The XY Model in One Dimension

Max A. Metlitski

I. INTRODUCTION

One of the oldest problems of quantum mechanics is the one dimensional spin-1/2 antiferromagnetic Heisenberg chain with the Hamiltonian $H = J\sum_i \vec{S}_i\vec{S}_{i+1}$. Although the spectrum of this Hamiltonian was found exactly by H. Bethe[1] in 1931, the solution is quite involved and does not shed much light on even such basic properties as long-range order. A much more natural approach to the problem of interacting spin-1/2's, stems from the similarity between spin-1/2 raising/lowering operators and fermion creation/annihilation operators. This correspondence, originally made precise in 1928 by Jordan and Wigner[2], can be used to convert spin-1/2 systems into problems of interacting spinless fermions. In this paper, I review the application of Jordan-Wigner transformations to a modification of the Heisenberg chain, known as the XY model, which was originally studied in great detail in [3]. The XY model, which can be obtained from the Heisenberg Hamiltonian by turning off the coupling between z spin components, reduces to a *free* theory of spinless fermions under the Jordan-Wigner transformations. Luckily, it turns out that the low-energy properties of the full anti-ferromagnetic Heisenberg chain, such as the presence of gapless excitations and absence of long range order are very similar to those of the XY model (see [4] and references therein).

The first part of this paper discusses the introduction of Jordan-Wigner transformations and the spectrum of the XY model. The second part of the paper is devoted to more advanced aspects of the XY model, such as the effects of anisotropy and study of short, intermediate and long range order.

II. JORDAN-WIGNER TRANSFORMATION OF THE XY MODEL

Consider the following Hamiltonian describing a chain of N spin-1/2's interacting antiferromagnetically with their nearest neighbors:

$$H = \sum_i (S^x{}_i S^x{}_{i+1} + S^y{}_i S^y{}_{i+1}) \tag{1}$$

Here $S^a{}_i$ are spin-1/2 operators, obeying the usual commutation relations $[S^a{}_i, S^b{}_j] = i\epsilon^{abc}\delta_{ij}S^c{}_i$. The scale of the coupling as well as $\hbar$ have been set to 1. We assume cyclic boundary conditions, i.e. the index i in the sum (1) runs over $1 \dots N$ with $\vec{S}_{N+1} = \vec{S}_1$.

We can obtain a ferromagnetic counterpart of (1), by defining $H_F = -H$. Thus, once we have solved the antiferromagnetic problem *exactly*, we can immediately read out the solution to the ferromagnetic problem.

As usual it is convenient to introduce raising and lowering operators: $a_i{}^\dagger = S^x{}_i + iS^y{}_i$, $a_i = S^x{}_i - iS^y{}_i$. These obey the algebra:

$$\{a_i, a_i{}^\dagger\} = 1,\ \{a_i, a_i\} = \{a_i{}^\dagger, a_i{}^\dagger\} = 0, \tag{2}$$

$$[a_i, a_j] = [a_i, a_j{}^\dagger] = [a_i{}^\dagger, a_j{}^\dagger] = 0,\ i \neq j \tag{3}$$

The Hamiltonian (1) then takes the form:

$$H = \frac{1}{2}\sum_i (a_i a_{i+1}^\dagger + a_{i+1}a_i{}^\dagger) \tag{4}$$

Hence the Hamiltonian is quadratic in a's. If *all* a's obeyed canonical anticommutation relations we would be done - it would be possible to diagonalize H by a linear transformation of the a's! Unfortunately, a's belonging to the same site obey anticommutaion relations, while a's on different sites obey commutation relations, so that unitary rotations of the a's obey neither bosonic nor fermionic algebra. The key to the solution of this problem is the Jordan-Wigner transformation. Let,

$$c_i = \exp(\pi i \sum_{j=1}^{i-1} a_j{}^\dagger a_j) a_i,\ \ c_i{}^\dagger = a_i{}^\dagger \exp(-\pi i \sum_{j=1}^{i-1} a_j{}^\dagger a_j) \tag{5}$$

The highly non-linear transformation (5) can be easily inverted. Observe,

$$c_i{}^\dagger c_i = a_i{}^\dagger a_i \tag{6}$$

and thus,

$$a_i = \exp\left(-\pi i \sum_{j=1}^{i-1} c_j{}^\dagger c_j\right) c_i, \;\; a_i{}^\dagger = c_i{}^\dagger \exp\left(\pi i \sum_{j=1}^{i-1} c_j{}^\dagger c_j\right) \tag{7}$$

The operators c_i, $c_i{}^\dagger$ obey the canonical fermion algebra:

$$\{c_i, c_j{}^\dagger\} = \delta_{ij}, \; \{c_i, c_j\} = 0, \; \{c_i{}^\dagger, c_j{}^\dagger\} = 0 \tag{8}$$

We will demonstrate explicitly, $\{c_i, c_j{}^\dagger\} = \delta_{ij}$ (the other anti-commutators in (8) can be computed in a similar fashion). Observe, $[a_i{}^\dagger a_i, a_j{}^\dagger \, a_j] = 0$, $(a_i{}^\dagger a_i)^2 = a_i{}^\dagger a_i$, $[a_i{}^\dagger a_i, a_j] = -\delta_{ij} a_j$, $[a_i{}^\dagger a_i, a_j{}^\dagger] = \delta_{ij} a_j{}^\dagger$ since a's on different sites commute and a's on the same site behave like fermions. Therefore,

$$\exp\left(\pm\pi i \sum_{j=n}^{m} a_j{}^\dagger a_j\right) = \prod_{j=n}^{m} \exp\left(\pm\pi i a_j{}^\dagger a_j\right) \tag{9}$$

where

$$\exp\left(\pm\pi i a_i{}^\dagger a_i\right) = \sum_{l=0}^{\infty} \frac{1}{l!} (\pm\pi i)^l (a_i{}^\dagger a_i)^l = 1 + \sum_{l=1}^{\infty} \frac{1}{l!} (\pm\pi i)^l a_i{}^\dagger a_i = 1 + (e^{\pm\pi i} - 1) a_i{}^\dagger a_i = 1 - 2 a_i{}^\dagger a_i \tag{10}$$

Also, observe that

$$\{a_i, 1 - 2a_i{}^\dagger a_i\} = a_i(1 - 2a_i{}^\dagger a_i) + (1 - 2a_i{}^\dagger a_i) a_i = 2a_i - 2a_i a_i{}^\dagger a_i = 2a_i - 2(1 - a_i{}^\dagger a_i) a_i = 0, \tag{11}$$

$$\{a_i{}^\dagger, 1 - 2a_i{}^\dagger a_i\} = \{a_i, 1 - 2a_i{}^\dagger a_i\}^\dagger = 0 \tag{12}$$

which implies

$$[\exp\left(\pm\pi i \sum_{j=n}^{m} a_j{}^\dagger a_j\right), a_i] = [\exp\left(\pm\pi i \sum_{j=n}^{m} a_j{}^\dagger a_j\right), a_i{}^\dagger] = 0, \; i \notin [n, m] \tag{13}$$

$$\{\exp\left(\pm\pi i \sum_{j=n}^{m} a_j{}^\dagger a_j\right), a_i\} = \{\exp\left(\pm\pi i \sum_{j=n}^{m} a_j{}^\dagger a_j\right), a_i{}^\dagger\} = 0, \; i \in [n, m] \tag{14}$$

