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Exact results for fidelity susceptibility of the quantum Ising model: the interplay between parity, system size, and magnetic field

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Abstract

We derive an exact closed-form expression for fidelity susceptibility of even- and odd-sized quantum Ising chains in a transverse field. To this aim, we diagonalize the Ising Hamiltonian and study the gap between its positive and negative parity subspaces. We derive an exact closed-form expression for the gap and use it to identify the parity of the ground state. We point out the misunderstanding in some of the former studies of fidelity susceptibility and discuss its consequences. Last but not least, we rigorously analyze the properties of the gap. For example, we derive analytical expressions showing its exponential dependence on the ratio between the system size and the correlation length.

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1. Introduction

Quantum phase transitions happen at zero absolute temperature when there are competing interactions trying to order the sample in different ways [1]. The balance between them is typically controlled by an external field such as a magnetic field acting on spins or the laser field imposing a periodic potential on cold atoms or ions [2, 3]. When this field reaches the critical value, the system is at the quantum critical point. Then, a small tilt of the field moves

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the system into one of the phases changing its properties significantly (e.g. magnetization, correlation functions, etc).

Several approaches to quantum phase transition have been proposed. The fairly recent one that we explore focuses on the (ground state) fidelity: $|\langle\psi(g)|\psi(g+\delta)\rangle|$, where $|\psi(g)\rangle$ is a ground-state wave-function of some Hamiltonian $\hat{H}(g)$, g is the external field whose variation induces a quantum phase transition, and δ is a small, but otherwise arbitrary, shift of this field [4]. This approach has been studied in a stunning variety of models. For example, numerous spin models (Ising, XY, XXZ, Heisenberg, Kitaev, Lipkin–Meshkov–Glick, etc), Hubbard, Bose–Hubbard, and Hubbard–Holstein models, Harper model, Dicke model, Luttinger liquid model, etc (see the review paper of Gu [5] and references therein). Dramatic change of the system’s properties across the critical point results in a drop of fidelity enabling both the location of the critical point and the determination of the universal critical exponent ν characterizing the divergence of the correlation length [4, 6–14].

We will study here fidelity susceptibility $\chi(g)$, which is defined through the Taylor expansion of fidelity in the field shift δ :

$$|\langle\psi(g)|\psi(g+\delta)\rangle| = 1 - \chi(g)\frac{\delta^2}{2} - \chi'(g)\frac{\delta^3}{4} + \mathcal{O}(\delta^4), \quad (1)$$

where we assumed that the ground states are normalized: $\langle\psi(g)|\psi(g)\rangle = 1$. This expansion is valid in the limit of $\delta \rightarrow 0$ taken at the fixed system size N . Fidelity approaches unity in this limit. Note that there exists the other limit of $N \rightarrow \infty$ taken at the fixed field shift δ [9–13]. In such limit fidelity approaches zero, which is known as the Anderson orthogonality catastrophe [15].

2. Model

We study fidelity susceptibility of the quantum Ising model in a transverse field. This is a paradigmatic model of a quantum phase transition [1] that can be experimentally realized in magnetic materials such as CoNb_2O_6 [16]. Its promising experimental emulation in an ion chain was proposed in [17]. The Hamiltonian that we study reads

$$\hat{H}(g) = - \sum_{i=1}^N (\sigma_i^x \sigma_{i+1}^x + g \sigma_i^z), \quad (2)$$

where g is the magnetic field, $N > 2$ is the number of spins, and we assume periodic boundary conditions $\vec{\sigma}_{N+1} = \vec{\sigma}_1$. For $|g| > 1$ the system is in the paramagnetic phase, while for $|g| < 1$ it is in the ferromagnetic phase. The critical points are at $g_c = \pm 1$.

A simple calculation leads to the following expression for fidelity susceptibility [4]

$$\chi(g) = \frac{1}{4} \sum_{k>0} \frac{\sin^2 k}{(g^2 - 2g \cos k + 1)^2}, \quad (3)$$

where k is the momentum of quasiparticles introduced to diagonalize the Hamiltonian (2).

Our goal is to derive an exact closed-form expression for fidelity susceptibility for *all* system sizes N and magnetic fields g (for some approximate studies of fidelity susceptibility in the Ising chain see e.g. [4–6]). The first step in this direction was done in [18], where even-sized chains were studied. We extend this result to the odd system sizes here. This requires precise determination of what momenta k should be placed into the sum (3), which we discuss in sections 3 and 4. The two choices that were employed in the past are

$$k = \frac{\pi}{N}, \frac{3\pi}{N}, \frac{5\pi}{N}, \dots \quad (4)$$

and

$$k = \frac{2\pi}{N}, \frac{4\pi}{N}, \frac{6\pi}{N}, \dots \quad (5)$$

We will *analytically* show in sections 5 and 6 that these two sets of momenta lead to significantly different results for fidelity susceptibility near the critical point (this difference was numerically pointed out in the context of Quantum Monte Carlo simulations of fidelity susceptibility in [7]). An exact closed-form expression for fidelity susceptibility in odd-sized systems will be derived in section 5 and combined with the even N result from [18], so that the complete expression for fidelity susceptibility in the Ising chain will be finally obtained. Finally, we will discuss in section 6 the consequences of incorrect quantization of momenta.

3. Diagonalization

All the steps discussed in this section are very elementary, but they are often presented incompletely in the literature. This presumably leads to misunderstandings discussed in section 6. As a matter of fact, the discussion of the ground state of the Hamiltonian (2) for all magnetic fields and system sizes is not as trivial as usually assumed (section 4). We mention in passing that none of the standard references to the Ising model diagonalization [1, 19–21] provides a complete discussion of the ground state determination in a *finite* system.

