Fidelity approach to frustrated quantum XY model

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Abstract

The XY chain in a transverse magnetic field is studied. Its quantum phase diagram is explored through fidelity of the ground state, an overlap function. This approach is based on phase transitions inducing a critical drop of the fidelity. The XY model is solved exactly, in the sense that the spectra, ground states in both parity sectors and elementary excitations are found. Two algorithms are used for determining the solution and their equivalence is proved; both relying on mapping the model to free fermions. Fidelity of the ground state is introduced and calculated numerically, correctly identifying quantum phase transitions of the model.

1 Introduction

The one-dimensional XY model in a transverse magnetic field, as a generalization of the Ising model, is a prototypical quantum mechanical model for magnetic-orderings in spin systems. It is interesting in a couple of ways; not only is it exactly solvable but it has an intriguing phase diagram which holds two non-trivial quantum phase transitions. Quantum phase transitions (QPTs), unlike classical phase transitions which are caused by thermal fluctuations, are caused by quantum fluctuations at absolute zero temperature. Although absolute zero is not achievable, even in principle, quantum phase transition properties can be detected in a system's behaviour near the critical point. QPTs can shed a light on exciting phenomena such as high-temperature superconductivity and offer a new perspective on treating (strongly) interacting quantum many-body systems. Furthermore, they can often be mapped to other problems, enabling us to reach a solution in a simpler manner, or even at all. For example, the two mentioned QPTs in the 1D XY model's phase diagram correspond to two universality classes; a free fermion system and the 1D quantum Ising model, respectively[1]. Last but not least, 1D models are experimentally achievable through, for example, trapped cold atoms in optical lattices[2, 3].

An interesting phenomena can occur in a XY chain under the right circumstances. First, picture an antiferromagnetic, square "chain" with four spins in its vertices. To satisfy antiferromagnetic conditions, all one needs to do is alternately put spins up or down, as shown on Figure 1a). In another setting, for example a triangle, when the same is tried, one finds it is impossible. We say the system is frustrated as it cannot meet its boundary conditions (point neighbouring spins in opposite directions). If a XY chain is closed, or has periodic boundary conditions, is antiferromagnetic and has an odd number of spins (i.e. lattice sites), it will experience frustration. At first, it seemed that this is a small effect that can be ignored, especially as the the chain becomes longer, as it stems from a single spin too many(or too few) but it turned out not to be the case. For example, it has been shown that under these conditions, a quantum phase transition can be observed which is not present in unfrustrated systems[4].

A novel way of approaching this problem is through fidelity analysis. Fidelity, a concept borrowed from quantum information theory, is a measure of "closeness" of two quantum states. One can think of it as an overlap function. It has been found that the boundaries between

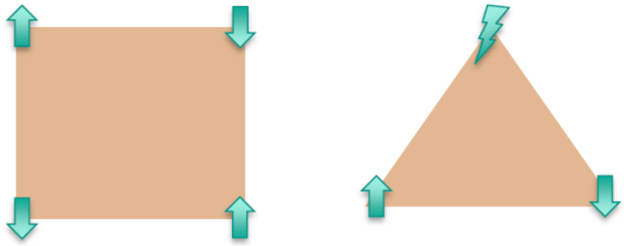

Fig. 1. A schematic depiction of frustration in a closed "chain" system. In a) we can see a normal antiferromagnetic system, where in b) the system cannot meet its boundary conditions.

different quantum phases can be analysed through the overlap between ground states (GSs) of systems with slightly differing coupling constants[5]. At critical points, the overlap shows a large, sometimes discontinuous drop. The virtue of this approach is in its generality; no *a priori* knowledge is needed of the system's specific physical properties (e.g. order parameters).

We use fidelity to reconstruct and analyse the quantum phase diagram of a 1D quantum XY model, for an even number of spins, providing a base for the next step which is expanding this analysis to the frustrated case.

First, in Section 2 we solve the XY chain using a series of transformations to bring it to diagonal form, find its spectra and ground state(s). In Section 3, a short overview of the relevant phase diagram for the XY model is given. Finally, in Section 4 a definition of fidelity is given, along with an alternative solution for a quadratic fermion model as it is relevant for fidelity calculations. Also in Section 4, a numerical algorithm is introduced and results of fidelity calculations are presented.

2 Solving the quantum XY model

The XY chain was introduced as an exactly solvable model similar to the Heisenberg model by Lieb, Schultz and Mattis in 1961 [6], where it was solved in the absence of a magnetic field. Works including a finite magnetic field apperead soon after[7, 8]. The problem is solved by mapping the chain to a system of free fermions. The XY Hamiltonian with anisotropy γ in a transverse magnetic field of strength h in terms of Pauli spin operators reads:

$$H = \frac{J}{2}\sum_{j=1}^{N}\left(\frac{1+\gamma}{2}\sigma_j^x\sigma_{j+1}^x + \frac{1-\gamma}{2}\sigma_j^y\sigma_{j+1}^y + h\sigma_j^z\right). \tag{2.1}$$

In a system described by this Hamiltonian, there is a 1D lattice with N sites, and on each site there is a $1/2$ spin with projections in 3 directions (x, y, z). In the presence of a magnetic field, the interaction between neighbours in the direction of the external magnetic field can be neglected. In (2.1), that direction is z. For $\gamma = 0$ the system reduces to a isotropic XX model, where for $\gamma = \pm 1$, one gets the 1D quantum Ising model.

2.1 Jordan Wigner transformation

Jordan-Wigner transformation is a mapping of spin operators to fermionic creation and annihilation operators. By transforming N spins to N fermions, we get a Hamiltonian that can be further simplified, in the end giving us a clean diagonal quadratic fermion Hamiltonian whose ground state and energy are easily acquired.