Now, we can compute the anti-commutator:

$$\{c_i, c_i{}^\dagger\} = a_i a_i{}^\dagger + a_i{}^\dagger a_i = 1 \tag{15}$$

and for $j > i$,

$$\{c_i, c_j{}^\dagger\} = a_i \exp(\pi i \sum_{k=1}^{i-1} a_k{}^\dagger a_k) \exp(-\pi i \sum_{k=1}^{j-1} a_k{}^\dagger a_k) a_j{}^\dagger + a_j{}^\dagger \exp(-\pi i \sum_{k=1}^{j-1} a_k{}^\dagger a_k) \exp(\pi i \sum_{k=1}^{i-1} a_k{}^\dagger a_k) a_i \tag{16}$$

$$= a_i \exp(\pi i \sum_{k=i}^{j-1} a_k{}^\dagger a_k) a_j{}^\dagger + a_j{}^\dagger \exp(\pi i \sum_{k=i}^{j-1} a_k{}^\dagger a_k) a_i = (a_i a_j{}^\dagger - a_j{}^\dagger a_i) \exp(\pi i \sum_{k=i}^{j-1} a_k{}^\dagger a_k) \tag{17}$$

$$= [a_i, a_j{}^\dagger] \exp(\pi i \sum_{k=i}^{j-1} a_k{}^\dagger a_k) = 0 \tag{18}$$

where we have used eqs. (13),(14). Similarly, for $j < i$,

$$\{c_i, c_j{}^\dagger\} = \{c_j, c_i{}^\dagger\}^\dagger = 0 \tag{19}$$

Let's rewrite the Hamiltonian in terms of c's using eq. (7). Since c's satisfy canonical anticommutation relations, $[c_i{}^\dagger c_i, c_j{}^\dagger c_j] = 0$, $(c_i{}^\dagger c_i)^2 = c_i{}^\dagger c_i$, $[c_i{}^\dagger c_i, c_j] = -\delta_{ij} c_j$, $[c_i{}^\dagger c_i, c_j{}^\dagger] = \delta_{ij} c_j{}^\dagger$, we have in complete analogy to eqs. (9),

$$\exp\left(\pm\pi i\sum_{j=n}^{m} {c_j}^\dagger c_j\right) = \prod_{j=n}^{m}\exp\left(\pm\pi i {c_j}^\dagger c_j\right) = \prod_{j=n}^{m}(1-2{c_j}^\dagger c_j) \tag{20}$$

$$\{1-2{c_i}^\dagger c_i, c_i\} = \{1-2{c_i}^\dagger c_i, {c_i}^\dagger\} = 0 \tag{21}$$

$$[\exp\left(\pm\pi i\sum_{j=n}^{m} {c_j}^\dagger c_j\right), c_i] = [\exp\left(\pm\pi i\sum_{j=n}^{m} {c_j}^\dagger c_j\right), {c_i}^\dagger] = 0,\ i\notin[n,m] \tag{22}$$

$$\{\exp\left(\pm\pi i\sum_{j=n}^{m} {c_j}^\dagger c_j\right), c_i\} = \{\exp(\pm\pi i\sum_{j=n}^{m} {c_j}^\dagger c_j), {c_i}^\dagger\} = 0,\ i\in[n,m] \tag{23}$$

Now, we can compute the various terms in the Hamiltonian (4). For $1\le i\le N-1$,

$$a_i {a^\dagger}_{i+1} = \exp(-\pi i\sum_{j=1}^{i-1} {c_j}^\dagger c_j) c_i {c^\dagger}_{i+1}\exp(\pi i\sum_{j=1}^{i} {c_j}^\dagger c_j) = c_i\exp(-\pi i\sum_{j=1}^{i-1} {c_j}^\dagger c_j)\exp(\pi i\sum_{j=1}^{i} {c_j}^\dagger c_j){c^\dagger}_{i+1} \tag{24}$$

$$= c_i\exp(\pi i {c_i}^\dagger c_i){c^\dagger}_{i+1} = c_i(1-2{c_i}^\dagger c_i){c^\dagger}_{i+1} = -(1-2{c_i}^\dagger c_i)c_i{c^\dagger}_{i+1} = -c_i{c^\dagger}_{i+1} = {c^\dagger}_{i+1}c_i \tag{25}$$

$$a_{i+1}{a_i}^\dagger = (a_i {a^\dagger}_{i+1})^\dagger = {c_i}^\dagger c_{i+1} \tag{26}$$

After similarly expressing the special cyclic boundary term $a_N {a_1}^\dagger + a_1 {a_N}^\dagger$ in terms of c's, the Hamiltonian becomes,

$$H = H_c + H_b, \tag{27}$$

$$H_c = \frac{1}{2}\sum_i ({c^\dagger}_{i+1}c_i + {c_i}^\dagger c_{i+1}) \tag{28}$$

$$H_b = -\frac{1}{2}({c_1}^\dagger c_N + {c_N}^\dagger c_1)(\exp\left(\pi i\sum_{j=1}^{N} {c_j}^\dagger c_j\right)+1) \tag{29}$$

The Hamiltonian H_c is quadratic in anticommuting operators c, and describes a free spinless fermion on a cyclic chain with nearest neighbor hopping. Hence H_c can be trivially diagonalized by solving the one particle Schrodinger equation, and making a unitary transformation of the c's. The effect of the boundary term H_b can be actually taken into account exactly (see section III A), but we choose to neglect it for now as it gives an $O(1/N)$ contribution to macroscopic physical quantities.

Observe, that in the original formulation the Hamiltonian conserves total spin along the z axis: $[H, S^z] = 0$. After the Jordan-Wigner transformation, this symmetry is manifested as conservation of the total fermion number $\mathcal{N} = \sum_i {c_i}^\dagger c_i,\ [H_c, \mathcal{N}] = 0$. Indeed,

$${S^z}_i = \frac{1}{2}[{a_i}^\dagger, a_i] = {a_i}^\dagger a_i - \frac{1}{2} = {c_i}^\dagger c_i - \frac{1}{2} \tag{30}$$

$$S^z = \sum_i {S_i}^z = \sum_i ({c_i}^\dagger c_i - \frac{1}{2}) = \mathcal{N} - \frac{N}{2} \tag{31}$$

Thus, each "spinless" fermion created by $c^\dagger$ carries $S^z = 1$.

It is instructive to see how the true 1D Heisenberg Hamiltonian $H_h = \sum_i \vec{S}_i\vec{S}_{i+1}$ transforms under the Jordan-Wigner transformation (5). Observe,

$$H_h = H + \sum_i {S_i}^z {S_{i+1}}^z = H + \sum_i ({c_i}^\dagger c_i - \frac{1}{2})({c^\dagger}_{i+1}c_{i+1} - \frac{1}{2}) \tag{32}$$

Thus, unlike the XY model, the Heisenberg Hamiltonian is no longer a free theory, but a theory of spinless fermions on a lattice with nearest neighbor hopping and nearest neighbor *interactions*.