The first step to diagonalize the Hamiltonian (2) is to perform the Jordan–Wigner transformation:

$$\sigma_i^z = 1 - 2\hat{c}_i^\dagger \hat{c}_i, \quad \sigma_i^x = (\hat{c}_i + \hat{c}_i^\dagger) \prod_{j<i} (1 - 2\hat{c}_j^\dagger \hat{c}_j), \quad \{\hat{c}_i, \hat{c}_j^\dagger\} = \delta_{ij}, \quad \{\hat{c}_i, \hat{c}_j\} = 0.$$

After this transformation and some additional manipulations one finds

$$\begin{aligned} \hat{H} &= - \sum_{i=1}^{N-1} \hat{f}_{i,i+1} + \hat{f}_{N,1} \hat{P} - g \sum_{i=1}^N (\hat{c}_i \hat{c}_i^\dagger - \hat{c}_i^\dagger \hat{c}_i), \quad \hat{f}_{i,j} = \hat{c}_i^\dagger \hat{c}_j - \hat{c}_i \hat{c}_j^\dagger - \hat{c}_i \hat{c}_j + \hat{c}_i^\dagger \hat{c}_j^\dagger, \\ \hat{P} &= \prod_{i=1}^N (1 - 2\hat{c}_i^\dagger \hat{c}_i), \end{aligned}$$

where \hat{P} is the parity operator, whose eigenvalues are either +1 (positive parity eigenstate) or −1 (negative parity eigenstate). This can be rewritten as

$$\hat{H} = \hat{H}^+ \hat{P}^+ + \hat{H}^- \hat{P}^-, \quad \hat{H}^\pm = - \sum_{i=1}^N [\hat{f}_{i,i+1} + g(\hat{c}_i \hat{c}_i^\dagger - \hat{c}_i^\dagger \hat{c}_i)], \quad \hat{P}^\pm = \frac{1}{2}(1 \pm \hat{P}),$$

where \hat{P}^+ and \hat{P}^- are the projectors onto the subspaces with an even and odd number of c -particles, respectively. The boundary conditions for \hat{H}^+ are antiperiodic

$$\hat{c}_{N+1} = -\hat{c}_1, \quad (6)$$

while for \hat{H}^- they are periodic

$$\hat{c}_{N+1} = \hat{c}_1. \quad (7)$$

Since the parity operator commutes with the Hamiltonian, one can find the eigenstates of both \hat{H} and \hat{P} . This allows for independent diagonalization in the subspaces of positive and negative parity. These simple calculations have to be done independently in even- and odd-sized chains.

Even number of spins, positive parity subspace. We perform the Fourier transform

$$\hat{c}_j = \frac{\exp(-i\pi/4)}{\sqrt{N}} \sum_k \hat{c}_k \exp(ikj), \quad (8)$$

where

$$k = \pm \frac{\pi}{N}, \pm \frac{3\pi}{N}, \dots, \pm \left(\pi - \frac{\pi}{N} \right)$$

to satisfy equation (6). This leads to the Hamiltonian

$$\hat{H}^+(\text{even } N) = \sum_k \hat{h}_k, \quad \hat{h}_k = [g - \cos(k)] [\hat{c}_k^\dagger \hat{c}_k - \hat{c}_{-k} \hat{c}_{-k}^\dagger] + \sin(k) [\hat{c}_k^\dagger \hat{c}_{-k}^\dagger + \hat{c}_{-k} \hat{c}_k],$$

which is diagonalized by the Bogolubov transformation

$$\hat{c}_k = \cos\left(\frac{\theta_k}{2}\right) \hat{\gamma}_k - \sin\left(\frac{\theta_k}{2}\right) \hat{\gamma}_{-k}^\dagger, \quad (\sin \theta_k, \cos \theta_k) = \left(\frac{\sin(k)}{\epsilon_k}, \frac{g - \cos(k)}{\epsilon_k} \right), \quad (9)$$

where another quasiparticle operator,

$$\hat{\gamma}_k = \cos\left(\frac{\theta_k}{2}\right) \hat{c}_k + \sin\left(\frac{\theta_k}{2}\right) \hat{c}_{-k}^\dagger, \quad \{\hat{\gamma}_k, \hat{\gamma}_{k'}^\dagger\} = \delta_{kk'}, \quad \{\hat{\gamma}_k, \hat{\gamma}_{k'}\} = 0,$$

has been introduced. Finally, the diagonalized Hamiltonian becomes

$$\hat{H}^+(\text{even } N) = \sum_k \epsilon_k (2\hat{\gamma}_k^\dagger \hat{\gamma}_k - 1), \quad \epsilon_k = \sqrt{[g - \cos(k)]^2 + \sin^2(k)}.$$

The ground-state is then annihilated by all the operators $\hat{\gamma}_k$. It can be written as

$$\prod_{k>0} \left(\cos\left(\frac{\theta_k}{2}\right) - \sin\left(\frac{\theta_k}{2}\right) \hat{c}_k^\dagger \hat{c}_{-k}^\dagger \right) |\text{vac}\rangle, \quad (10)$$

where $|\text{vac}\rangle$ is annihilated by all \hat{c}_k operators. This ground state contains an even number of c -particles. It belongs to the positive parity subspace. Its eigenenergy is

$$\varepsilon^+(\text{even } N) = - \sum_k \epsilon_k. \quad (11)$$

Combining equations (10), (9), and (1) one obtains equation (3). The same summand appears for all parities and system sizes.

