Variational GS energy error

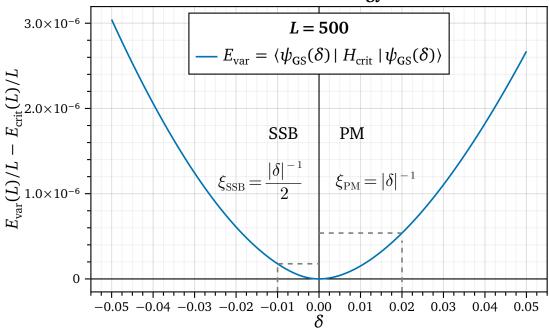


Figure 1: Plot of the variational ground-state energy density error (1) as a function of the perturbation coupling δ , defined in (2). System size is L = 500.

Figure 1 displays the variational ground-state energy density error,

$$\frac{E_{\text{var}} - E_{\text{crit}}}{L},\tag{1}$$

plotted as a function of the perturbative coupling δ in system size L=500. $E_{\rm var}(L)$ reads as $E_{\rm var}(L)=\langle \psi_{\rm GS}(\delta)|H_{\rm crit}|\psi_{\rm GS}(\delta)\rangle$, whereas $\psi_{\rm GS}(\delta)$ is the ground state of the Hamiltonian,

$$H(\delta) = -\sum_{n=1}^{L-1} \sigma_n^x \sigma_{n+1}^x - (1+\delta) \sum_{n=1}^{L} \sigma_n^z,$$
 (2)

and $H_{\text{crit}} = H(0)$. Furthermore, $E_{\text{crit}}(L) = -2/\sin(\pi/(2L))$.

We solve the quadratic Hamiltonian (2) with its free fermion representation and obtain its ground state and ground state energy density numerically exactly [1], allowing us to measure observable (1) numerically.

One can observe a small bias towards the paramagnetic (PM) phase ($\delta > 0$) in terms of lower energies as opposed to the spontaneous-symmetry breaking (SSB) phase ($\delta < 0$) as a function of δ .

The grey dashed lines are a guide to the eye, visualizing lines of constant correlation length $\xi(\chi)$ (vertical part), and therefore constant bond dimension χ , $\xi(\chi) \propto |\delta|^{-\nu}$. As discussed in the main text, the correlation length in the SSB phase scales with a factor of 1/2 of that in the trivial PM phase, since the excitations in the SSB phase are domain walls, and one therefore needs two quasiparticles to create nontrivial correlations on top of the ground state, as opposed to a single quasiparticle in the PM phase. That implies, in the Ising model, $\xi(\chi) = a_{\delta \leq 0} |\delta|^{-1}$ with $a_{\delta < 0} = 1/2$ and $a_{\delta > 0} = 1$. Hence, we show a case where the perturbation, induced by a finite bond dimension (or correlation length), takes an amplitude of $\delta_{\rm SSB} = -0.01$, and $\delta_{\rm PM} = +0.02$, leading to their respective variational ground-state energy density error. Of these two candidates, the SSB GS energy is lower than that of the PM candidate (horizontal part). This shows the fact that the different proportionality constants $a_{\delta \leq 0}$ result in a clear preferred ground state when it comes to the variational optimization performed by the DMRG algorithm: the variational ground state in the SSB phase, which coincidentally is the case of higher entanglement entropy; see Fig. 2 for L=500, where we display the half-chain von Neumann entanglement entropy,

$$\rho_{A}(\delta) = \text{Tr}_{\neg A}(|\psi(\delta)\rangle\langle\psi(\delta)|) \tag{3}$$

$$S_A(\delta) = -\text{Tr}(\rho_A \log(\rho_A)) \tag{4}$$

Half-chain entanglement entropy of the variational GS

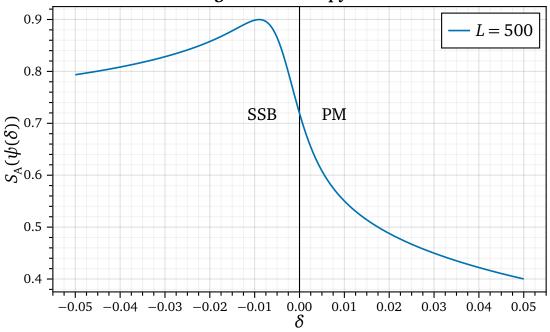


Figure 2: Plot of the half-chain von Neumann entanglement entropy of the variational ground state of (2) as a function of the perturbation coupling δ . System size is L = 500. Subsystem A comprises sites $A = 1, \ldots, L/2$, and we partially trace over its complement.

The limiting behavior of the half-chain entanglement entropy is $\lim_{\delta \to -\infty} S_A(\psi(\delta)) = \log(2) \approx 0.693$ and $\lim_{\delta \to +\infty} S_A(\psi_{GS}(\delta)) = 0$. This is because the limiting SSB GS $(\delta \to -\infty)$ is doubly degenerate and given in terms of the maximally mixed two Néel states, which are product states, while the limiting PM GS $(\delta \to +\infty)$ is a trivial, fully polarized product state. In the thermodynamic limit, the entanglement entropy diverges logarithmically with the correlation length at $\delta = 0$, as $S = c \log(\xi)/6 + \text{const} \propto -c \nu \log(|\delta|)$.

References

[1] J. Surace and L. Tagliacozzo, *Fermionic Gaussian states: An introduction to numerical approaches*, SciPost Physics Lecture Notes p. 054 (2022), 10.21468/SciPostPhysLectNotes.54.