Let's proceed with diagonalization of H_c. We rewrite,

$$H_c = \sum_{ij} {c_i}^\dagger A_{ij} c_j, \quad A_{ij} = \frac{1}{2}(\delta_{i,j+1} + \delta_{j,i+1}) \tag{33}$$

Letting $\{\phi_k\}$ be a complete and orthonormal set of eigenvectors of $\mathbf{A}$ with eigenvalues $\{\Lambda_k\}$, define:

$$\eta_k = \sum_i \phi^*{}_{ki} c_i, \quad \eta_k{}^\dagger = \sum_i \phi_{ki} c_i{}^\dagger \tag{34}$$

which imply canonical anticommutation relations of η's, and conversely:

$$c_i = \sum_k \phi_{ki} \eta_k, \quad c_i{}^\dagger = \sum_k \phi^*{}_{ki} \eta_k{}^\dagger \tag{35}$$

Expressing H_c in terms of η's:

$$H_c = \sum_k \Lambda_k \eta_k{}^\dagger \eta_k \tag{36}$$

Some of the eigenvalues of $\mathbf{A}$ will be negative, so it is convenient to make an additional transformation:

$$\xi_k = \eta_k, \ \Lambda_k \geq 0; \quad \xi_k = \eta_k{}^\dagger, \ \Lambda_k < 0 \tag{37}$$

leading to

$$H_c = \sum_{k,\Lambda_k \geq 0} \Lambda_k \xi_k{}^\dagger \xi_k + \sum_{k,\Lambda_k<0} \Lambda_k \xi_k \xi_k{}^\dagger = \sum_k |\Lambda_k| \xi_k{}^\dagger \xi_k - \sum_{k,\Lambda_k<0} |\Lambda_k| = \sum_k |\Lambda_k| (\xi_k{}^\dagger \xi_k - \frac{1}{2}) \tag{38}$$

where we've used, $tr(\mathbf{A}) = \sum_k \Lambda_k = 0$. The ξ's are again canonical fermi operators. Hence the ground state $|\Omega\rangle$ satisfies,

$$\xi_k |\Omega\rangle = 0, \ \forall k \tag{39}$$

and operators $\xi_k{}^\dagger$ generate elementary fermionic excitations with energy $|\Lambda_k|$ above the ground state.

Utilizing translational invariance, we find the eigenvectors and eigenvalues of $\mathbf{A}$ to be:

$$\phi_{kj} = \frac{1}{\sqrt{N}} e^{ikj}, \ \ \Lambda_k = \cos(k); \qquad k = \frac{2\pi n}{N}, \ \ -N/2 \leq n \leq N/2 - 1 \tag{40}$$

So, in thermodynamic limit $N \to \infty$ there are always gapless excitations near $k = \pm\frac{\pi}{2}$ (see Fig. 1 for a plot of the dispersion relation). These have a dispersion, $k = \pm\pi/2 + q$, $\epsilon(k) = |\sin(q)| \approx |q|$ as $q \to 0$. The ground state energy per spin becomes:

$$\frac{U}{N} = -\frac{1}{N} \sum_k \frac{1}{2} |\Lambda_k| \to -\int_{-\pi}^{\pi} \frac{dk}{2\pi} \frac{1}{2} |\cos(k)| = -\frac{1}{4\pi} 4 \int_0^{\pi/2} \cos(k) dk = -\frac{1}{\pi} \tag{41}$$

Let's investigate the spin properties. For simplicity we assume that N is even and not divisible by 4, so that the ground state is non-degenerate[1](at any rate, the ground state of H_c is at most 4 times degenerate). Notice,

$$S^z = \sum_i c_i{}^\dagger c_i - \frac{N}{2} = \sum_k \eta_k{}^\dagger \eta_k - \frac{N}{2} = \sum_{k,\Lambda_k \geq 0} \xi_k{}^\dagger \xi_k + \sum_{k,\Lambda_k<0} \xi_k \xi_k{}^\dagger - \frac{N}{2} \tag{42}$$

$$= \sum_{k,\Lambda_k \geq 0} \xi_k{}^\dagger \xi_k + \sum_{k,\Lambda_k<0} (1 - \xi_k{}^\dagger \xi_k) - \frac{N}{2} = \sum_k sgn(\Lambda_k) \xi_k{}^\dagger \xi_k + \sum_{k,\Lambda_k<0} 1 - \frac{N}{2} \tag{43}$$

Hence, excitations with $|k| < \frac{\pi}{2}$ carry $S^z = +1$, while excitations with $|k| > \frac{\pi}{2}$ carry $S^z = -1$. The total spin of the ground state is,

$$S^z |\Omega\rangle = (\sum_{k,\Lambda_k<0} 1 - \frac{N}{2}) |\Omega\rangle = 0 \tag{44}$$

---

[1] Another reason for considering the case N - even, not divisible by 4, is that in this case the ground state of H_c is actually an exact eigenstate of H with the same eigenvalue.

So the ground state is non-degenerate and carries $S^z = 0$ - this is the same result as in the full Heisenberg model.

Our above results can be trivially generalized to the case of ferromagnetic coupling. In that case,

$$H_F = -H \approx -H_c = \sum_k -|\Lambda_k|(\xi_k{}^\dagger \xi_k - \frac{1}{2}) = \sum_k |\Lambda_k|(\xi_k \xi_k{}^\dagger - \frac{1}{2}) \tag{45}$$

So the new ground state satisfies, $\xi_k{}^\dagger |\Omega_F\rangle = 0$, $\forall k$. Hence $|\Omega_F\rangle$ can be obtained from the antiferromagnetic ground state by turning on all the excitations, and the ferromagnetic excitations are obtained by removing the antiferromagnetic ones. In particular, the ground state energy and the excitation spectrum are the same as in the antiferromagnetic case. Hence, the ground state is still non-degenerate and

$$S^z|\Omega_F\rangle = (\sum_k sgn(\Lambda_k)\xi_k{}^\dagger \xi_k + \sum_{k,\Lambda_k<0} 1 - \frac{N}{2})|\Omega_F\rangle = (\sum_k sgn(\Lambda_k) + \sum_{k,\Lambda_k<0} 1 - \frac{N}{2})|\Omega_F\rangle = (\sum_{k,\Lambda_k\geq 0} 1 - \frac{N}{2})|\Omega_F\rangle = 0 \tag{46}$$

This is in clear contrast to the full ferromagnetic Heisenberg model, where the ground state is greatly degenerate, and one of the ground states carries $S^z = N/2$.

III. PROPERTIES OF THE XY MODEL

A. Anisotropy Effects

It is first interesting to generalize the discussion of section II to the case when the interaction in the XY plane is not isotropic, i.e

$$H_\gamma = \sum_i ((1+\gamma) S_i{}^x S_{i+1}{}^x + (1-\gamma) S_i{}^y S_{i+1}{}^y) \tag{47}$$

where $-1 \leq \gamma \leq 1$ is the anisotropy parameter. In section II, we considered the fully isotropic case $\gamma = 0$, which has an additional symmetry $[H, S^z] = 0$. The opposite limit $\gamma = 1$ corresponds to the classical Ising model, in which the ground state is Neel ordered, i.e $S_i^x|\Omega\rangle = (-1)^i|\Omega\rangle\ \forall i$. The methods developed in section II allow us to explicitly study how the system properties change as we go from the totally ordered state at $\gamma = 1$ to the isotropic limit $\gamma = 0$.