Even number of spins, negative parity subspace. We perform the Fourier transform (8) with momenta

$$k = 0, \pm \frac{2\pi}{N}, \pm \frac{4\pi}{N}, \dots, \pm \left(\pi - \frac{2\pi}{N} \right), \pi$$

to ensure that equation (7) holds. The transformed Hamiltonian reads:

$$\hat{H}^-(\text{even } N) = \sum_{k \in \{0, \pi\}} \hat{h}_k + (g-1)(\hat{c}_0^\dagger \hat{c}_0 - \hat{c}_0 \hat{c}_0^\dagger) + (g+1)(\hat{c}_\pi^\dagger \hat{c}_\pi - \hat{c}_\pi \hat{c}_\pi^\dagger).$$

The $k \in \{0, \pi\}$ part of the Hamiltonian is diagonalized with the Bogolubov transformation (9). Thus, there is an even number of quasiparticles in those modes (see the wave-function (10)). Therefore, the negative parity ground state will have either the $k = 0$ or the $k = \pi$ mode excited. Minimizing the eigenenergy we find that the $k = 0$ mode is occupied, the $k = \pi$ one is empty, and the eigenenergy is

$$\varepsilon^-(\text{even } N) = - \sum_{k \in \{0, \pi\}} \epsilon_k - 2. \quad (12)$$

Odd number of spins, positive parity subspace. We perform the Fourier transform (8) with momenta

$$k = \pm \frac{\pi}{N}, \pm \frac{3\pi}{N}, \dots, \pm \left(\pi - \frac{2\pi}{N} \right), \pi$$

to ensure that equation (6) holds. The transformed Hamiltonian reads:

$$\hat{H}^+(\text{odd } N) = \sum_{k \setminus \{\pi\}} \hat{h}_k + (g+1)(\hat{c}_\pi^\dagger \hat{c}_\pi - \hat{c}_\pi \hat{c}_\pi^\dagger).$$

The $k \setminus \{\pi\}$ part of the Hamiltonian is diagonalized with the Bogolubov transformation (9). Thus, there is an even number of quasiparticles in those modes. Therefore, the positive parity ground state will have to have the $k = \pi$ mode empty. Its eigenenergy is

$$\varepsilon^+(\text{odd } N) = - \sum_{k \setminus \{\pi\}} \epsilon_k - g - 1. \quad (13)$$

Odd number of spins, negative parity subspace. We perform the Fourier transform (8), but this time the summation goes over momenta

$$k = 0, \pm \frac{2\pi}{N}, \pm \frac{4\pi}{N}, \dots, \pm \left(\pi - \frac{\pi}{N}\right)$$

to satisfy equation (7). After this transform

$$\hat{H}^-(\text{odd } N) = \sum_{k \setminus \{0\}} \hat{h}_k + (g-1)(\hat{c}_0^\dagger \hat{c}_0 - \hat{c}_0 \hat{c}_0^\dagger).$$

The $k \setminus \{0\}$ part of the Hamiltonian is diagonalized by the Bogolubov transformation (9). This implies that the number of quasiparticles in the $k \setminus \{0\}$ modes is even. The total number of quasiparticles in the negative parity ground state is odd. Therefore, the diagonal $k = 0$ mode has to be occupied. The eigenenergy of such a ground state is

$$\varepsilon^-(\text{odd } N) = - \sum_{k \setminus \{0\}} \epsilon_k + g - 1. \quad (14)$$

Next, we will compare the ground state energies in the positive and negative parity subspaces to find out the ground state of the whole (not just the *parity-projected*) Hamiltonian.

4. Ground state and gap

We have identified ground states in the positive and negative parity subspaces. Next, we find that

$$\varepsilon^- - \varepsilon^+ = g^N \int_0^1 dt \frac{4N t^{N-3/2} \sqrt{(1-t)(1-g^2 t)}}{1 - (gt)^{2N}} \quad \text{for } |g| < 1, \quad (15)$$

$$\varepsilon^- - \varepsilon^+ = \text{sign}(g^N)(2|g| - 2) + g^{-N} \int_0^1 dt \frac{4N t^{N-3/2} \sqrt{(1-t)(g^2 - t)}}{1 - t^{2N}/g^{2N}} \quad \text{for } |g| > 1, \quad (16)$$

$$\varepsilon^- - \varepsilon^+ = 2 \tan\left(\frac{\pi}{4N}\right) \text{sign}(g^N) \quad \text{at } g = \pm 1. \quad (17)$$

Expressions (15)–(17) are valid for any system size $N > 2$. Two remarks are presented below.

First, these expressions show that

$$\text{sign}(\varepsilon^- - \varepsilon^+) = \text{sign}(g^N),$$

which holds for all magnetic fields g and system sizes N . Therefore, the ground state of the Hamiltonian (2) has positive parity when N is even. On the other hand, when N is odd, the parity of the ground state is positive for $g > 0$ and negative for $g < 0$. This has interesting consequences for fidelity susceptibility (section 5). These remarks are summarized in table 1; see also [7], where the Perron–Frobenius theorem is employed to argue that the parity of the ground state is positive for $g > 0$.

Table 1. Parity of the Ising chain ground state.