It is convenient to write Hamiltonian (2.1) using Pauli raising and lowering operators:

$$\sigma^{+,-} = \frac{1}{2}(\sigma^x \pm i\sigma^y). \tag{2.2}$$

Then, (2.1) reads (h.c. stands for the hermitian conjugate of the expression in brackets) :

$$H = \frac{J}{2}\sum_{j=1}^{N}\left[(\sigma_j^+\sigma_{j+1}^- + \gamma\sigma_j^+\sigma_{j+1}^+ + \text{h.c.}) + h\sigma_j^z\right]. \tag{2.3}$$

Reviewing the known properties of Pauli spin operators, we can see they are not Fermi operators:

$$[\sigma_j^\alpha, \sigma_j^\beta] = 2i\epsilon_{\alpha\beta\gamma}\,\sigma_j^\gamma, \tag{2.4a}$$
$$[\sigma_i^\alpha, \sigma_j^\beta] = 0 \quad \text{for} \quad i \neq j. \tag{2.4b}$$
$$\{\sigma_j^\alpha, \sigma_j^\beta\} = 2\delta_{\alpha\beta}, \tag{2.4c}$$
$$\tag{2.4d}$$

Latin letters i, j stand for particular sites, while Greek letters α, β, γ stand for x, y or z. $\epsilon_{\alpha\beta\gamma}$ is the Levi-Civita symbol and $\delta_{\alpha\beta}$ the Kronecker delta. As these relations show, Pauli spins satisfy fermionic anti-commutation relations only on a particular site (2.4c), while between different sites they act bosonically. Furthermore, it can be shown (using (2.2) and (2.4)) that the set of operators σ_j^-, σ_j^+ and σ_j^z is also not a set of Fermi operators.

That is why we introduce the Jordan-Wigner transformation for the XY model; the Fermi annihilation and creation operators are, respectively:

$$\psi_j = \left(\prod_{l=1}^{j-1}\sigma_l^z\right)\sigma_j^+, \tag{2.5a}$$
$$\psi_j^\dagger = \left(\prod_{l=1}^{j-1}\sigma_l^z\right)\sigma_j^-, \tag{2.5b}$$

for $j = 1, 2, ..N$. The product $\prod$ is used in place of tensor product symbol $\otimes$ for simplicity. Using the definition of these Fermi operators and properties of Pauli operators, it can be shown that ψ_j and $\psi_j^\dagger$ are Fermi operators:

$$\{\psi_i, \psi_j\} = 0, \tag{2.6a}$$
$$\{\psi_i, \psi_j^\dagger\} = \delta_{ij}. \tag{2.6b}$$

This system's Hilbert space is a tensor product of N spin $1/2$ Hilbert spaces, and its basis are product spin states $|n_1\rangle \otimes |n_2\rangle \otimes ... |n_N\rangle$ or shortly $|n_1\, n_2 ... n_N\rangle$. The n_i stands for $\uparrow$ or $\downarrow$. If we identify $\uparrow$ with 0 and $\downarrow$ with 1, and use $\sigma^z\,|\uparrow\rangle = |\uparrow\rangle$ and $\sigma^z\,|\downarrow\rangle = -\,|\downarrow\rangle$, it follows:

$$\psi_j^\dagger\psi_j = n_j\,|n_1\, n_2 ... n_j ... n_N\rangle\,. \tag{2.7}$$

As it naturally stems from (2.5), spin downs $\downarrow$ correspond to particles and spin ups $\uparrow$ to holes. It is convenient to define also the inverse relations for Pauli operators in terms of Fermi operators for $j = 1, .., N$:

$$\sigma_j^z = 1 - 2\psi_j^\dagger \psi_j, \tag{2.8a}$$

$$\sigma_j^+ = \left(\prod_{l=1}^{j-1} 1 - 2\psi_l^\dagger \psi_l \right) \psi_j, \tag{2.8b}$$

$$\sigma_j^- = \left(\prod_{l=1}^{j-1} 1 - 2\psi_l^\dagger \psi_l \right) \psi_j^\dagger. \tag{2.8c}$$

Applying (2.8) to (2.3) we obtain:

$$\begin{aligned} H = &-\frac{J}{2} \sum_{j=1}^{N-1} \left(\psi_j \psi_{j+1}^\dagger + \gamma \psi_j \psi_{j+1} + \text{ h.c. } \right) + \frac{J}{2} P \left(\psi_N \psi_1^\dagger + \gamma \psi_N \psi_1 + \text{ h.c. } \right) \\ &- Jh \sum_{j=1}^{N} \psi_j^\dagger \psi_j + \frac{1}{2} JNh. \end{aligned} \tag{2.9}$$

We isolated the $j = N$ case because defining a ψ_{N+1} operator would tamper with the Fermi commutation relations. We also introduced the Hermitian parity operator:

$$P = \prod_{l=1}^{N} \sigma_l^z = \prod_{l=1}^{N} \left(1 - 2\psi_l^\dagger \psi_l \right). \tag{2.10}$$

The parity operator simply gives a plus (minus) sign on a state with even (odd) number of particles. Since the Hamiltonian (2.9) only has terms quadratic in Fermi operators (they come in pairs such as $\psi_i \psi_j$), the number of particles also only changes in pairs. Therefore, the Hamiltonian commutes with the parity operator $[H, P] = 0$. We see that (2.9) is not quadratic in Fermi operators, but if we separate our problem into two sectors based on parity P, we will have a quadratic form Hamiltonian in each sector, bringing us closer to the final diagonal form. We can do this by writing the Hamiltonian (2.9) as follows:

$$H = \frac{1+P}{2} H^+ + \frac{1-P}{2} H^-. \tag{2.11}$$

Explicitly, H^+ and H^- are equal to (2.9), substituting P with ± 1:

$$\begin{aligned} H^\pm = &-\frac{J}{2} \sum_{j=1}^{N-1} \left(\psi_j \psi_{j+1}^\dagger + \gamma \psi_j \psi_{j+1} + \text{ h.c. } \right) \pm \frac{J}{2} \left(\psi_N \psi_1^\dagger + \gamma \psi_N \psi_1 + \text{ h.c. } \right) \\ &- Jh \sum_{j=1}^{N} \psi_j^\dagger \psi_j + \frac{1}{2} JNh, \end{aligned} \tag{2.12}$$