First, we rewrite the Hamiltonian H_γ in terms of operators $a, a^\dagger$.

$$H_\gamma = \frac{1}{2}\sum_i ((a_i a^\dagger{}_{i+1} + a_{i+1} a_i{}^\dagger) + \gamma(a_i a_{i+1} + a^\dagger{}_{i+1} a_i{}^\dagger)) \tag{48}$$

Now we apply the Jordan-Wigner transformation (7), to express H_γ in terms of c's:

$$H_\gamma = H_c + H_b \tag{49}$$

$$H_c = \frac{1}{2}\sum_i ((c^\dagger{}_{i+1} c_i + c_i{}^\dagger c_{i+1}) + \gamma(c_i{}^\dagger c^\dagger{}_{i+1} + c_{i+1} c_i)) \tag{50}$$

$$H_b = -\frac{1}{2}(c_1{}^\dagger c_N + c_N{}^\dagger c_1 + \gamma(c_N{}^\dagger c_1{}^\dagger + c_1 c_N))(P+1),\ P = \exp(\pi i \sum_{j=1}^N c_j{}^\dagger c_j) = \exp(\pi i \mathcal{N}) \tag{51}$$

We again for now neglect the boundary term H_b as it has little effect on macroscopic physical quantities (we indicate how to take H_b exactly into account at the end of this section). The Hamiltonian H_c is still quadratic in c's, but now for $\gamma \neq 0$, $[H_c, \mathcal{N}] \neq 0$ because of the new $c\,c$, $c^\dagger c^\dagger$ terms in the Hamiltonian. Recalling the correspondence, between $\mathcal{N}$ and S^z, the non-conservation of fermion number $\mathcal{N}$ simply reflects the non-conservation of S^z.

Hamiltonian H_c can be diagonalized with a linear transformation of the canonical fermion operators $c, c^\dagger$. Indeed, write

$$H_c = \sum_{i,j} (c_i{}^\dagger A_{ij} c_j + \frac{1}{2}(c_i^\dagger B_{ij} c_j^\dagger - c_i B_{ij} c_j)) \tag{52}$$

$$A_{ij} = \frac{1}{2}(\delta_{i,j-1} + \delta_{i,j+1}),\ \ B_{ij} = \frac{\gamma}{2}(\delta_{i,j-1} - \delta_{i,j+1}) \tag{53}$$

where A is a real symmetric matrix and B is a real antisymmetric matrix. Defining,

$$\eta_k = \sum_i (g_{ki} c_i + h_{ki} {c_i}^\dagger), \tag{54}$$

$${\eta^\dagger}_k = \sum_i (g_{ki} {c_i}^\dagger + h_{ki} c_i) \tag{55}$$

we wish to find real constants g_{ki}, h_{ki}, s.t. the η's obey canonical anti-commutation relations and,

$$H_c = \sum_k \Lambda_k {\eta_k}^\dagger \eta_k + const \tag{56}$$

Using the equation of motion technique, $[H, {\eta^\dagger}_k] = \Lambda_k {\eta^\dagger}_k$, we obtain:

$$\mathbf{A} g_k + \mathbf{B} h_k = \Lambda_k g_k \tag{57}$$

$$-\mathbf{B} g_k - \mathbf{A} h_k = \Lambda_k h_k \tag{58}$$

Letting,

$$\phi_{ki} = g_{ki} + h_{ki}, \;\; \psi_{ki} = g_{ki} - h_{ki} \tag{59}$$

$$(\mathbf{A} + \mathbf{B})\phi_k = \Lambda_k \psi_k, \tag{60}$$

$$(\mathbf{A} - \mathbf{B})\psi_k = \Lambda_k \phi_k \tag{61}$$

which implies,

$$(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})\phi_k = \Lambda_k^2 \phi_k, \tag{62}$$

$$(\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B})\psi_k = \Lambda_k^2 \psi_k \tag{63}$$

Assuming $det(A-B) \neq 0$[2], all eigenvalues Λ_k^2 of the real symmetric matrix $R = (A-B)(A+B)$ are strictly positive, and hence N real orthonormal eigenvectors ϕ_k of R, generate N real solutions of eqs. (57), (58) with $\Lambda_k > 0$, if we let $\psi_k = {\Lambda_k}^{-1}(A+B)\phi_k$.

After transformations (54), (55), the Hamiltonian becomes,

$$H_c = \sum_k \Lambda_k ({\eta_k}^\dagger \eta_k - \frac{1}{2}) \tag{64}$$

The ground state is again defined as $\eta_k |\Omega\rangle = 0, \forall k$, and the spectrum is that of free fermions with excitation energies Λ_k.

It remains to diagonalize the matrix $((A-B)(A+B))_{ij} = \frac{1-\gamma^2}{4}(\delta_{i+1,j-1} + \delta_{i-1,j+1}) + \frac{1+\gamma^2}{2}\delta_{ij}$. Due to translational invariance, we find[3],

$$\Lambda_k \;=\; (1 - (1-\gamma^2)\sin^2 k)^{1/2} \tag{65}$$

$$\phi_{kj} = \sqrt{\frac{2}{N}}\sin(kj),\; k > 0, \quad \phi_{kj} \;=\; \sqrt{\frac{2}{N}}\cos(kj),\; k \leq 0, \;\; k = \frac{2\pi n}{N},\; -\frac{N}{2} \leq n \leq \frac{N}{2} - 1 \tag{66}$$

The corresponding ψ_k can be calculated from eq. (60):

$$\psi_{kj} \;=\; \frac{1}{\Lambda_k}(A+B)_{jn}\phi_{kn} = \frac{1}{2\Lambda_k}((\phi_{k,j+1} + \phi_{k,j-1}) + \gamma(\phi_{k,j+1} - \phi_{k,j-1})) \tag{67}$$

$$\;=\; \frac{1}{\Lambda_k}(\cos(k)\phi_{kj} + \gamma \sin(k)\phi_{-k,j}) \tag{68}$$

---

[2] if $det(A-B) = 0$ we can still represent the Hamiltonian in the form (56)

[3] Actually, ϕ_k for $k = 0$, and $k = -\pi$ have a normalization factor $\sqrt{\frac{1}{N}}$. The effect of these two modes, is however, negligible in the limit $N \to \infty$

We observe that for any asymmetry $\gamma \neq 0$, the excitation spectrum develops a gap $\Delta = \Lambda(\pm\frac{\pi}{2}) = |\gamma|$ (see Fig. (1) for a plot of the dispersion relation). The ground state energy per spin becomes,

$$\frac{U}{N} = -\frac{1}{N}\sum_k \frac{1}{2}\Lambda_k \to -\frac{1}{\pi}\int_0^{\pi/2} dk(1-(1-\gamma^2)\sin^2(k))^{1/2} = -\frac{1}{\pi}\mathcal{E}(\sqrt{1-\gamma^2}) \tag{69}$$

where $\mathcal{E}$ is an elliptic E function.