	$g > 0$	$g < 0$
Even N	+	+
Odd N	+	−

Second, the above expressions quantify the gap between positive and negative parity ground states, which is important in understanding symmetry breaking in the Ising model, as well as in other contexts including adiabatic driving across the first order phase transition [22]. The gap in the ferromagnetic phase is bounded by the following inequalities

$$\max \left(g^N \frac{2}{\sqrt{\pi}} \frac{\sqrt{1-g^2}}{\sqrt{N}}, g^N \frac{4g}{\pi N} \right) \leq \varepsilon^- - \varepsilon^+ \leq g^N 2 \frac{\sqrt{1-g^2}}{\sqrt{N-1}} + g^N \frac{\pi g}{2N-1}, \quad (18)$$

where equality happens at $g = 0$ (see appendix A for details; we assumed here that $0 \leq g \leq 1$ for convenience). Written in such a way, inequality (18) shows two limits.

In the thermodynamic limit—i.e., when the correlation length in the infinite Ising chain [23]

$$\xi \sim 1/|\ln g|$$

is much smaller than the size of the system—we see from inequality (18) that the gap is exponentially small in N :

$$\varepsilon^- - \varepsilon^+ = \mathcal{O}(\exp(-N/\xi)/\sqrt{N}).$$

This result is in agreement with the estimation from [22], where it is stated that the gap is smaller than any power law in N . It quantitatively shows how the two fold degeneracy of the ground state emerges when the system size increases.

When the size of the system is smaller than the correlation length, inequality (18) shows that

$$\varepsilon^- - \varepsilon^+ = \mathcal{O}(1/N).$$

The gap disappears then in the ferromagnetic phase as if the system would be at the critical point (17). It is so because this is the limit where finite-system size effects dominate physics.

We mention also that one can use equation (15) to prove that the gap is monotonically increasing from $g = 0$ to $g = \pm 1$, which is discussed in appendix A. Finally, we notice that the gap is always ‘macroscopic’ on the paramagnetic side (16)—the symmetry breaking does not occur there.

The qualitative content of these remarks about the disappearance of the gap is, of course, discussed in standard textbooks such as [1]. The novelty here is that we managed to obtain the closed-form expression for the gap, which allowed us to rigorously quantify its behavior. This adds another piece of the exact analytical insight to the plethora of already known analytical results for the quantum Ising model.

We will now discuss derivation of equations (15)–(17). We start from writing ϵ_k as $\sum_{\ell=0}^{\infty} a_{\ell} \cos(\ell k)$. Next, we substitute this expansion into equations (11)–(14) and use the identity $\sum_{s=0}^{n-1} \cos(x + sy) = \cos(x + (n-1)y/2) \sin(ny/2) \operatorname{cosec}(y/2)$ to obtain

$$\varepsilon^- - \varepsilon^+ = \operatorname{sign}(g^N) \Theta(|g| - 1) (2|g| - 2) - 2N(a_N + a_{3N} + a_{5N} + \dots), \quad (19)$$

where Θ is the Heaviside step function. This expression holds for any system size $N > 2$ and any magnetic field g .

Subsequently, we assume that $0 < g < 1$ (the derivation for different values of g proceeds in almost identical way and we will only quote the final result later). We write the Fourier coefficients for $\ell > 0$ as

$$a_\ell = \frac{1}{\pi} \int_{-\pi}^{\pi} dk \cos(k\ell) \sqrt{[g - \cos(k)]^2 + \sin^2(k)}.$$

Introducing $z = e^{ik}$, it is equivalent to

$$a_\ell = -\frac{1}{\pi} \oint_{|z|=1} dz \sqrt{\frac{(z-g)(gz-1)}{z}} z^{\ell-1},$$

with branch cuts along $(0, g) \cup (1/g, \infty)$. By deforming the integration contour, this leads to

$$a_\ell = -\frac{2g^\ell}{\pi} \int_0^1 dt \sqrt{(1-t)(1-g^2t)} t^{\ell-3/2}. \quad (20)$$

Substituting equation (20) into equation (19), one obtains equation (15). The derivation for $-1 < g < 0$ involves slightly different branch cuts and leads to the same final result. Thus, equation (15) holds for any $|g| < 1$.

The gap in the paramagnetic phase can be obtained through the Kramers–Wannier duality mapping

$$g \leftrightarrow \frac{1}{g} \quad (21)$$

from the gap in the ferromagnetic phase. This duality symmetry follows from the symmetry of the classical two dimensional Ising model discussed in the seminal [24]. The map between the two dimensional classical model and the one dimensional quantum model that we consider is described in [25]. The basics of the duality symmetry in the quantum context are discussed in [26], while its implications for fidelity and fidelity susceptibility are discussed in [11] and [18], respectively.

For the gap, we find that

$$\varepsilon^-(g) - \varepsilon^+(g) = \text{sign}(g^N)(2|g| - 2) + |g| \left[\varepsilon^-\left(\frac{1}{g}\right) - \varepsilon^+\left(\frac{1}{g}\right) \right] \quad \text{for } |g| > 1. \quad (22)$$

One can show this by performing the mapping (21) on equations (11)–(14), and then noting that $\epsilon_k(1/g) = \epsilon_k(g)/|g|$. Combining equations (22) and (15) one obtains equation (16).

Equation (17) can be directly evaluated with $\sum_{s=0}^{n-1} \sin(x + sy) = \sin(x + (n-1)y/2) \sin(ny/2) \text{cosec}(y/2)$. The same result can be obtained by taking the limit of $g \rightarrow \pm 1$ in equations (15) and (16).