Also, now there is a convenient way to define ψ_{N+1} that will allow us to write (2.12) in a more concise way:

$$\psi_{N+1} \left| P = 1 \right\rangle = -\psi_1 \left| P = 1 \right\rangle, \tag{2.13a}$$

$$\psi_{N+1} \left| P = -1 \right\rangle = \psi_1 \left| P = -1 \right\rangle, \tag{2.13b}$$

brings us:

$$H^{\pm} = -\frac{J}{2}\sum_{j=1}^{N}(\psi_j\psi_{j+1}^{\dagger} + \gamma\psi_j\psi_{j+1} + \text{h.c.}) - Jh\sum_{j=1}^{N}\psi_j^{\dagger}\psi_j + \frac{1}{2}JNh. \tag{2.14}$$

2.2 Fourier transform of Fermi operators

We can define new operators ψ_q that play a role of a Fourier transform(for confirmation and informal proof see Appendix A.1):

$$\psi_q := \frac{1}{\sqrt{N}}\sum_{l=1}^{N}\psi_l e^{-i\frac{2\pi}{N}ql}, \tag{2.15}$$

for any $q \in X_N$, with $X_N = \{x_0, x_0+1, x_0+2, ..., x_0+N-1\}$ and $x_0 = 1/2$ in the even sector and $x_0 = 0$ in the odd sector. These operators are periodic with period N $\psi_q = \psi_{q+N}$ so we can technically talk about all $q \in X_N + \mathbb{Z}$. It can be shown using (2.15), (2.6) and (A.1) that ψ_q are also Fermi operators:

$$\{\psi_q, \psi_{q'}\} = 0 \tag{2.16a}$$

$$\{\psi_q, \psi_{q'}^{\dagger}\} = \delta_{qq'} \tag{2.16b}$$

Now, using (2.15), (2.16) and (A.1) we obtain the following:

$$\sum_{j=1}^{N}\psi_j^{\dagger}\psi_{j+1} = \sum_q \psi_q^{\dagger}\psi_q e^{i\frac{2\pi}{N}q}, \tag{2.17a}$$

$$\sum_{j=1}^{N}\psi_j^{\dagger}\psi_{j+1}^{\dagger} = \sum_q \psi_q^{\dagger}\psi_{-q}^{\dagger}e^{i\frac{2\pi}{N}q} = i\sum_q \sin\left(\frac{2\pi}{N}q\right)\psi_q^{\dagger}\psi_{-q}^{\dagger}, \tag{2.17b}$$

$$\sum_{j=1}^{N}\psi_j^{\dagger}\psi_j = \sum_q \psi_q^{\dagger}\psi_q, \tag{2.17c}$$

Furthermore, we will redefine ψ_q by adding a phase factor (not harmful to Fermi relations (2.16)) to get rid of the imaginary unit:

$$\psi_q := \frac{e^{i\pi/4}}{\sqrt{N}}\sum_{l=1}^{N}\psi_l e^{-i\frac{2\pi}{N}ql}. \tag{2.18}$$

We now have Hamiltonians (2.14) in a form that is simpler to diagonalize:

$$H^{\pm} = J\sum_q\left[\cos\left(\frac{2\pi}{N}q\right) - h\right]\left(\psi_q^{\dagger}\psi_q - \frac{1}{2}\right) + \frac{1}{2}J\gamma\sum_q \sin\left(\frac{2\pi}{N}q\right)\left(\psi_q^{\dagger}\psi_{-q}^{\dagger} + \psi_{-q}\psi_q\right). \tag{2.19}$$

An extra term $-\frac{J}{2}\sum_q \cos\frac{2\pi}{N}q = 0$ was added for aesthetic reasons.

2.3 Bogoliubov transformation

Bogoliubov transformation is a transformation that can be thought of as essentially a rotation of phase space which allows us to change Hamiltonian basis to one in which the Hamiltonian is diagonal. In the process, it will give us new creation and annihilation operators which will tell us the structure of the elementary excitations in our system. It will be the final step that will bring us to the free fermionic Hamiltonian in diagonal form.

The last formulation of Hamiltonians (2.19) can now be written in simple matrix notation:

$$H^{\pm} = -\frac{1}{2}J\sum_{q}\begin{pmatrix}\psi_q^{\dagger} & \psi_{-q}\end{pmatrix} M_q \begin{pmatrix}\psi_q \\ \psi_{-q}^{\dagger}\end{pmatrix}, \tag{2.20}$$

where M_q are 2×2 symmetric matrices:

$$M_q = \begin{pmatrix} h-\cos\left(\frac{2\pi}{N}q\right) & -\gamma\sin\left(\frac{2\pi}{N}q\right) \\ -\gamma\sin\left(\frac{2\pi}{N}q\right) & -\left[h-\cos\left(\frac{2\pi}{N}q\right)\right] \end{pmatrix} = \begin{pmatrix} a_q & b_q \\ b_q & -a_q \end{pmatrix}, \tag{2.21}$$

with coefficients:

$$a_q \coloneqq h-\cos\left(\frac{2\pi}{N}q\right), \tag{2.22a}$$

$$b_q \coloneqq -\gamma\sin\left(\frac{2\pi}{N}q\right). \tag{2.22b}$$

It is obvious that the matrix M_q is diagonal for $q=0$ in the odd sector, while for $q=N/2$ it depends on the parity of N. Let us examine the case(s) when $q\neq 0, N/2$. In this case(s) the matrix M_q is not diagonal but it is symmetric so it can be diagonalized by an orthogonal matrix O_q:

$$M_q = O_q^T D_q O_q, \tag{2.23}$$

with D_q being a diagonal matrix. We can define O_q as a rotation matrix:

$$O_q = \begin{pmatrix} \cos\theta_q & -\sin\theta_q \\ \sin\theta_q & \cos\theta_q \end{pmatrix}, \tag{2.24}$$

which allows us to write:

$$O_q\begin{pmatrix}\psi_q \\ \psi_{-q}^{\dagger}\end{pmatrix} = \begin{pmatrix} \cos\theta_q\psi_q - \sin\theta_q\psi_{-q}^{\dagger} \\ \sin\theta_q\psi_q + \cos\theta_q\psi_{-q}^{\dagger}\end{pmatrix}. \tag{2.25}$$