Finally, let's discuss how to take the boundary term H_b into account. We observe, that even though for arbitrary γ, $[\mathcal{N}, H_c] \neq 0$, we have $[P, H_c] = [P, H] = 0$, where $P = \exp(\pi i \mathcal{N})$. This corresponds to the symmetry with respect to rotations around z axis by π. Thus, we can diagonalize H_c and P simultaneously. Notice, that P has eigenvalues ± 1, and $\{P, {\eta_k}^\dagger\} = 0$. So if the ground state $|\Omega\rangle$ of H_c with energy E_0 carries $P = -1$, then $H_b|\Omega\rangle = 0$ and hence $|\Omega\rangle$ is an eigenstate of full H with the same energy E_0. In addition, all eigenstates of H_c with an even number of excitations also have $P = -1$ and hence are exact eigenstates of H. As shown in section II, for $\gamma = 0$, N even, and not divisible by 4, the ground state of H_c carries $S^z = 0$, and hence $\mathcal{N} = \frac{N}{2}$ is odd, and $P = -1$. By continuity, this is true for all γ. Therefore, in this case, the ground state of H_c is guaranteed to be a true eigenstate of H. Notice, that these complications could be avoided if we considered a chain with free ends. In this case, no extra boundary term arises in transformation from a's to c's. Yet, this case has no translational invariance, making ϕ_k's somewhat ugly.

B. Magnetic Order

Let's investigate the magnetic order properties of the XY model. We know that for $\gamma = \pm 1$ the ground state has *long range* Neel order, i.e. ${S_i}^x|\Omega\rangle = (-1)^i|\Omega\rangle$ (and in the ferromagnetic case, ${S_i}^x|\Omega\rangle = |\Omega\rangle$). It is interesting to understand what happens as γ decreases from 1 to 0. It is clear that states with spin-x components ordered and spin-y components ordered start to compete, yet it is not obvious, whether the ground state has any long and/or short range order at $\gamma = 0$.

It is best to define the magnetic order in terms of correlators

$${\rho^a}_{ij} = \langle {S_i}^a {S_j}^a\rangle, \;\; \rho_{ij} = \sum_a \langle \vec{S}_i \vec{S}_j\rangle = \sum_a {\rho^a}_{ij} \tag{70}$$

where the expectation values are taken in the ground state of H (or in the canonical ensemble if we are working at finite temperature). This way, our definition is not sensitive to the degeneracy of the ground state, which can affect the single spin expectations $\langle {S_i}^a\rangle$. The correlators can be easily expressed in terms of fermionic operators c, $c^\dagger$. For $j > i$, we obtain,

$$\begin{aligned}
\rho^x_{ij} &= \frac{1}{4}\langle ({a_i}^\dagger + a_i)({a_j}^\dagger + a_j)\rangle = \frac{1}{4}\langle ({c_i}^\dagger + c_i)\exp(\pi i \sum_{n=i}^{j-1} {c_n}^\dagger c_n)({c_j}^\dagger + c_j)\rangle & (71)\\
&= \frac{1}{4}\langle ({c_i}^\dagger + c_i)\prod_{n=i}^{j-1}(1-2{c_n}^\dagger c_n)({c_j}^\dagger + c_j)\rangle & (72)\\
&= \frac{1}{4}\langle ({c_i}^\dagger + c_i)(1-2{c_i}^\dagger c_i)\prod_{n=i+1}^{j-1}(({c_n}^\dagger + c_n)({c_n}^\dagger - c_n))({c_j}^\dagger + c_j)\rangle & (73)\\
&= \frac{1}{4}\langle ({c_i}^\dagger - c_i)\prod_{n=i+1}^{j-1}(({c_n}^\dagger + c_n)({c_n}^\dagger - c_n))({c_j}^\dagger + c_j)\rangle & (74)
\end{aligned}$$

We introduce the operators,

$$A_i = {c_i}^\dagger + c_i, \; B_i = {c_i}^\dagger - c_i \tag{75}$$

These obey the algebra,

$$\{A_i, A_j\} = \delta_{ij}, \; \{B_i, B_j\} = -2\delta_{ij}, \; \{A_i, B_j\} = 0 \tag{76}$$

In terms of A, B, eq. (71) becomes,

$$\rho^x_{ij} = \frac{1}{4}\langle B_i A_{i+1} B_{i+1} A_{i+2} \ldots A_{j-1} B_{j-1} A_j\rangle \tag{77}$$

Similarly, for y and z correlators,

$$\rho^y_{ij} = (-1)^{j-i}\frac{1}{4}\langle A_i B_{i+1} A_{i+1} B_{i+2} \dots B_{j-1} A_{j-1} B_j\rangle \tag{78}$$

$$\rho^z_{ij} = \frac{1}{4}\langle A_i B_i A_j B_j\rangle \tag{79}$$

Now since A's and B's are anticommuting variables, their expectation values can be evaluated with Wick's theorem, in terms of sums of all possible contractions of pairs of operators. Observe,

$$\langle A_i A_j\rangle = \sum_{k,k'} \phi_{ki}\phi_{k'j}\langle(\eta_k{}^\dagger + \eta_k)(\eta_{k'}{}^\dagger + \eta_{k'})\rangle = \sum_{k,k'} \phi_{ki}\phi_{k'j}\langle\eta_k\eta_{k'}{}^\dagger\rangle = \sum_k \phi_{ki}\phi_{kj} = \delta_{ij} \tag{80}$$

$$\langle B_i B_j\rangle = \sum_{k,k'} \psi_{ki}\psi_{k'j}\langle(\eta_k{}^\dagger - \eta_k)(\eta_{k'}{}^\dagger - \eta_{k'})\rangle = -\sum_k \psi_{ki}\psi_{kj} = -\delta_{ij} \tag{81}$$

$$\langle B_i A_j\rangle = \sum_{k,k'} \psi_{ki}\phi_{k'j}\langle(\eta_k{}^\dagger - \eta_k)(\eta_{k'}{}^\dagger + \eta_{k'})\rangle = -\sum_k \psi_{ki}\phi_{kj} = -(\psi^T\phi)_{ij} = G_{ij} \tag{82}$$

The matrix G acts as a Green's function in our calculations. Notice that in expressions for correlators (77), (78), (79), all A's live on different sites, and hence contractions of A's always give 0 by (80). Similarly, contractions of B's are always 0. Hence, only contractions of A's with B's appear when we evaluate our correlators with Wick's theorem. Summing all these contractions we obtain:

$$\rho^x_{ij} = \frac{1}{4}\sum_{p\in S[i+1,j]} sgn(p)(G_{i,p(i+1)}G_{i+1,p(i+2)}\dots G_{j-1,p(j)}) = \frac{1}{4}\det G^{ij}_x \tag{83}$$

$$\rho^y_{ij} = \frac{1}{4}\sum_{p\in S[i,j-1]} sgn(p)(G_{i+1,p(i)}G_{i+2,p(i+1)}\dots G_{j,p(j-1)}) = \frac{1}{4}\det G^{ij}_y \tag{84}$$

$$\rho^z_{ij} = \frac{1}{4}(G_{ii}G_{jj} - G_{ij}G_{ji}) \tag{85}$$

where $S[a,b]$ is the group of permutations of integers $\{n : a \le n \le b\}$ and matrices G^{ij}_x, G^{ij}_y are given by

$$(G^{ij}_x)_{nm} = G_{i+n-1,i+m},\ (G^{ij}_y)_{nm} = G_{i+n,i+m-1},\ 1 \le n,m \le j-i \tag{86}$$

So the various correlators are just subdeterminants of the Green's function G. It now remains to evaluate these subdeterminants. Before we perform this calculation, let's indicate how to generalize our results to the case of ferromagnetic coupling, $H_F = -H$. In that case, we have as explained in section II, $\eta \leftrightarrow \eta^\dagger$, and hence $g_{ki} \leftrightarrow h_{ki}$, which implies $\phi_{ki} \to \phi_{ki}$, $\psi_{ki} \to -\psi_{ki}$. It follows from eq. (82), that $G \to -G$, and hence by eqs. (83), (84) $\rho^{x,y}_{ij} \to (-1)^{j-i}\rho^{x,y}_{ij}$, $\rho^z_{ij} \to \rho^z_{ij}$.

