is conserved ($[H^\pm, \Pi] = 0$); the Hamiltonian in Eq. (S-3) does not mix the parity subspaces. Initialising the system in a state with zero projection onto, say, the odd subspace then restricts the dynamics to the even subspace only. For an initial Gibbs state, the system is a mixture of positive and negative parity states and both subspaces must be accounted for. Despite this we restrict our attention to the even parity subspace only. This treatment becomes exact in the thermodynamic limit where boundary effects become negligible. This is the correct limit in which to discuss phase transitions, however a discussion of the fluctuation theorems is more suited to a finite chain. The analysis of a chain of arbitrary length in which both parity subspaces are accounted follows from a straightforward extension of what is presented here at the expense of more cumbersome expressions and provides little extra insight. Note that, in the main text, the fact that we consider the even subspace only is denoted by the summation over the set of positive parity pseudomomenta $k \in K^+$ in all relevant expressions. In the main text the ‘+’ superscript that is used here to explicitly distinguish between the positive and negative parity subspaces is dropped for the sake of brevity.

The diagonalisation of the Hamiltonian is completed by application of a Fourier transformation followed by a Bogolyubov transformation, which factorizes over the spaces with different pseudomomentum k . For the positive parity contribution to the Hamiltonian the Fourier transformation is

defined as

$$c_j = \frac{e^{-i\pi/4}}{\sqrt{N}} \sum_{k \in K^+} c_k e^{ikj},$$

where the values of pseudomomentum are

$$K^+ = \left\{ k = \pm \frac{\pi}{N} (2n-1), \quad n = 1, \dots, \frac{N}{2} \right\}.$$

After this transformation the Hamiltonian Eq. (S-3) takes the form

$$H^+ = \sum_{k \in K^+} 2(\lambda - \cos(k)) c_k^\dagger c_k + \sin(k) (c_k^\dagger c_{-k}^\dagger + c_{-k} c_k) - \lambda.$$

Note that all the terms preserve pseudomomentum so that the remaining step of the diagonalization can be performed within each subspace with assigned value of $\pm k$. The last step is the Bogolyubov transformation

$$c_{\pm k} = \gamma_{\pm k} \cos\left(\frac{\phi_k}{2}\right) \mp \gamma_{\mp k}^\dagger \sin\left(\frac{\phi_k}{2}\right), \quad (\text{S-4})$$

where

$$\begin{aligned} \cos(\phi_k) &= \frac{\lambda - \cos(k)}{\sqrt{\sin^2(k) + [\lambda - \cos(k)]^2}}, \\ \sin(\phi_k) &= \frac{\sin(k)}{\sqrt{\sin^2(k) + [\lambda - \cos(k)]^2}}. \end{aligned} \quad (\text{S-5})$$

With this, the Hamiltonian can be written in the form

$$H^+ = \sum_{k \in K^+} \epsilon_k \left(\gamma_k^\dagger \gamma_k - \frac{1}{2} \right),$$

with the dispersion relation

$$\epsilon_k = 2\sqrt{\sin^2(k) + [\lambda - \cos(k)]^2}.$$

Note that $\epsilon_k = \epsilon_{-k} > 0$ and that the total spectrum is symmetric with respect to the zero of energy.

Appendix B: Connecting the initial and final Hamiltonians

To evaluate the characteristic function explicitly, the eigenstates of the initial Hamiltonian $H^+(\lambda_0)$ must be written in terms of the eigenstates of the final Hamiltonian $H^+(\lambda_\tau)$. Inverting Eq. (S-4) and its hermitian conjugate it is possible to relate the sets of pre- and post-quench Bogolyubov operators. Hence,

$$\begin{aligned} \tilde{\gamma}_k &= \gamma_k \cos\left(\frac{\Delta_k}{2}\right) + \gamma_{-k}^\dagger \sin\left(\frac{\Delta_k}{2}\right), \\ \tilde{\gamma}_{-k} &= \gamma_{-k} \cos\left(\frac{\Delta_k}{2}\right) - \gamma_k^\dagger \sin\left(\frac{\Delta_k}{2}\right). \end{aligned}$$