Since the columns of O_q^T are the eigenvectors of M_q, we get the expressions for $\cos\theta_q$ and $\sin\theta_q$ by solving the eigenvalue problem for the matrix M_q (2.21). By this procedure we will also get the diagonal matrix D_q. Here are the results:

$$\cos\theta_q = \frac{b_q}{\sqrt{2}\sqrt{a_q^2+b_q^2-a_q\sqrt{a_q^2+b_q^2}}}, \tag{2.26a}$$

$$\sin\theta_q = \frac{a_q-\sqrt{a_q^2+b_q^2}}{\sqrt{2}\sqrt{a_q^2+b_q^2-a_q\sqrt{a_q^2+b_q^2}}}, \tag{2.26b}$$

and

$$D_q = \begin{pmatrix} \Lambda_q & 0 \\ 0 & -\Lambda_q \end{pmatrix} \tag{2.27}$$

with Λ_q:

$$\Lambda_q := \Lambda\left(\frac{2\pi}{N}q\right) := \sqrt{\left[h - \cos\left(\frac{2\pi}{N}q\right)\right]^2 + \gamma^2 \sin^2\left(\frac{2\pi}{N}q\right)}. \tag{2.28}$$

Now, looking at (2.25) and considering the property $\cos\theta_{-q} = -\cos\theta_q, \quad \sin\theta_{-q} = \sin\theta_q$ we can see it is convenient to define operators:

$$\chi_q \equiv \cos\theta_q \psi_q - \sin\theta_q \psi^\dagger_{-q}, \tag{2.29}$$

because then we have:

$$O_q \begin{pmatrix} \psi_q \\ \psi^\dagger_{-q} \end{pmatrix} = \begin{pmatrix} \chi_q \\ -\chi^\dagger_{-q} \end{pmatrix}. \tag{2.30}$$

It can be shown that operators χ_q are also fermionic (see discussion for special cases $q = 0, N/2$ in Appendix A.2, along with definition of χ_q in special cases) and periodic with period N:

$$\{\chi_q, \chi_{q'}\} = 0 \tag{2.31a}$$

$$\{\chi_q, \chi^\dagger_{q'}\} = \delta_{qq'}. \tag{2.31b}$$

By reformulating the Hamiltonian (2.19) using operators (2.29) we finally get a diagonal free fermion Hamiltonian:

$$H^\pm = -J \sum_q \Lambda_q \left(\chi^\dagger_q \chi_q - \frac{1}{2}\right). \tag{2.32}$$

2.4 Ground state and energy spectrum

The next and final step in solving the XY model is finding its spectra and ground state. We will focus on the ferromagnetic case and take the coupling constant to be negative $J = -1$, as we are not dealing with frustration yet. Before starting, it is important to remind ourselves that the Hamiltonian from 2.3 is actually two Hamiltonians, H^+ and H^- and the Hamiltonian that describes our system is actually (2.11). To solve the full Hamiltonian, we need to solve both H^+ and H^-. Each of them have 2^N eigenstates, but as they go into the full Hamiltonian only if they satisfy the parity condition, and that happens half the time for the respective $H^{+,-}$, in the end we will have $2^{N-1} + 2^{N-1} = 2^N$ eigenstates for the full Hamiltonian, exactly as we should.

As mentioned, we will look separately at the even and odd sector. We start with the even sector. The ground state of the H^+ Hamiltonian is its vacuum state, we'll label it by $|GS^+\rangle$:

$$\chi_q |GS^+\rangle = 0 \quad \text{for any } q \in \left\{\frac{1}{2}, \frac{1}{2} + 1, ..., \frac{1}{2} + N - 1\right\}. \tag{2.33}$$

As we can see from (2.32), the ground state energy is given by:

$$E_0^+ = -\frac{1}{2}\sum_{q=0}^{N-1} \Lambda_{q+1/2}. \tag{2.34}$$

We need to find the explicit expression for the ground state. We start by using operators (2.18) and their property:

$$\psi_q \left|0\right\rangle = 0 \quad \text{for any } q. \tag{2.35}$$

By expanding this equation using (2.31), and using properties of $\sin\theta_q$ and $\cos\theta_q$, we get:

$$\chi_q(\cos\theta_q + \sin\theta_q\, \psi_q^\dagger \psi_{-q}^\dagger) \left|0\right\rangle = 0. \tag{2.36}$$

Given equation (2.36), one can check that the ground state of the even sector Hamiltonian H^+, normalized, is:

$$\left|GS^+\right\rangle = \prod_{q=0}^{\left\lfloor \frac{N}{2} \right\rfloor -1} \left(\cos\theta_{q+1/2} + \sin\theta_{q+1/2}\, \psi_{q+1/2}^\dagger \psi_{q+1/2}^\dagger\right) \left|0\right\rangle . \tag{2.37}$$

As we can see, the operators ψ_q occur in pairs. By the definition (2.18), that means that ψ_j also occur in pairs, which leads to $\left|GS^+\right\rangle$ (2.37) having even parity. An even parity ground state in the even sector means (2.37) is also an eigenstate of the Hamiltonian (2.11).