We can't make any further progress without calculating the Green's function G defined in eq. (82). Recall,

$$G_{ij} = -\sum_k \psi_{ki}\phi_{kj} = -\sum_k \frac{1}{\Lambda_k}(\cos(k)\phi_{ki} + \gamma\sin(k)\phi_{-k,i})\phi_{kj} \tag{87}$$

$$= \frac{1+(-1)^{i-j+1}}{2}\left(-\frac{2}{\pi}\right)\int_0^{\pi/2} dk\frac{1}{\Lambda_k}(\cos(k)\cos(k(i-j)) - \gamma\sin(k)\sin(k(i-j))) \tag{88}$$

where we've obtained the last line by some trivial algebra, from eqs. (66), (67). Notice that G_{ij} depends only on the difference $i-j$ as should be expected for a cyclic chain due to translational invariance. Hence, we write $G_{ij} = G_{i-j}$. Also, G_{ij} vanishes when $i-j$ is even.

We can evaluate G_r analytically in the isotropic case $\gamma = 0$ and in the Ising limit $\gamma = 1$. For $\gamma = 0$, we have

$$G_r = -\frac{2}{\pi}\int_0^{\pi/2}\cos(kr) = (-1)^{(r+1)/2}\frac{2}{\pi r},\ \text{ r-odd} \tag{89}$$

while for $\gamma = 1$,

$$G_r = -\frac{2}{\pi}\int_0^{\pi/2} dk\cos(k(r+1)) = -\delta_{r,-1} \tag{90}$$

Now we are ready to investigate order in the ground state of the XY chain.

1. Short Range Order

Let's find out what are the correlations in the XY model between nearest neighbors at finite anisotropy. This requires calculating,

$$\rho_1^x = \rho_{i,i+1}^x = \frac{1}{4}G_{i,i+1} = \frac{1}{4}G_{-1} \tag{91}$$

$$\rho_1^y = \rho_{i,i+1}^y = \frac{1}{4}G_{i+1,i} = \frac{1}{4}G_1 \tag{92}$$

$$\rho_1^z = \rho_{i,i+1}^z = \frac{1}{4}(G_{ii}G_{i+1,i+1} - G_{i,i+1}G_{i+1,i}) = -\frac{1}{4}G_{-1}G_1 \tag{93}$$

and involves only the nearest neighbor Greens's functions $G_{\pm 1}$, which can be calculated in terms of elliptic E and K functions:

$$G_{\pm 1} = -\frac{2}{\pi}\frac{1}{1\mp\gamma}(\mathcal{E}(\sqrt{1-\gamma^2}) \mp \gamma\mathcal{K}(\sqrt{1-\gamma^2})) \tag{94}$$

The correlators, ρ_1^x, ρ_1^y, ρ_1^z are plotted in Fig. 2. Observe, that for any γ all of these are negative, and hence the nearest neighbors clearly display anti-ferromagnetic correlations. When $\gamma = 1$, we have as expected from Ising model, $\rho_x = -\frac{1}{4}$, $\rho_y = 0$, $\rho_z = 0$. As γ decreases, we see that anti-ferromagnetic correlations between y components of neighboring spins start to develop, competing with the correlations of S^x. The appearance of correlations between y components also seems to induce an anti-ferromagnetic correlation between z components. Finally, in the isotropic case $\gamma = 0$, the correlations between x and y components of neighboring spins become equal (as expected from symmetry reasons), and $\rho_1^x = \rho_1^y = -\frac{1}{2\pi}$, $\rho_1^z = -\frac{1}{\pi^2}$. So anti-ferromagnetic short-range order persists in the isotropic limit $\gamma = 0$. Finally, if the coupling is ferromagnetic, then as indicated above, $\rho_1^{x,y} \to -\rho_1^{x,y}$ and $\rho_1^z \to \rho_1^z$. Hence, for the ferromagnetic XY model, the x and y components of spins display ferromagnetic correlations, while the z components of spins display anti-ferromagnetic correlations.

2. Intermediate Range Order

We can numerically evaluate the determinants (83), (84) using the Green function (87). We display the resulting correlators $\rho_r^x = \rho_{i,i+r}^x$, $\rho_r^y = \rho_{i,i+r}^y$, $\rho_r^z = \rho_{i,i+r}^z$ in Figs. 3, 4, 5 for several values of $\gamma > 0$. The correlations of x and y spin components are clearly anti-ferromagnetic as $\rho_r^{x,y} \propto (-1)^r$. The z spin components are also correlated anti-ferromagnetically, but only for sites i, $i + r$, where r is odd. It seems that for $\gamma = 0$, ρ_r^x tends to 0 as $r \to \infty$, and for $\gamma \neq 0$, ρ_r^x tends to a non-zero constant as $r \to \infty$. On the other hand both ρ^y and ρ^z tend to 0 as $r \to \infty$. In the next two sections we indicate how to prove these claims analytically.

3. Absence of Long Range Order in Isotropic XY model

It can be shown analytically that in the isotropic ($\gamma = 0$) XY model $\lim_{r\to\infty}\rho_r^a = 0$, i.e. there is no long range order. For ρ^z this statement is trivial, as

$$\rho_r^z = -\frac{1}{\pi^2 r^2},\ \text{r-odd},\ \ \rho_r^z = 0,\ \text{r-even}\ \ \Rightarrow\ \lim_{r\to\infty}\rho_r^z = 0 \tag{95}$$

However, for x, y spin components there is some work to be done estimating the subdeterminants of matrices $G_{x,y}^r = G_{x,y}^{i,i+r}$ given in eqs. (83), (84). It is easy to see, using $G_r = G_{-r}$ for $\gamma = 0$, that $G_y^r = (G_x^r)^T$, and hence $\rho_r^x = \rho_r^y = \frac{1}{4}\det(G_x^r)$ as expected for symmetry reasons. One can use Hadamard's Theorem to bound the determinant of G_x^r by the product of norms of its rows:

$$\det(G_x^r)^2 \le \prod_{i=1}^{r}\sum_{j=1}^{r}(G_x^r)_{ij}^2 \tag{96}$$

One can further use the orthogonality of matrix G and the explicit form of $G_r = (-1)^{(r+1)/2}\frac{2}{\pi r}$ for r-odd, to bound the norm of each row of G_x^r, obtaining at the end,

$$\rho_r^{x,y} = \frac{1}{4}\det(G_x^r) \le r^{-2/\pi^2} \times const \to 0,\ \text{as}\ r \to \infty \tag{97}$$

Finally, let us remark that a similar argument using Hadamard's Theorem can be used to show that at any finite temperature, the correlators ρ_r^a fall off exponentially as $r \to \infty$, and no long range order exists for *any* anisotropy γ. For further details see the original paper [3].

