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Article

Parity dependent quantum phase transition in the quantum Ising chain in a transverse field

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Abstract: Phase transitions- both in the classical and in the quantum version- are the perfect playground for appreciating universality at work. Indeed, the fine details become unimportant and a classification in very few universality classes is possible. Very recently, a striking deviation from this picture has been discovered: some antiferromagnetic spin chains with competing interactions show a different set of phase transitions depending on the parity of number of spins in the chain. The aim of this article is to demonstrate that the same behavior also characterizes the most simple quantum spin chain: the Ising model in a transverse field. By means of an exact solution based on a Wigner-Jordan transformation, we show that a first order quantum phase transition appears at zero applied field in the odd spin case, while it is not present in the even case. A hint of a possible physical interpretation is given by the combination of two fact: at the point of the phase transition, the degeneracy of the ground state in the even and the odd case substantially differ, being respectively 2 and $2N$, with N the number of spins; the spin of the most favorable kink states changes at that point.

Keywords: Ising model; quantum phase transitions; frustrated boundary conditions

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1. Introduction

In the non-relativistic microscopic world, the fundamental laws of physics regulate the interaction within pairs of constituents [1]. In the macroscopic scenario, emergent phenomena such as the onset of order parameters, the appearance of phase transitions, and the development of dissipation, are observed [2]. Connecting the two counterparts is a central aim of statistical mechanics. Conceptually, the procedure is the following: one calculates the properties of the system under inspection for an arbitrary number N of constituents, and then performs the thermodynamic limit N to infinity. In such a highly nontrivial limit, the emergent properties show up. Although it is most often not possible to apply this strategy directly, this paradigm has proven extremely useful. Indeed, it led to the description of the different phases of matter and the transitions between them. This statement holds true for both the symmetry related phases of matter [2], and for the topological phases [3–5]. At the same time, it applies to both thermal [2] and quantum [6] phase transitions.

Very recently, a striking discovery was made: there are models in which the result of the limit, at zero temperature, crucially depends on the parity of N [7–13]. We will here call this phenomenon even-odd criticality. More specifically, what has been shown is that, depending on the parity of N, the system is gapless or gapped. Moreover, again depending on the parity, quantum phase transitions can be present or not. All the models known to show this spectacular behavior are antiferromagnetic spin chains with competing orders and subject to compactifying (periodic or twisted) boundary conditions. The physics behind the phenomenon is the competition between the local antiferromagnetic order and the global constraints posed by the boundary conditions. In this respect, the main difference between the even and the odd N cases is that only in the odd N case at least one link between spins must be in the energetically unfavorable condition; in other words, at least one kink is present in the ground state.

Since the discovery is extremely recent, not much is known about even-odd criticality. However, its potential is huge. From the theoretical side, it challenges the definition of

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phases, even thermal phases if classical models with even-odd criticality will be found, and represents a strikingly new playground for the study of the quantum quench dynamics of many-body physics and relaxation [14–28]. From a more practical perspective, it opens the way to unprecedented possibilities for quantum technologies: spin chains represent the typical models for the quantum buses transferring quantum information. Even-odd critical systems are in principle able to allow or stop the flow of information by switching on or off a single site.
In this work, we show for the first time that even the most simple, yet fruitful and inspiring, spin chain shows even-odd criticality: we analyze the antiferromagnetic Ising spin chain with N sites in a transverse field to show, by means of the exact solution based on the Wigner-Jordan transformation, the presence of a first order quantum phase transition that is only present in the case of odd N. Such quantum phase transition is manifested in a discontinuity of the first derivative of the ground state energy with respect to the applied field, calculated at zero field.
The rest of the article is structured as follows: in Sec. 2. we outline the Ising model in the antiferromagnetic regime and its solution; in Sec. 3. we analyze the ground state and its energy, and show that a quantum phase transition is only present in the odd N case. Finally, in Sec. 3. we discuss the result and we draw our conclusions.