We continue with the odd sector. We can start like in the even sector, but we will brand the vacuum state as $\left|GS^*\right\rangle$ for reasons that will become clear later:

$$\chi_q \left|GS^*\right\rangle = 0 \quad \text{for any } q \in \Big\{0, 1, ..., N-1\Big\}. \tag{2.38}$$

As now we have a $q = 0$ term, we need to separately look at cases $h < 1$ and $h > 1$ according to the definition for χ_q in the $q = 0$ case (A.4). In the $h > 1$ case we have an analogous situation to the even sector with (2.36), and the ground state for the Hamiltonian H^- for $h > 1$ is:

$$\left|GS^*,\, h > 1\right\rangle = \prod_{q=0}^{\left\lfloor \frac{N-1}{2} \right\rfloor} \left(\cos\theta_q + \sin\theta_q \psi_q^\dagger \psi_{-q}^\dagger\right) \left|0\right\rangle . \tag{2.39}$$

As this is essentially the same expression as the ground state of the even sector (2.37), it also has even parity, which means that it is not an eigenstate of the full Hamiltonian (2.11) as it gets canceled by the operator $1 - P$. Therefore, to find the eigenstate of the full Hamiltonian, we need to add an excitation. If we minimize the expression (2.28) we get that the lowest energy excitation is for $q = 0$, so the common eigenstate of the odd sector and full Hamiltonian with the lowest energy is gained by adding an excitation at $q = 0$ to (2.39):

$$\left|GS^-,\, h > 1\right\rangle = \chi_{q=0}^\dagger \left|GS^*,\, h > 1\right\rangle = \psi_{q=0}^\dagger \prod_{q=0}^{\left\lfloor \frac{N-1}{2} \right\rfloor} \left(\cos\theta_q + \sin\theta_q \psi_q^\dagger \psi_{-q}^\dagger\right) \left|0\right\rangle . \tag{2.40}$$

For $h < 1$, with a little manipulation of (2.36), we get the state (2.38) in the form:

$$|GS^*,\, h < 1\rangle = \psi^\dagger_{q=0} \prod_{q=0}^{\left\lfloor \frac{N-1}{2} \right\rfloor} \left(\cos\theta_q + \sin\theta_q \psi^\dagger_q \psi^\dagger_{-q}\right) |0\rangle \,. \tag{2.41}$$

The parity of (2.41) is odd, as it should be so:

$$|GS^*,\, h < 1\rangle = |GS^-,\, h < 1\rangle \,. \tag{2.42}$$

Finally, the common odd sector and full Hamiltonian eigenstate with the lowest energy, for any magnetic field h, is given by:

$$|GS^-\rangle = \psi^\dagger_{q=0} \prod_{q=0}^{\left\lfloor \frac{N-1}{2} \right\rfloor} \left(\cos\theta_q + \sin\theta_q \psi^\dagger_q \psi^\dagger_{-q}\right) |0\rangle \,. \tag{2.43}$$

The corresponding energies are:

$$E_0^- = \begin{cases} -\frac{1}{2}\sum_{q=0}^{N-1} \Lambda_q & \text{for } h \leq 1 \\ -\frac{1}{2}\sum_{q=0}^{N-1} \Lambda_q + (h-1) & \text{for } h \geq 1. \end{cases} \tag{2.44}$$

This concludes the solving of the XY model. The rest of the eigenstates can be reached by applying the creation operators χ_q in pairs, on states (2.37) and (2.43).

3 Phase diagram

The phase diagram of the 1D XY model at zero temperature, described by the Hamiltonian (2.3) is parametrized by γ and h. γ is the aforementioned anisotropy parameter which speaks of the relative strength of coupling in x and y spin components. h is the parameter describing the strength of the external magnetic field that is directed along the z-axis. Since the other cases can be easily determined using the system symmetries it is enough to examine only the quadrant $(y \geq 0, h \geq 0)$, . It is easy to see that by a $\pi/2$ rotation along the z-axis, a $\gamma \to -\gamma$ equivalent transformation is achieved, whereas a spin reflection across the x-y plane corresponds to $h \to -h$.

As was mentioned in Section 1, this phase diagram contains two non-trivial quantum phase transitions. One is located on the $\gamma = 0$ line for $|h| \leq 1$ and belongs to the universality class of the isotropic XX model (Heisenberg chain), as can be seen from the Hamiltonian (2.3). It corresponds to free fermions aligning on a lattice. The other transition is an Ising transition, along the critical line $h = 1$. The diagram is shown in Figure 2.

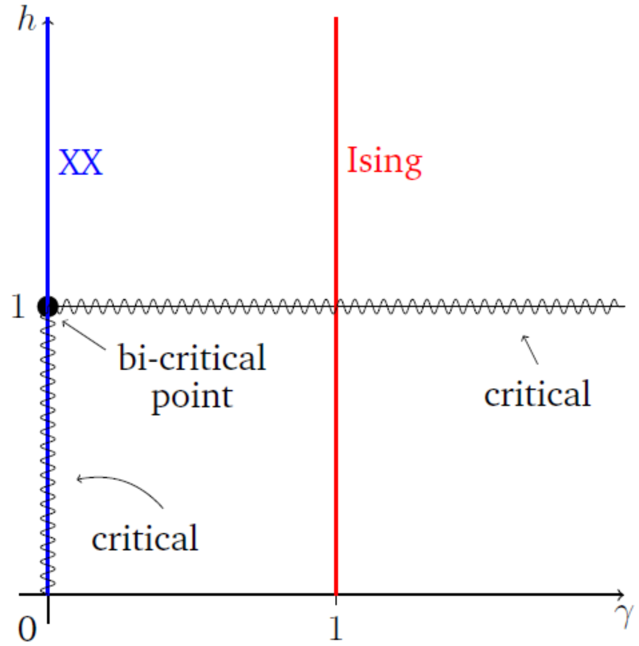

Fig. 2. Phase diagram at T=0 for the 1D XY chain. The $\gamma = 0$ line matches the XX model, and it is critical for $|h| \leq 1$. The $\gamma = 1$ line corresponds to the Ising model and it intersects the critical $h = 1$ line.[9]

4 Fidelity

Fidelity is, as introduced in Section 1, is a function of overlap between two quantum states. Given two quantum states described by density operators ρ and σ, fidelity is defined as [10]:

$$F(\rho, \sigma) := \mathrm{tr}\left(\sqrt{\rho^{1/2}\sigma\rho^{1/2}}\right). \tag{4.1}$$