4. End-to-End Order

Although the subdeterminants $\det(G^{ij}_{x,y})$ are difficult to analyze for arbitrary γ and i, j, they greatly simplify for $i = 1, j = N$, i.e. when we are computing the correlations between the first and the last spin in the chain. Indeed, from eq. (71), we see that

$$\rho^x_{1N} = \frac{1}{4}\langle (c_1{}^\dagger + c_1)(c_N{}^\dagger - c_N) \exp(\pi i \sum_n c_n{}^\dagger c_n)\rangle = \frac{1}{4}\langle A_1 B_N P\rangle \tag{98}$$

where $P = \exp(\pi i \mathcal{N})$. As was noted in section III A, $P|\Omega\rangle = \pm|\Omega\rangle$, so we obtain,

$$\rho^x_{1N} = -\frac{1}{4} G_{N1} P \tag{99}$$

and similarly,

$$\rho^y_{1N} = -\frac{1}{4} G_{1N} P \tag{100}$$

So the complicated subdeterminants reduce to just a single Green's function. However, for the cyclic chain this is not telling us much about the long range order, since sites 1 and N are nearest neighbors. For the chain with free ends, however, the end-to-end order is a meaningful indication of long range order (although the two need not agree numerically exactly, due to end effects). Computing the Green's function's for a chain with free ends (by solving eqs. (60), (61) to find ϕ_k, ψ_k, and then using the definition of Green's function (82)), one obtains [3] in the limit $N \to \infty$

$$\rho^y_{1N} = 0, \;\; \rho^x_{1N} = -\frac{\gamma}{(1+\gamma)^2}, \;\; \gamma > 0 \tag{101}$$

Hence, there is no end-to-end order of the y spin components for any $\gamma > 0$, while there is end-to-end order of the x spin components for any positive anisotropy γ. Also, the end-to-end order vanishes in the isotropic case $\gamma = 0$. These results support our numerical computations of section III B.2, and the analytical results of section III B.3.

---

[1] H. Bethe, Z. Phys., **71**, 205 (1931).
[2] P. Jordan and E. Wigner, Z. Physik **47**, 631 (1928).
[3] E. Lieb, T. Schultz, D. Mattis, Ann. of Phys., **16**, 407 (1961);
E. Lieb, D. Mattis, *Mathematical Physics in One Dimension.* Academic Press, New York and London, (1966).
[4] A. Tsvelik, *Quantum Field Theory in Condensed Matter Physics.* Cambridge University Press, Cambridge, (1995).

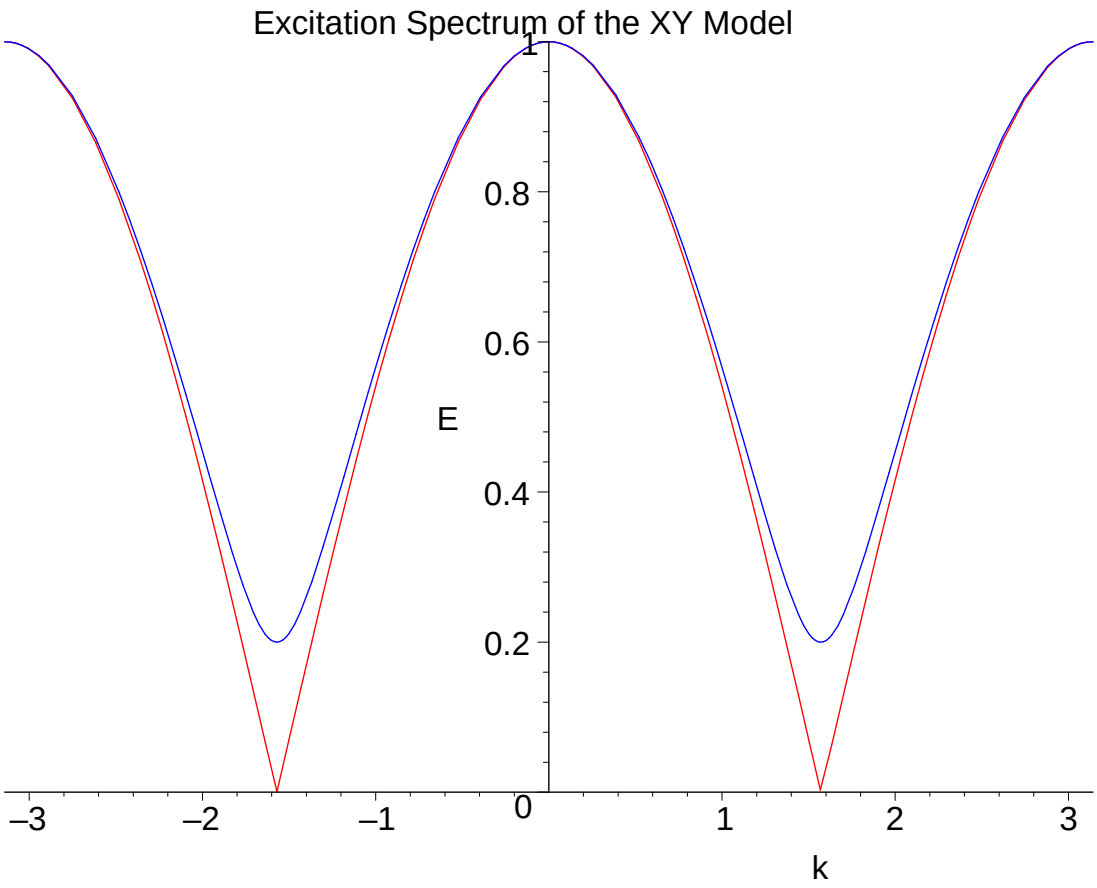

FIG. 1: In this figure we show the spectrum of the excitations of the XY model for different values of the anisotropy γ. The red curve corresponds to $\gamma = 0$, while the blue curve corresponds to $\gamma = 0.2$. The spectrum is gapless in the isotropic case, and acquires a gap γ in the anisotropic case.