Finally, we mention that it would be interesting to apply the above summation technique to compute the gap between the positive and negative parity ground states of the XY model. This gap was studied in [27], but no exact closed-form expressions were derived. It was found numerically in [27] that the parity of the ground state changes as the magnetic field is varied. This happens in the XY model for both even- and odd-sized systems at different magnetic fields. It would be quite interesting to provide an analytical characterization of this phenomenon coined in [27] as vacua competition.

5. Fidelity susceptibility

We can finally focus on our main goal: The computation of fidelity susceptibility. Using the results from section 3, we find that for any $N > 2$ and any magnetic field g , fidelity susceptibility of the lowest energy eigenstate in the positive parity subspace is

$$\chi^+(g) = \frac{N^2}{16g^2} \frac{g^N}{(g^N + 1)^2} + \frac{N}{16g^2} \frac{g^N - g^2}{(g^N + 1)(g^2 - 1)}, \quad (23)$$

while in the negative parity subspace it is

$$\chi^-(g) = -\frac{N^2}{16g^2} \frac{g^N}{(g^N - 1)^2} + \frac{N}{16g^2} \frac{g^N + g^2}{(g^N - 1)(g^2 - 1)}. \quad (24)$$

Thus, employing the results of section 4, we find that fidelity susceptibility of the *ground state* of the Ising Hamiltonian is the following. For even system sizes $\chi(g) = \chi^+(g)$ for any g , while for odd system sizes $\chi(g) = \chi^+(g)$ for $g > 0$ and $\chi(g) = \chi^-(g)$ for $g < 0$ (table 1). This can be written as

$$\chi(g) = \frac{N^2}{16g^2} \frac{|g|^N}{(|g|^N + 1)^2} + \frac{N}{16g^2} \frac{|g|^N - g^2}{(|g|^N + 1)(g^2 - 1)}$$

for any system size $N > 2$ and any magnetic field g . This result provides the ultimate expression for fidelity susceptibility of the Ising chain in a transverse field. It is worth to stress that its derivation required not only the ability to compute the sum (3), but also the careful diagonalization of the Ising Hamiltonian followed by the rigorous analysis of the gap between its positive and negative parity subspaces. We also mention that the difference between fidelity susceptibility of the positive and negative parity ground states was numerically quantified in [7].

We will now discuss the key steps allowing for the derivation of equations (23) and (24) for $g > 0$. The results for $g < 0$ can be obtained from the $g > 0$ ones by changing the summation in equation (3) from k to $\pi - k$.

The positive parity result (23) for even N was obtained in [18]. Since an analogous calculation can be performed for odd N and its outcome is exactly the same, we will not repeat it here.

Thus, we focus on the derivation of the negative parity result, i.e., equation (24). Since the calculations for even and odd N are similar and lead to the same final result, equation (24), we will sketch the derivation of the odd N result only. Our calculation starts from the identity [28]

$$\sum_k \left[\frac{\sin^2(k/2)}{\sinh(z)} + \frac{\tanh(z/2)}{2} \right]^{-1} = N \coth\left(\frac{Nz}{2}\right) - \coth\left(\frac{z}{2}\right), \quad k = \frac{2\pi}{N}, \frac{4\pi}{N}, \dots, \pi - \frac{\pi}{N}. \quad (25)$$

We multiply both sides of equation (25) by $\tanh(z/2)$ and take the derivative of the resulting equation with respect to z

$$\sum_k \frac{\sin^2(k/2)}{[\sinh^2(z/2) + \sin^2(k/2)]^2} = \frac{N}{\sinh(z)} \frac{d}{dz} \left[\coth\left(\frac{Nz}{2}\right) \tanh\left(\frac{z}{2}\right) \right]. \quad (26)$$

Then, we multiply equation (26) by $\cosh^4(z/2)$ and differentiate the resulting equation with respect to z to get

$$\frac{d}{dz} \sum_k \frac{\sin^2 k}{[\sinh^2(z/2) + \sin^2(k/2)]^2} = \frac{2N}{\cosh^2(z/2)} \frac{d}{dz} \left(\frac{\cosh^3(z/2)}{\sinh(z/2)} \frac{d}{dz} \left[\coth\left(\frac{Nz}{2}\right) \tanh\left(\frac{z}{2}\right) \right] \right). \quad (27)$$

Finally, we integrate equation (27) over z from 0 to x , use equation (26) in the limit of $z \rightarrow 0$ to compute $\sum_k \sin^{-2}(k/2) = (N^2 - 1)/6$, and rearrange the terms to obtain

$$\sum_k \frac{\sin^2 k}{[\sinh^2(x/2) + \sin^2(k/2)]^2} = 2N \left(\frac{\coth(Nx/2)}{\tanh(x)} - 1 \right) - \frac{N^2}{\sinh^2(Nx/2)}. \quad (28)$$

Equation (24) follows from the substitution of $x = \ln g$ into equation (28).

6. Discussion

We will discuss here the importance of proper quantization of momenta in fidelity susceptibility calculations. If one evaluates fidelity susceptibility (3) over momenta (4) then it equals $\chi^+(g)$. The evaluation of sum (3) over momenta (5) leads to $\chi^-(g)$. The two expressions are different. Their difference comes from shifting the summation over momenta by mere π/N , which may seem to be insignificant for $N \gg 1$. This impression is incorrect near the critical point and correct far away from it. Two problems arise from the improper quantization of momenta.