2. Model

The model under inspection is the antiferromagnetic quantum Ising chain in a transverse field [6]. Explicitly, we consider the Hamiltonian

$$H = \frac{J}{2}\sum_{j=1}^{N}\left[\sigma_j^x\sigma_{j+1}^x + h\sigma_j^z\right]. \tag{1}$$

Here, we impose periodic boundary conditions $\sigma_{N+1}^\alpha = \sigma_1^\alpha$. Moreover, in the Hamiltonian, $J > 0$ parametrizes the antiferromagnetic coupling and sets the energy scale, h parametrizes the transverse magnetic field (we will only consider $|h| < 1$), j is an index running over the lattice sites, N is the number of lattice sites, and σ_j^α with $\alpha = x, y, z$ are the three Pauli matrices defined on the j-th site.
The Hamiltonian can be exactly diagonalized by means of a Wigner-Jordan transformation to free fermions [29,30]. To do so, previously we define

$$\sigma_j^\pm \equiv \frac{\sigma_j^x \pm i\sigma_j^y}{2}. \tag{2}$$

Then, the transformation to free fermions is introduced, namely

$$\sigma_j^+ \equiv e^{i\pi\sum_{l=1}^{j-1}\psi_l^\dagger\psi_l}\psi_j\,, \tag{3}$$

$$\sigma_j^- = e^{-i\pi\sum_{l=1}^{j-1}\psi_l^\dagger\psi_l}\psi_j^\dagger\,, \tag{4}$$

$$\sigma_j^z = 1 - 2\psi_j^\dagger\psi_j\,, \tag{5}$$

where $\{\psi_j^\dagger, \psi_l\} = \delta_{j,l}$ and $\{\psi_j^\dagger, \psi_l^\dagger\} = \{\psi_j, \psi_l\} = 0$. Here $\{\cdot,\cdot\}$ is the anticommutator and ψ_j is the spinless fermionic operator associated to a particle on the site j. From the interpretation point of view, it is fruitful to note that the number $n_j = \psi_j^\dagger\psi_j$ of spinless femions on the j-th site equals one or zero if the z projection of the spin on that site j is 1 or -1 respectively. The advantage brought by this transformation is that the Hamiltonian, written in terms of the fermions, can be diagonalized by simple Bogoliubov transformations. Indeed, one finds

$$H = \mathcal{P}H^{(+)}\mathcal{P} + \mathcal{Q}H^{(-)}\mathcal{Q}\,. \tag{6}$$

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Here $\mathcal{P}$ is the projector onto the even parity sector of the fermionic Fock space, given by

$$\mathcal{P} \equiv \frac{1 + \prod_{j=1}^{N}\left(1 - 2\psi_j^\dagger \psi_j\right)}{2}, \tag{7}$$

that satisfies $[\mathcal{P}, H] = 0$, with $[\cdot,\cdot]$ the commutator. Furthermore, $\mathcal{Q} \equiv 1 - \mathcal{P}$. The Hamiltonians $H^{(\pm)}$ are given by

$$H^{(\pm)} = \frac{J}{2}\sum_{j=1}^{N}\left[\psi_j^{(\pm)\dagger}\psi_{j+1}^{(\pm)} + \psi_j^{(\pm)\dagger}\psi_{j+1}^{(\pm)\dagger} - h\psi_j^{(\pm)\dagger}\psi_j^{(\pm)} + \frac{h}{2}\right] + \text{h.c.}. \tag{8}$$