In the case of pure states, (4.1) reduces to the overlap between two states. Given $\rho = |\psi_Z\rangle\langle\psi_Z|$ and $\sigma = |\psi_{\tilde{Z}}\rangle\langle\psi_{\tilde{Z}}|$, the fidelity of pure states is then:

$$F(Z, \tilde{Z}) = |\langle\psi_Z|\psi_{\tilde{Z}}\rangle| \tag{4.2}$$

By noting that these fermionic states must be coherent (after all, the Hamiltonian (2.32) is essentially a Hamiltonian of N independent quantum harmonic oscillators), we can motivate writing the ground state of a XY chain as a(n) (unormalized) Gaussian state $|\psi_Z\rangle$:

$$|\psi_Z\rangle = \exp\left(\frac{1}{2}\sum_{i,j=0}^{N} c_i^\dagger G_{ij} c_j^\dagger\right)|0\rangle. \tag{4.3}$$

The state $|0\rangle$ is the vacuum state $c_i|0\rangle = 0$, where c_i's are fermionic operators. G is a $N \times N$ anti-symmetric matrix that is obtained through a different algorithm of solving the XY chain (the whole class of free fermion systems, to be exact). Let us justify this expression of the ground state (4.3) and show it is equivalent to the ground state with even parity (2.37). We will also keep the number of particles/spins N to be even. The odd parity state, as well as odd N, are a bit more complicated and are left as the next step after this work.

4.1 Different solving algorithm for XY chain

It might be the most clear to start with a reduced version, notation wise, of the starting Hamiltonian, as the process is general and does not depend on our specific factors. We can write the general quadratic Hamiltonian as:

$$H = \sum_{i,j}^{N} c_i^\dagger A_{ij} c_j + \tfrac{1}{2} \sum_{i,j}^{N} \left(c_i^\dagger B_{ij} c_j^\dagger + \text{h.c.} \right). \tag{4.4}$$

The c_i's ($c_i^\dagger$)'s are the annihilation (creation) operators, A and B are $N \times N$ real, symmetric and anti-symmetric matrices respectively. There is a real matrix Z defined by:

$$A = \frac{Z + Z^T}{2}, \quad B = \frac{Z^T - Z}{2} \quad \Rightarrow Z = A - B. \tag{4.5}$$

Solving the eigenvalue equation:

$$ZZ^\dagger \Phi = \Lambda^2 \Phi, \quad \Lambda = \sqrt{\Lambda^2} = \text{diag}(\Lambda_1, .., \Lambda_N), \tag{4.6}$$

with Λ being a diagonal matrix with single-particle energies as its elements, and Φ a matrix consisting of eigenvectors for every Λ_i, we get the energy spectra and its corresponding eigenvectors in form of Φ. We get another matrix Ψ solving:

$$\Lambda \Psi = \Phi Z. \tag{4.7}$$

Now we can define matrices g and h:

$$g = \frac{\Phi + \Psi}{2}, \quad h = \frac{\Phi - \Psi}{2}. \tag{4.8}$$

Elements of these matrices are coefficients to a canonical linear transformation which would transform the Hamiltonian (4.4) into a diagonal form.
The matrix G from expression (4.3) is now obtained from the equation:

$$gG + h = 0. \tag{4.9}$$

With a little bit of algebra, and a convenient shorthand $\Lambda_\Phi := \Phi^{-1}\Lambda\Phi$, it follows:

$$G = \frac{\Lambda_\Phi^{-1} Z - \mathbb{I}}{\Lambda_\Phi^{-1} Z + \mathbb{I}} = \frac{T-1}{T+1} = \frac{T^{1/2} - T^{-1/2}}{T^{1/2} + T^{-1/2}}. \tag{4.10}$$

It is also important to notice that by manipulating (4.6) slightly it is obvious that the newly defined matrix $T := \Lambda_\Phi^{-1} Z$ is the unitary part of the polar decomposition of Z: $Z = \Lambda_\Phi T$.

4.2 Ground state equivalence

The matrix G can be brought, by unitary transformation U, to a block diagonal form[11]:

$$G = U(\mathbf{0}_{N-2M} \oplus G_D)U^T, \quad G_D = \mathrm{i} \oplus_{\nu=1}^{M} t_\nu \sigma^y_{(\nu)}, \tag{4.11}$$

where 0_{L-2M} is a null matrix of dimension $N - 2M$, $\sigma^y_{(\nu)}$ is a Pauli matrix acting on a 2D space of two single-particle modes ν and $-\nu$, and $t_\nu \neq 0$ is real. ν and $-\nu$ are used as a counting mechanism, as we're counting in pairs/every other indice. A counter with even and odd indices also could have been used.

If we allow $t_\nu = 0$, we can reduce the notation to $G = UG_DU^T$ with the sum over ν now going to $N/2$ and just keep the first $N-2M$ t_ν zero. In this moment it is important to remind ourselves that this procedure is valid for only the even sector, and only for even N. An odd number of rows would make this more complicated as t_ν's obviously come in pairs.
Starting from (2.39), using the fact that in the XY chain only neighbours interact $i = j \pm 1$ and the decomposition of G (4.11) in the discussed form, a little bit of algebra gets us the following expression:

$$|\Psi_Z\rangle = \otimes_{\nu=1}^{N/2} \left[\left(1+t_\nu^2\right)^{-1/2} |00\rangle_{\nu,-\nu} + t_\nu \left(1+t_\nu^2\right)^{-1/2} |11\rangle_{\nu,-\nu} \right]. \tag{4.12}$$

This form is normalized; factor $(1+t_\nu)^{-1/2}$ comes from the norm. Now, we need to find out what is t_ν equal to. First, from the block form, we know that the spectre of G is $\mathrm{Sp}(G) = \{\pm \mathrm{i} t_\nu\}_{\nu=1}^{N/2}$. Furthermore, since T is unitary, we can write its spectra as $\mathrm{Sp}(T) = \{e^{\mathrm{i}\theta_\mu}\}$. Using (4.10) we see that we can also write the spectra of G as $\mathrm{Sp}(G) = \{\mathrm{i}\tan(\theta_\mu/2)\}_{\mu=1}^{N/2}$.
Applying another property of unitarity, we can write T as $T = e^K$, with K an anti-symmetric matrix. Then we can decompose it like G: $K_D = U^\mathrm{T} K U = \oplus_{\nu=1}^{N/2} \mathrm{i}\theta_\nu \sigma^y_{(\nu)}$. Just like t_ν, $\theta_\nu \in \mathbb{R}$.
It follows that $\mathrm{Sp}(T) = \left\{ \mathrm{e}^{\pm i\theta_\nu} \right\}_{\nu=1}^{N/2}$ and $t_\nu = \tan(\theta_\nu/2)$, which plugged into (4.12) gives:

$$|\Psi_Z\rangle = \otimes_{\nu=1}^{N/2} \left[\cos(\theta_\nu/2) |00\rangle_{\nu,-\nu} + \sin(\theta_\nu/2) |11\rangle_{\nu,-\nu} \right]. \tag{4.13}$$

If we applied the operators of creation in (2.37), and redefined $\theta_q \to \theta_\nu/2$, we would have this form (4.13). Here, a $\otimes$ symbol was used (unlike in Section 2) because it was necessary to emphasise the blocks of matrices used.