Here $\Delta_k = \tilde{\phi}_k - \phi_k$ and the expressions for the pre- and post-quench Bogolyubov angles, ϕ_k and $\tilde{\phi}_k$, have the form given

in Eq.(S-5) with $\lambda = \lambda_0$ and λ_τ respectively. Using this, the vacuum states in the two representations are related by

$$|0_k, 0_{-k}\rangle = \left(\cos\left(\frac{\Delta_k}{2}\right) + \sin\left(\frac{\Delta_k}{2}\right) \tilde{\gamma}_k^\dagger \tilde{\gamma}_{-k}^\dagger \right) |\tilde{0}_k, \tilde{0}_{-k}\rangle. \quad (\text{S-6})$$

The expressions for higher energy eigenstates $|n_k, n_{-k}\rangle$ are then obtained by applying the appropriate creation operators to Eq. (S-6).

Appendix C: Calculation of the average work

The calculation for the average work done on a quenched transverse Ising model takes advantage of the factorization of $H^+(\lambda_0)$ and $H^+(\lambda_\tau)$ into blocks of paired pseudomomenta with labels $\pm k$. We start by writing the density matrix of the system as $\rho = \bigotimes_{k>0} \rho_{\pm k}$, so that

$$\langle W \rangle = \text{Tr} \left[\sum_{k>0} (H_{\pm k}^+(\lambda_\tau) - H_{\pm k}^+(\lambda_0)) \bigotimes_{k'>0} \rho_{\pm k'} \right], \quad (\text{S-7})$$

where $H_{\pm k}^+(\lambda_\tau) = \epsilon_k(\lambda_\tau)(\tilde{\gamma}_k^\dagger \tilde{\gamma}_k + \tilde{\gamma}_{-k}^\dagger \tilde{\gamma}_{-k} - 1)$ and $H_{\pm k}^+(\lambda_0) = \epsilon_k(\lambda_0)(\gamma_k^\dagger \gamma_k + \gamma_{-k}^\dagger \gamma_{-k} - 1)$. With a little effort, Eq. (S-7) can be rewritten as

$$\langle W \rangle = \sum_{k>0} \text{Tr} \left[(H_{\pm k}^+(\lambda_\tau) - H_{\pm k}^+(\lambda_0)) \prod_{k'>0} \sigma_{\pm k'} \right], \quad (\text{S-8})$$

where,

$$\sigma_{\pm k} = \sum_{n_{\pm k}=0,1} |n_k, n_{-k}\rangle \langle n_k, n_{-k}| \frac{e^{-\beta \epsilon_k(\lambda_0)(n_k + n_{-k} - 1)}}{4 \cosh^2(\beta \epsilon_k(\lambda_0)/2)}.$$

Noting that $\text{Tr} \left[\prod_{k'>0} \sigma_{\pm k'} \right] = 1$, Eq.(S-8) reduces to the form $\langle W \rangle = \sum_{k>0} \langle W_k \rangle$, with

$$\langle W_k \rangle = \text{Tr} \left[(H_{\pm k}^+(\lambda_\tau) - H_{\pm k}^+(\lambda_0)) \sigma_{\pm k} \right].$$

In order to calculate the trace we note that we need only keep the terms of $H_{\pm k}^+(\lambda_\tau)$ that are diagonal in the basis of $H_{\pm k}^+(\lambda_0)$;

$$[H_{\pm k}^+(\lambda_\tau)]_{\text{diag}} = \epsilon_k(\lambda_\tau) \cos(\Delta_k) (\gamma_k^\dagger \gamma_k + \gamma_{-k}^\dagger \gamma_{-k} - 1).$$

With this, $\langle W_k \rangle$ takes form

$$\langle W_k \rangle = (\cos(\Delta_k) \epsilon_k(\lambda_\tau) - \epsilon_k(\lambda_0)) \text{Tr} [(n_k + n_{-k} - 1) \sigma_{\pm k}],$$

which leads straightforwardly to the expression for the average work in the main text.