Wrong symmetry of fidelity susceptibility in odd-sized systems. Fidelity susceptibility of the Ising chain in the ground state should be symmetric with respect to the

$$g \leftrightarrow -g \quad (29)$$

mapping because the spin–spin interactions in the Hamiltonian (2) order the system in the $\pm x$ direction and so it should not matter whether the magnetic field points in the $+z$ or $-z$ direction.

For even-sized systems the quantization of momenta (parity of the ground state) does not have to change after reflection (29) to ensure the symmetry of fidelity susceptibility: $\chi^+(g) = \chi^+(-g)$ when N is even.

For odd-sized systems the situation is more complicated because neither $\chi^+(g)$ nor $\chi^-(g)$ is symmetric with respect to the mapping (29). Thus, one needs a different quantization of momenta (parity of the ground state) for positive and negative magnetic fields to ensure the symmetry of fidelity susceptibility (table 1). When properly calculated, ground state fidelity susceptibility is symmetric with respect to reflection (29) in odd-sized systems due to the

$$\chi^+(g) = \chi^-(-g)$$

relation. The wrong symmetry of fidelity susceptibility implies its wrong magnitude near *at least* one of the critical points, which brings us to the second problem.

Wrong magnitude of fidelity susceptibility near the critical point. We need to define first what we mean by near and away from the critical point. We express the distance from the critical point through the parameter $y = N \ln g \sim \text{sgn}(g - 1)N/\xi(g)$ (we assume $g > 0$ from now on). We say that the system is near the critical point when $|y| < 1$ and away from it when $|y| > 1$.

To quantify for $g > 0$ the difference between the correct (incorrect) expression for ground state fidelity susceptibility given by χ^+ (χ^-), we study the ratio between the two expressions. As discussed in appendix B, this ratio is unchanged by duality mapping (21) and it has a maximum at the critical point, where

$$\left. \frac{\chi^+}{\chi^-} \right|_{y=0} = 3 \frac{N}{N-2}.$$

In other words, χ^+ is roughly larger than χ^- by the factor of three near the critical point (figure 1; see also figure 2 of [7], where a similar plot is presented). This discrepancy happens even when $N \gg 1$. The ratio of χ^+/χ^- monotonically goes to unity away from the critical point (appendix B and figure 1), and one can easily verify that for $|y| \gg \ln N$

$$\frac{\chi^+}{\chi^-} - 1 \simeq 4 \exp\left(-|y| + \frac{|y|}{N}\right) \left[N \sinh\left(\frac{|y|}{N}\right) - \cosh\left(\frac{|y|}{N}\right) \right].$$

Therefore, far away from the critical point the difference between the correct and incorrect expression for fidelity susceptibility becomes negligible.

Both problems can be found in the literature. We will focus below on popular [4, 6, 29]. In [4] the system size is odd and momenta (5) are used for both positive and negative magnetic

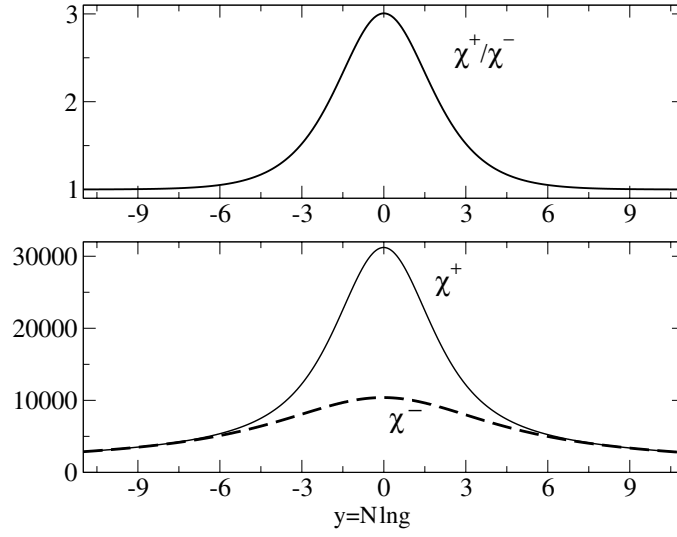


Figure 1. Illustration of the difference between fidelity susceptibility of the positive and negative parity ground states. The former, i.e., $\chi^+(g)$, is given by equation (23). The latter, i.e., $\chi^-(g)$ is given by equation (24). Upper panel: χ^+/χ^- as a function of $y = N \ln g \sim \text{sign}(g-1)N/\xi(g)$, where $\xi(g)$ is the correlation length of the infinite Ising chain. Lower panel: χ^+ (solid line) versus χ^- (dashed line). Both panels are for $N = 1000$. Near the critical point, $|y| < 1$, χ^+ differs from χ^- significantly. Far away from the critical point, $|y| \gg 1$, the two curves perfectly merge. The system is in the ferromagnetic (paramagnetic) phase for $y < 0$ ($y > 0$).

fields. The expression for fidelity susceptibility derived in [4] does not preserve the $g \leftrightarrow -g$ symmetry⁵. The same problem appears in [29] (see⁶ for a brief discussion). In [6], the system size is odd, positive magnetic fields are considered, and momenta (5) instead of (4) are used to compute fidelity susceptibility. Thus, the magnitude of fidelity susceptibility in figure 2 of [6] is underestimated around the critical point by the factor of about three⁷.

Summarizing, we have (i) comprehensively discussed the ground state of the quantum Ising model in a transverse field; (ii) computed and analyzed an exact closed-form expression for the energy gap between the positive and negative parity eigenstates of the Ising chain; (iii) calculated an exact closed-form expression for fidelity susceptibility of the Ising chain for all system sizes and magnetic fields; and (iv) discussed the consequences of the incorrect quantization of momenta in fidelity susceptibility studies.