4.3 Calculating fidelity

Fidelity in form (4.2) is not very practical. Considering the fact that this system's ground state is coherent (which we've motivated in Subsection 4.1), we can write the fidelity in the following form [12]:

$$F(Z, \tilde{Z} = \langle \Psi_{\tilde{Z}} \mid \Psi_Z \rangle = \frac{\det\left(\mathbb{I} + G^\dagger \tilde{G}\right)^{1/2}}{\det\left(\mathbb{I} + G^\dagger G\right)^{1/4} \det\left(\mathbb{I} + \tilde{G}^\dagger \tilde{G}\right)^{1/4}}. \tag{4.14}$$

It is possible to further simplify this form [5] to get:

$$F(Z, \tilde{Z}) = \left| \det \frac{T + \tilde{T}}{2} \right|^{1/2} \tag{4.15}$$

Comparing (4.4) and (2.11), we construct matrices A and B. Following the algorithm described in Subsection 4.1, we are able to procure T we need for calculating fidelity according to equation (4.15). As demonstrated in 3, it is enough to examine behaviour for $h \geq 0, \gamma \geq 0$. We varied γ in range $\gamma = [-0.2, 1.0]$ and h in range $h = [0.0, 1.2]$. The reason for going slightly into negative values for γ is the fact that we expect interesting behaviour at $\gamma = 0$. We used the *numpy* package from Python for calculations.

4.4 Results

Graphs showing fidelity of XY chain for even number of particles (N) in the even sector are seen in Figures 3 and 4.

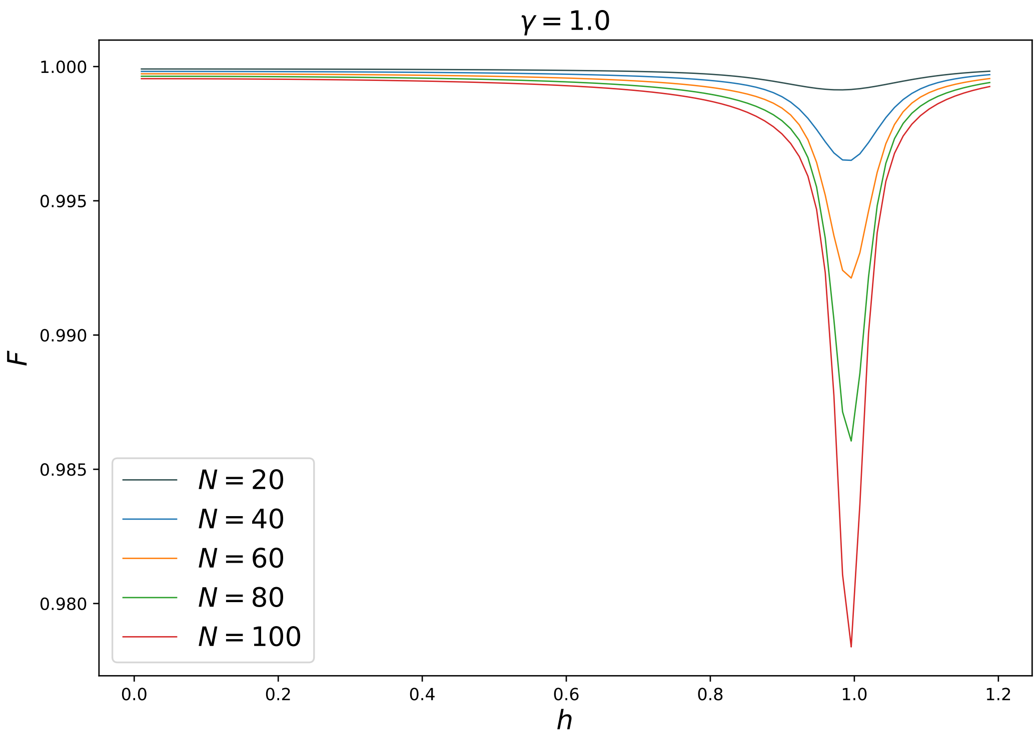

Fig. 3. Fidelity for $\gamma = 1.0$ in range $h = [0.0, 1.2]$. A clear dip is seen at $h = 1.0$ that increases with increasing N.

The numerical results perfectly coincide with expected phase transitions (See Figure 2). As can be seen in Figure 3, by varying h for $\gamma = 1.0$ we can clearly see a dip for $h = 1.0$, corresponding to the Ising transition, as mentioned in Section 3. The dip would also show for other values of γ, but $\gamma = 1.0$ is chosen as it matches the Ising model. On the other hand, Figure 4 shows fidelity calculated by varying γ. There is also a distinct dip of fidelity at $\gamma = 0$, corresponding to a transition to XX model. h is taken to be $h = 0.5$, but fidelity would show the same behavior for any $|h| \leq 1$. Both graphs display that the dip sharpens and increases with increasing N. This is a signature of the fact that in the thermodynamic limit $N \to \infty$ this dip becomes a real discontinuity.