It is important to underline that the number of fermions, and hence their parity, is not related to the number of sites N, but rather to the magnetization in the z direction.
Although $H^{(+)}$ and $H^{(-)}$ have the same form, they are not the same operator. Indeed, the fermionic operators obey different boundary conditions. One has

$$\psi_{N+1}^{(\pm)} = \mp\psi_1^{(\pm)}. \tag{9}$$

The origin of the different boundary conditions is the non-locality of the Wigner Jordan transformation, that produces a different coupling between the $j = 1$ and the $j = N$ sites in the even and the odd N cases.
The different boundary conditions imply a different Fourier series for the diagonalization, namely we define

$$\psi_j^{(\pm)} \equiv \frac{e^{i\frac{\pi}{4}}}{\sqrt{N}}\sum_{q\in\Gamma^{(\pm)}} e^{iqj}\tilde{\psi}_q^{(\pm)}, \tag{10}$$

where $\Gamma^{(+)} \equiv \left\{\frac{\pi}{N}(2k+1)\right\}$ and $\Gamma^{(-)} \equiv \left\{\frac{2\pi}{N}k\right\}$, with $k = 0, \ldots, N-1$. We find

$$H^{(\pm)} = -J\sum_{q\in\Gamma^{(\pm)}}\left[(h - \cos(q))\tilde{\psi}_q^{(\pm)\dagger}\tilde{\psi}_q^{(\pm)} + \frac{1}{2}\sin(q)\left(\tilde{\psi}_{-q}^{(\pm)\dagger}\tilde{\psi}_q^{(\pm)\dagger} + \tilde{\psi}_q^{(\pm)}\tilde{\psi}_{-q}^{(\pm)}\right)\right] + \frac{JhN}{2}. \tag{11}$$

It is here crucial to notice that two values of q need to be treated with particular care: $q = 0$ and $q = \pi$. In those cases, no superconducting-like coupling is present and they need to be treated separately. However, this fact only generates subtleties for $q = 0$. Subsequently, we rotate the fields introducing

$$\tilde{\psi}_q^{(+)} \equiv \cos(\theta_q)\chi_q^{(+)} + \sin(\theta_q)\chi_{2\pi-q}^{(+)\dagger}, \tag{12}$$

$$\tilde{\psi}_{q\neq 0}^{(-)} \equiv \cos(\theta_q)\chi_q^{(-)} + \sin(\theta_q)\chi_{2\pi-q}^{(-)\dagger}, \tag{13}$$

$$\tilde{\psi}_0^{(-)} \equiv \chi_0^{(-)}, \tag{14}$$

with θ_q satisfying

$$\tan 2\theta_q = \frac{\sin(q)}{h - \cos(q)}. \tag{15}$$

We thus find

$$H^{(+)} = -J\sum_{q\in\Gamma^{(+)}}\left[\epsilon(q)\left(\chi_q^{(+)\dagger}\chi_q^{(+)} - \frac{1}{2}\right)\right] \tag{16}$$

and

$$H^{(-)} = -J\sum_{q\in\Gamma^{(-)}, q\neq 0}\left[\epsilon(q)\left(\chi_q^{(-)\dagger}\chi_q^{(-)} - \frac{1}{2}\right)\right] + J\epsilon(0)\left(\chi_0^{(-)\dagger}\chi_0^{(-)} - \frac{1}{2}\right), \tag{17}$$

with

$$\epsilon(q) \equiv \sqrt{(h - \cos(q))^2 + \sin^2(q)}. \tag{18}$$

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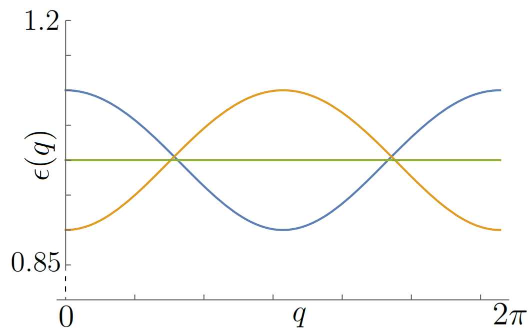

Figure 1. Energy dispersion $\epsilon(q)$ as a function of q for $h = 0$ (green), $h = 0.1$ (orange) and $h = -0.1$ (blue).