The (i)–(ii) results analytically illustrate the symmetry breaking phenomenon in the Ising model, i.e., the disappearance of the energy gap leading to the degeneracy of the ground state. We show rigorously that the gap decays exponentially fast with the system size in the thermodynamic limit. The (iii) result completes the former studies of fidelity susceptibility providing a textbook-quality expression. It analytically shows how the fidelity susceptibility

⁵ For example, one can verify that the discrete sum for $S_N^\lambda(\lambda, \gamma = 1)$ —equations (7) and (8) of [4]—is equal to $4\chi^-(\lambda)$, whose asymmetry for odd N with respect to the $\lambda \leftrightarrow -\lambda$ transformation is easily seen from our equation (24).

⁶ After setting $\gamma = 1$ in equation (6) of [29] the g_{11} component of the metric tensor represents fidelity susceptibility of the Ising chain. The expression given for it right under equation (6) of [29] is not symmetric under the transformation $h \leftrightarrow -h$, which can be easily checked (e.g., by plotting it). In fact, the discrete sum for $g_{11}(h, \gamma = 1)$ from [29] equals $\chi^-(h)$, whose lack of reflection symmetry for odd-sized systems is evident from our equation (24).

⁷ One can show using our results that the expression for fidelity susceptibility plotted in figure 2 of [6] equals $\chi^-(\lambda)$, while the correct result is $\chi^+(\lambda)$.

approach to quantum phase transitions works in the Ising model. The (iv) discussion corrects misunderstanding in some former calculations resulting from incorrect identification of the parity of the ground state. This misunderstanding leads to a wrong expression for fidelity susceptibility near the critical point.

Finally, we mention two additional applications of our results. First, we expect that our exact analytical summation technique will be useful in the future studies of various concepts in the Ising model: The harmonic oscillator of many-body physics. Second, our results for fidelity susceptibility can be used to benchmark numerical results, e.g., quantum Monte Carlo simulations, where the complications arise due to the very existence of the two parity subspaces that we discuss [7].

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Appendix A. Gap

We will prove here some properties of the gap mentioned in section 4. We will focus on the ferromagnetic phase, because the results for the paramagnetic phase gap can be obtained through duality mapping (22). Moreover, we will assume that the magnetic field $g > 0$, because the gap has a well-defined parity with respect to the $g \leftrightarrow -g$ reflection. This leaves us with $g \in (0, 1)$, which we assume through this section.

We will use below two textbook inequalities. The first one comes from [30]

$$a^r - b^r > rb^{r-1}(a - b) \quad \text{for } r > 1 \vee r < 0, \quad (\text{A.1})$$

where $a, b > 0$ (equality happens when $a = b$, $r = 0$, or $r = 1$). The second one is the Wendel's inequality [31]

$$\left(\frac{x}{x+s}\right)^{1-s} < \frac{\Gamma(x+s)}{x^s \Gamma(x)} < 1 \quad \text{for } s \in (0, 1) \wedge x \in (0, \infty). \quad (\text{A.2})$$

Monotonicity of the gap. We will now prove that the gap increases monotonically from $g = 0$ to $g = 1$. Since

$$\frac{d}{dg}(\varepsilon^- - \varepsilon^+) = \int_0^1 dt \frac{4N}{\pi} t^{N-3/2} \sqrt{\frac{1-t}{1-g^2t}} \frac{g^{N-1}}{[1-(gt)^{2N}]^2} f(g, t),$$

it suffices to show that $f(g, t) > 0$:

$$\begin{aligned} f(g, t) &= [1 - (gt)^{2N}][N - (N+1)g^2t] + 2N(1 - g^2t)(gt)^{2N} \\ &\geq 2N(gt)^{2N} \left[1 - g + N \left(\frac{1}{gt} - 1 - g + g^2t \right) \right] \\ &\geq 2N(gt)^{2N} (1 - g)[1 + N(1 - gt)] > 0 \quad \text{for } t \in (0, 1) \wedge g \in (0, 1). \end{aligned}$$

The first inequality follows from bounding of $1 - (gt)^{2N}$ with inequality (A.1), where we substituted $a = 1$, $b = gt$, and $r = 2N$. The second one results from bounding $1/gt - 1$ with inequality (A.1), where now $a = gt$, $b = 1$, and $r = -1$.

Lower bound on the gap.

$$\begin{aligned}\varepsilon^- - \varepsilon^+ &= -2N(a_N + a_{3N} + a_{5N} + \dots) > -2Na_N \\ &\geq 2N \max \left(\frac{\sqrt{1-g^2}}{\sqrt{\pi}} \frac{\Gamma(N-1/2)}{\Gamma(N+1)} g^N, \frac{2}{\pi} \frac{g^{N+1}}{N^2 - 1/4} \right) \\ &> \max \left(g^N \frac{2}{\sqrt{\pi}} \frac{\sqrt{1-g^2}}{\sqrt{N}}, g^N \frac{4g}{\pi N} \right).\end{aligned}$$

The first inequality holds because $a_\ell < 0$ (20). The second follows from bounding integral (20) with inequality

$$\sqrt{(1-t)(1-g^2t)} = \sqrt{(1-g^2)(1-t) + g^2(1-t)^2} \geq \max(\sqrt{1-g^2}\sqrt{1-t}, g(1-t)).$$

The final step employs $1/(N^2 - 1/2) > 1/N^2$ and $\Gamma(N-1/2)/\Gamma(N+1) > 1/N^{3/2}$ following from inequality (A.2).