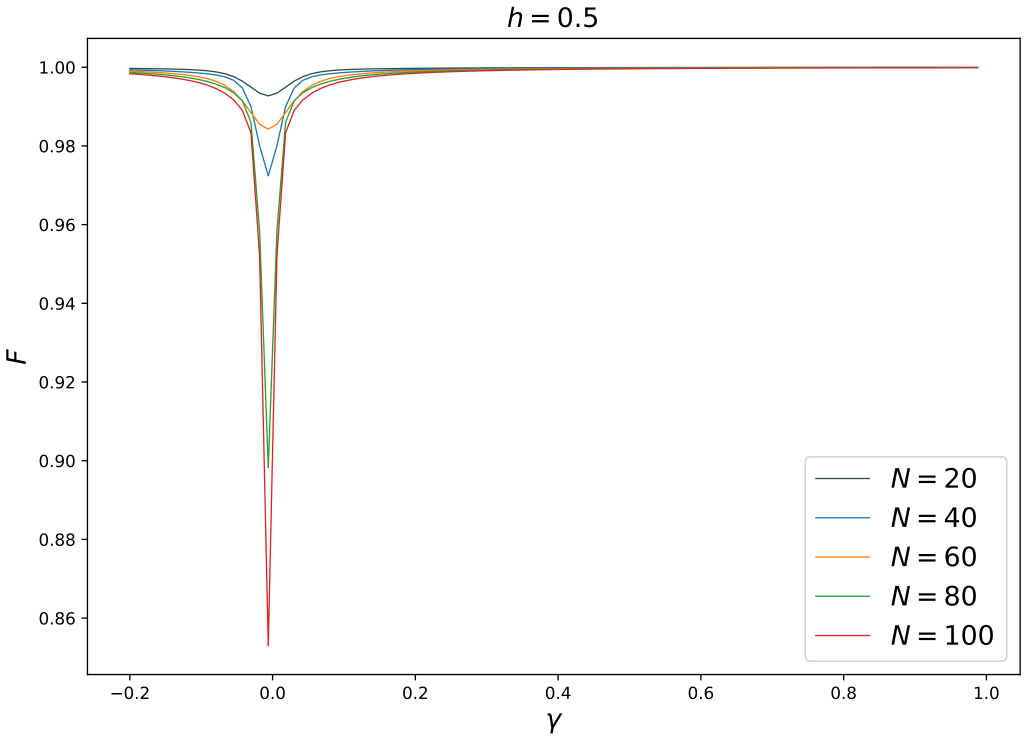

Fig. 4. Fidelity for $h = 0.5$ in range $\gamma = [-0.2, 1.0]$. A clear dip is seen at $\gamma = 0.0$ that increases with increasing N.

5 Conclusion

In conclusion, in this work, we have analyzed the ground-state fidelity for the unfrustrated 1D XY model. As was expected, such a quantity remains near to 1 except for the values close to the quantum critical points, i.e. for $h = 1$ and/or for $\gamma = 0$, in which it reaches a minimum that becomes deeper and deeper as the number of the spins of the system increases hence signaling the presence of a critical region. As it is well known in the literature [13, 14] this kind of behavior is shared by all gapped spin models and, as well as the existence of a local order parameter of the Ginzburg-Landau theory, it is assumed to be independent of the particular choice of the boundary conditions. However, in the last year, such independence was challenged by several studies on topologically frustrated one-dimensional spin models that have unveiled new phases that have no counterparts in the associated unfrustrated models[4, 15]. In this optics, in the future, our target is to extend the analysis presented in this work to frustrated models with the goal to unveil the different structures of the ground-state manifold between frustrated and unfrustrated systems.

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A Appendix

A.1 Fourier transform operators

If we notice that:

$$x_0 \in \mathbb{Z} \Rightarrow \frac{1}{N} \sum_{x \in X_N} e^{i \frac{2\pi}{N} xn} = \begin{cases} 1, & n = kN, k \in \mathbb{Z} \\ 0, & \text{else} \end{cases}$$
$$x_0 = \tfrac{1}{2} \Rightarrow \frac{1}{N} \sum_{x \in X_N} e^{i \frac{2\pi}{N} xn} = \begin{cases} (-1)^k, & n = kN, k \in \mathbb{Z} \\ 0, & \text{else} \end{cases} \tag{A.1}$$

We can write the operator ψ_j for all $j = 1, .., N$ like:

$$\psi_j = \sum_{l=1}^{N} \left[\psi_l \frac{1}{N} \sum_{x \in X_N} e^{\frac{2\pi}{N} x(j-l)} \right]. \tag{A.2}$$

It is not important what we take for x_0, an integer or $1/2$. However, by choosing $x_0 = 1/2$ in the even sector and $x_0 = 0$ in the odd sector, we're able to continue with periodic boundary conditions and define ψ_{N+1} in line with (A.2). Now we see why it's convenient to define operators ψ_q like (2.15) and why we call them Fourier transform of ψ_j.

A.2 Special cases operator definitions

It is sometimes convenient to rearrange equations (2.26) into a different form:

$$\tan 2\theta_q = \frac{\gamma \sin\left(\frac{2\pi}{N} q\right)}{h - \cos\left(\frac{2\pi}{N} q\right)}, \tag{A.3a}$$

$$e^{i2\theta_q} = \frac{h - \cos\left(\frac{2\pi}{N} q\right) + i\gamma \sin\left(\frac{2\pi}{N} q\right)}{\sqrt{\left[h - \cos\left(\frac{2\pi}{N} q\right)\right]^2 + \gamma^2 \sin^2\left(\frac{2\pi}{N} q\right)}}. \tag{A.3b}$$

For example, in the case when $q = 0$ or $N/2$, the matrix (2.21) is already diagonal and (2.26) are not well defined. Therefore, we simply define operators χ_q so (A.3b) is fulfilled and take any $\cos\theta_q$ and $\sin\theta_q$ that are consistent with that. The suitable definition of χ_q for $q = 0, N/2$ then is:

$$\chi_{q=0} := \begin{cases} \psi^\dagger_{q=0}, & \text{for } h < 1 \\ \psi_{q=0}, & \text{for } h > 1. \end{cases} \tag{A.4}$$

$$\chi_{q=N/2} := \psi_{q=N/2}. \tag{A.5}$$