Importantly, $\epsilon(q)$ is flat for $h = 0$, while it has its minimum for $q = 0 \in \Gamma^{(-)}$ ($q = \pi \in \Gamma^{(+)}$) for $h > 0$ ($h < 0$). This fact is shown in Fig.1. Note that we did not have to treat separately the $q = \pi$ case since, in the parameter range we inspect, $h + 1 = \epsilon(\pi)$. This was not the case for $q = 0$. Indeed, $\lim_{q\to 0}$ does not converge to the energy contribution related to the occupation of the fermion $\chi_0^{(-)}$, but rather to its opposite. Finally, it is worth to stress that the parity of the fermions ψ is the same as the parity of the fermions χ.

3. Results

In order to demonstrate the presence of the first order quantum phase transition, we need to study the ground state energy as a function of h and of the parity of N. To do so, we have to address the lowest energy state of both $H^{(+)}$ and $H^{(-)}$ that is compatible with the parity requirements and can hence contribute to the eigenstates of H. We will hence analyze, the eight energies $E^{(\pm)}_{g/l,e/o}$ of the lowest energy eigenstates of H emerging from $H^{(+)}$ and $H^{(-)}$, for even (e) and odd (o) N, and for $h > 0$ (g) and $h < 0$ (l). We now proceed to the assessment of the eight cases.

1) For N even and $h > 0$, the lowest energy state of $H^{(+)}$ with an even number of fermions is simply obtained by occupying all the energy levels, so

$$E^{(+)}_{g,e} = -\frac{J}{2} \sum_{q\in\Gamma^{(+)}} \epsilon(q). \tag{19}$$

2) For N even and $h > 0$, the lowest energy state of $H^{(-)}$ with an odd number of fermions is the one obtained by occupying all the fermionic states, except for one. Since $\Gamma^{(-)}$ contains $q = 0$, and $q = 0$ is the only state with positive energy, it is indeed favorable to keep it empty. By doing so, and by noticing that the energy contribution of keeping the $q = 0$ empty is $J\epsilon(0)$, the energy becomes

$$E^{(-)}_{g,e} = -\frac{J}{2} \sum_{q\in\Gamma^{(-)}} \epsilon(q). \tag{20}$$

3) For N even and $h < 0$, the lowest energy state of $H^{(+)}$ with an even number of fermions is simply obtained by occupying all the energy levels, so

$$E^{(+)}_{l,e} = -\frac{J}{2} \sum_{q\in\Gamma^{(+)}} \epsilon(q). \tag{21}$$

4) For N even and $h < 0$, the lowest energy state of $H^{(-)}$ with an odd number of fermions is the one obtained by occupying all the fermionic states, except for one. Since $\Gamma^{(-)}$ contains

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$q = 0$, and $q = 0$ is the only state with positive energy, it is indeed favorable to keep it empty. By doing so, and by noticing that the energy contribution of keeping the $q = 0$ empty is $J\epsilon(0)$, the energy becomes

$$E^{(-)}_{l,e} = -\frac{J}{2} \sum_{q \in \Gamma^{(-)}} \epsilon(q). \tag{22}$$

5) For N odd and $h > 0$, the lowest energy state of $H^{(+)}$ with an even number of fermions is the one obtained by filling all the states except for the one with the smallest energy in modulus (note that all energies are negative). For $h > 0$ such minimum is for $q = \frac{\pi}{N}, 2\pi - \frac{\pi}{N}$. We hence get

$$E^{(+)}_{g,o} = -\frac{J}{2} \sum_{q \in \Gamma^{(+)}} \epsilon(q) + J\epsilon\left(\frac{\pi}{N}\right). \tag{23}$$

6) For N odd and $h > 0$, the lowest energy state of $H^{(-)}$ with an even number of fermions is the one obtained by filling all the states. We get

$$E^{(-)}_{g,o} = -\frac{J}{2} \sum_{q \in \Gamma^{(-)}} \epsilon(q) + J\epsilon(0). \tag{24}$$