Upper bound on the gap.

$$\begin{aligned}\varepsilon^- - \varepsilon^+ &= -2N \sum_{\ell=N, 3N, \dots} a_\ell \\ &\leq \frac{4N}{\pi} g^{N+1} \sum_{\ell=N, 3N, \dots} \frac{g^{\ell-N}}{\ell^2 - 1/4} + \frac{2N}{\sqrt{\pi}} g^N \sqrt{1-g^2} \sum_{\ell=N, 3N, \dots} \frac{\Gamma(\ell-1/2)}{\Gamma(\ell+1)} g^{\ell-N} \\ &< \frac{4N}{\pi} g^{N+1} \frac{N}{N-1/2} \sum_{\ell=N, 3N, \dots} \frac{g^{\ell-N}}{\ell^2} + \frac{2N}{\sqrt{\pi}} g^N \sqrt{1-g^2} \sqrt{\frac{N}{N-1}} \sum_{\ell=N, 3N, \dots} \frac{g^{\ell-N}}{\ell^{3/2}} \\ &< g^N \frac{\pi g}{2N-1} + g^N 2 \frac{\sqrt{1-g^2}}{\sqrt{N-1}}.\end{aligned}$$

The first inequality follows from the substitution of

$$\sqrt{(1-t)(1-g^2t)} = \sqrt{(1-g^2)(1-t) + g^2(1-t)^2} \leq \sqrt{1-g^2}\sqrt{1-t} + g(1-t)$$

into integral (20). The second inequality follows from

$$\frac{1}{\ell^2 - 1/4} < \frac{1}{\ell^2} \frac{2N}{2N-1}, \quad \frac{\Gamma(\ell-1/2)}{\Gamma(\ell+1)} < \frac{1}{\ell^{3/2}} \sqrt{\frac{N}{N-1}},$$

both valid for $\ell \geq N$ (the latter follows from inequality (A.2)). In the final step, the sums are evaluated at $g = 1$.

Appendix B. χ^+/χ^-

We will discuss here the properties of χ^+/χ^- , which were only briefly mentioned in section 6. Without loss of generality, we consider magnetic fields $g > 0$.

Duality of the ratio. It can be shown using equations (23) and (24) that

$$\frac{\chi^+(g)}{\chi^-(g)} = \frac{\chi^+(1/g)}{\chi^-(1/g)}. \quad (\text{B.1})$$

This ferromagnetic–paramagnetic duality implies that we can focus on the studies of χ^+/χ^- in one of the phases. Symmetry (B.1) should not be taken for granted, because neither χ^+ nor χ^- is symmetric with respect to the $g \leftrightarrow 1/g$ mapping (see [18] for the detailed discussion of the symmetries and properties of χ^+). Thus, we will further restrict the discussion to $g \geq 1$. The duality symmetry also implies that there is an extremum of χ^+/χ^- at the critical point $g_c = 1$. Indeed, the calculation of the first and second derivative of χ^+/χ^- shows that there

is a maximum at $g_c = 1$ for $N > 2$. Note that neither χ^+ nor χ^- has maximum exactly at the critical point.

Monotonicity of the ratio. From now on, it is convenient to parameterize the ratio with $y = N \ln g$:

$$\frac{\chi^+}{\chi^-} = \tanh^2\left(\frac{y}{2}\right) \frac{\sinh(y - y/N) + (N - 1) \sinh(y/N)}{\sinh(y - y/N) - (N - 1) \sinh(y/N)}. \quad (\text{B.2})$$

To prove that the ratio monotonically decreases in $y \in (0, \infty)$, we investigate its derivative

$$\begin{aligned} \frac{d}{dy} \left(\frac{\chi^+}{\chi^-} \right) &= \frac{\tanh(y/2)}{\cosh^2(y/2)} \frac{f(y)}{2[\sinh(y - y/N) - (N - 1) \sinh(y/N)]^2}, \\ f(y) &= (N + 1) \sinh^2\left(y - \frac{y}{N}\right) - (N - 1)(N - 2) \sinh^2(y)/N \\ &\quad - (2N - 1)(N - 1) \sinh^2\left(\frac{y}{N}\right). \end{aligned}$$

Next, we Taylor-expand the hyperbolic functions to get

$$f(y) = -\frac{1}{2} \sum_{k=3}^{\infty} \frac{(2y)^{2k}}{(2k)!} \frac{N - 1}{N^{2k}} a_k, \quad a_k = (N - 2)N^{2k-1} - (N + 1)(N - 1)^{2k-1} + 2N - 1.$$

Finally, one can prove by induction that $a_k > 0$ for all $N > 2$ and $k \geq 3$. Indeed, $a_3 = 2N(N^2 - 1)(N - 2)(N - 1/2) > 0$ and if $a_k > 0$ then $a_{k+1} > (2N - 1)(N^2 - 1)[(N - 1)^{2k-2} - 1] > 0$. Therefore, $f(y > 0) < 0$ and so $d(\chi^+/\chi^-)/dy < 0$ for $y > 0$ and $N > 2$, which we wanted to show.

Calculating the ratio at $g = 0, 1, \infty$ and taking into account the $y \leftrightarrow -y$ symmetry of equation (B.2), we see that χ^+/χ^- is monotonically decreasing from $3N/(N - 2)$ at $g = 1$ to unity at $g = 0$ and $g = \infty$.

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