7) For N odd and $h < 0$, the lowest energy state of $H^{(+)}$ with an even number of fermions is the one obtained by filling all the states except for the one with the smallest energy in modulus (note that all energies are negative), given by $q = \pi$. We hence get

$$E^{(+)}_{l,o} = -\frac{J}{2} \sum_{q \in \Gamma^{(+)}} \epsilon(q) + J\epsilon(\pi). \tag{25}$$

8) For N odd and $h < 0$, the lowest energy state of $H^{(-)}$ is the one obtained by leaving both $q = 0$ and $q = p$ empty, where p is the nearest to π element in $\Gamma^{(-)}$. We hence get

$$E^{(-)}_{l,o} = -\frac{J}{2} \sum_{q \in \Gamma^{(-)}} \epsilon(q) + J\epsilon(p). \tag{26}$$

In the thermodynamic limit $N \to \infty$, $E^{(+)}_{g,e}$ and $E^{(-)}_{g,e}$ are degenerate and constitute the ground state manifold for N even and $h > 0$. The same holds for $E^{(+)}_{l,e}$ and $E^{(-)}_{l,e}$ for $h < 0$. It is clear that the ground state energy is smooth in $h = 0$.
As far as the odd N is concerned, and again considering the thermodynamic limit, $E^{(+)}_{l,o}$ and $E^{(-)}_{l,o}$ are degenerate, as well as $E^{(+)}_{g,o}$ and $E^{(-)}_{g,o}$. However, here a peculiar effect happens: the ground state energy is not smoothly connected between $h < 0$ and $h > 0$. Indeed we find, and this is the central result of the present study, that

$$\lim_{N\to\infty} \left(\frac{\partial E^{(+)}_{g,o}}{\partial h}\bigg|_{h\to 0^+} - \frac{\partial E^{(+)}_{l,o}}{\partial h}\bigg|_{h\to 0^-} \right) = -2J. \tag{27}$$

We have indeed found that a first order quantum phase transition appears for odd N only in the quantum Ising chain in a transverse field.

4. Discussion and conclusion

In this work we have analytically demonstrated that a first order quantum phase transition (a discontinuity of the derivative of the ground state energy) is present as a function of the applied field in the case of an odd number of spins, while this is not the case

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for even N.
The crucial mathematical point is that in the odd case only, for $h = 0$, the degeneration of the ground state is remarkably different from the $h \neq 0$ case. Indeed, while in both cases the energy dispersion $\epsilon(q)$ becomes flat for $h = 0$, only in the odd N case that fact influences the ground state degeneracy, due to the parity constraints posed by the projectors $\mathcal{P}$ and $\mathcal{Q}$ appearing in the fermionic description of H. A further ingredient that is crucial for the existence of the effect is that the minimum of $\epsilon(q)$ switches from $q = 0$ to $q = \pi$ as h goes from positive to negative.
From the physical point of view such mathematical statements translate into the following considerations: in the even N case for every h the ground state is doubly degenerate, gapped, antiferromagnetic and no feature appears. On the other hand, in the odd N case the spectrum is not gapped since at least one kink must be present. Moreover, the kink states form a metallic band. This fact is due to the fact that not all the antiferromagnetic nearest neighbour interactions can be fulfilled. In the classical $h = 0$ case this reflect into a degeneracy $2N$ of the ground state, since such a kink can be equivalently positioned anywhere in the chain and a full spin flip does not change the energy. For finite h the degeneracy is lifted by hybridization. In switching from $h < 0$ to $h > 0$ the most favorable majority spin orientation changes, and this reorganization of the ground state, allowed by the degeneracy at $h = 0$, has the first order quantum phase transition as a signature.
The implications and opportunities for further inspections that are opened by our discovery are, in our opinion, remarkable. Indeed the finite temperature effects of the phenomenon, the quantum quench related thermodynamics of the model, the search for even-odd criticality without classical point and its physical interpretation and the quest for even-odd thermal phase transitions are all possible follow ups of our finding in the prototypical quantum Ising chain.

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