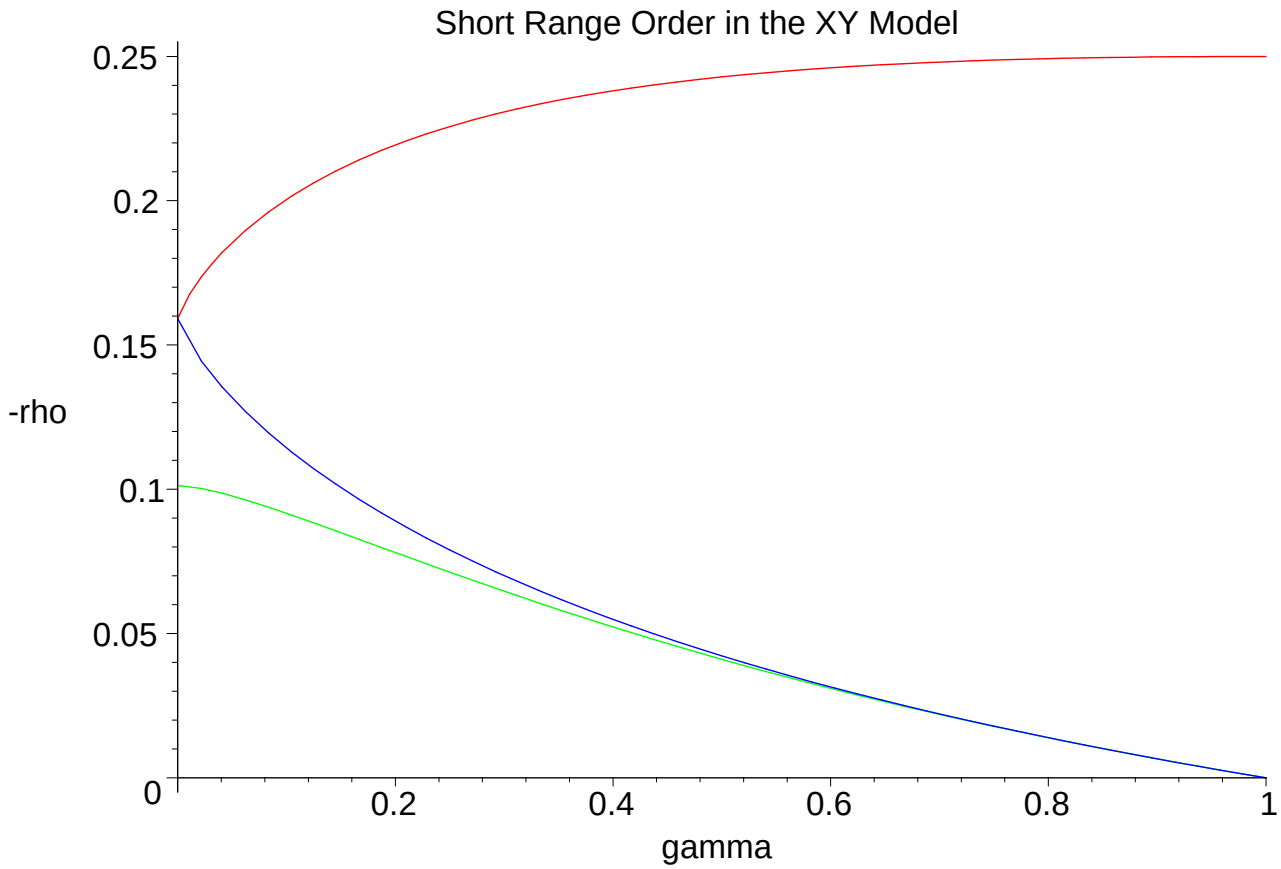

FIG. 2: In this figure we display the nearest neighbor spin correlations in the XY model as a function of anisotropy γ. The red curve corresponds to ρ_1^x, the blue curve corresponds to ρ_1^y and the green curve to ρ_1^z. We clearly see that the competition between x and y spin correlations as $\gamma \to 0$.

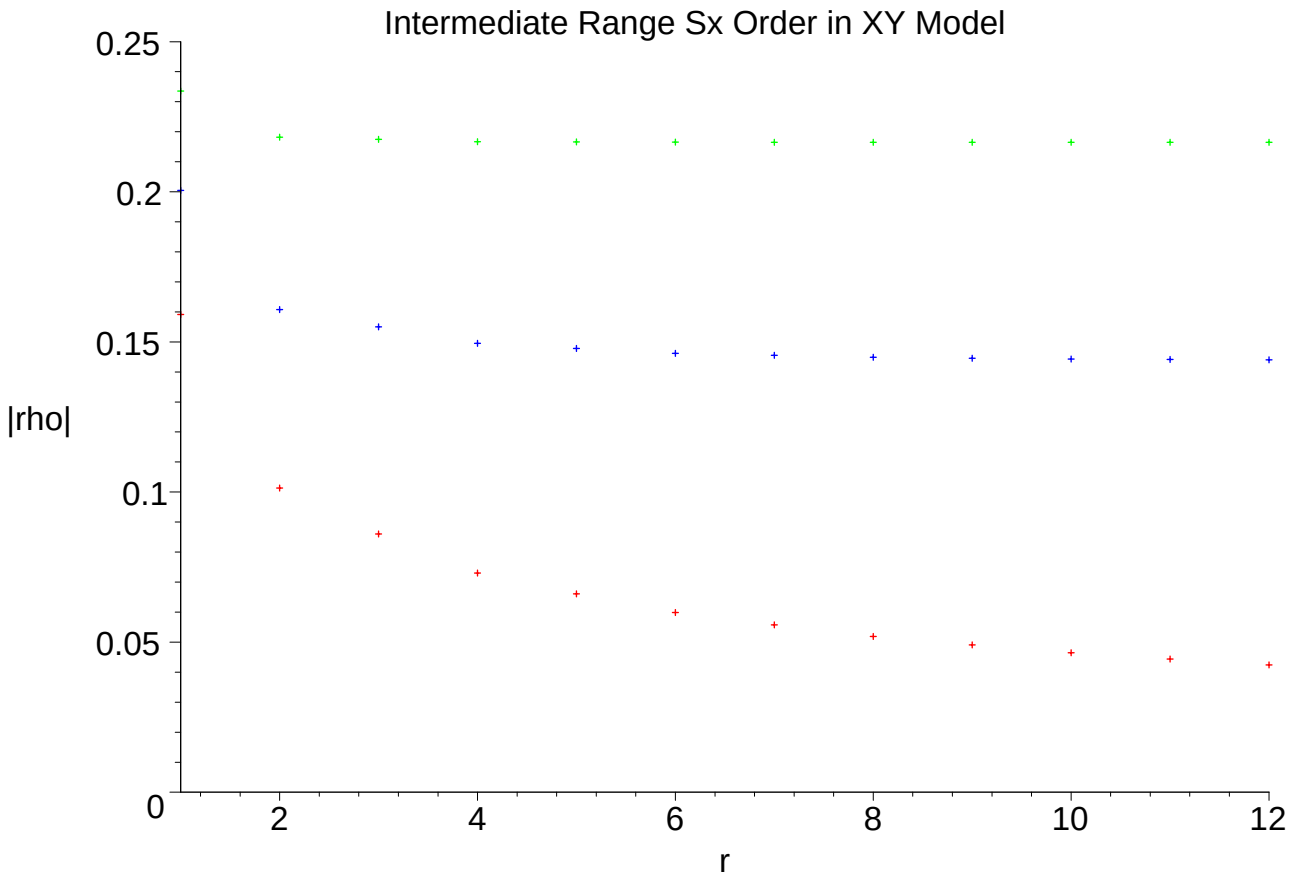

FIG. 3: In this figure we display correlations between x components of spins $(-1)^r \rho_r^x$ as a function of their separation r for several values of anisotropy γ. The red curve corresponds to $\gamma = 0$, the blue curve corresponds to $\gamma = 0.1$ and the green curve to $\gamma = 1/3$. We see that for the isotropic case $\gamma = 0$, the correlator slowly tends to 0, while for non-zero anisotropy γ, the correlator tends to a non-zero limit.

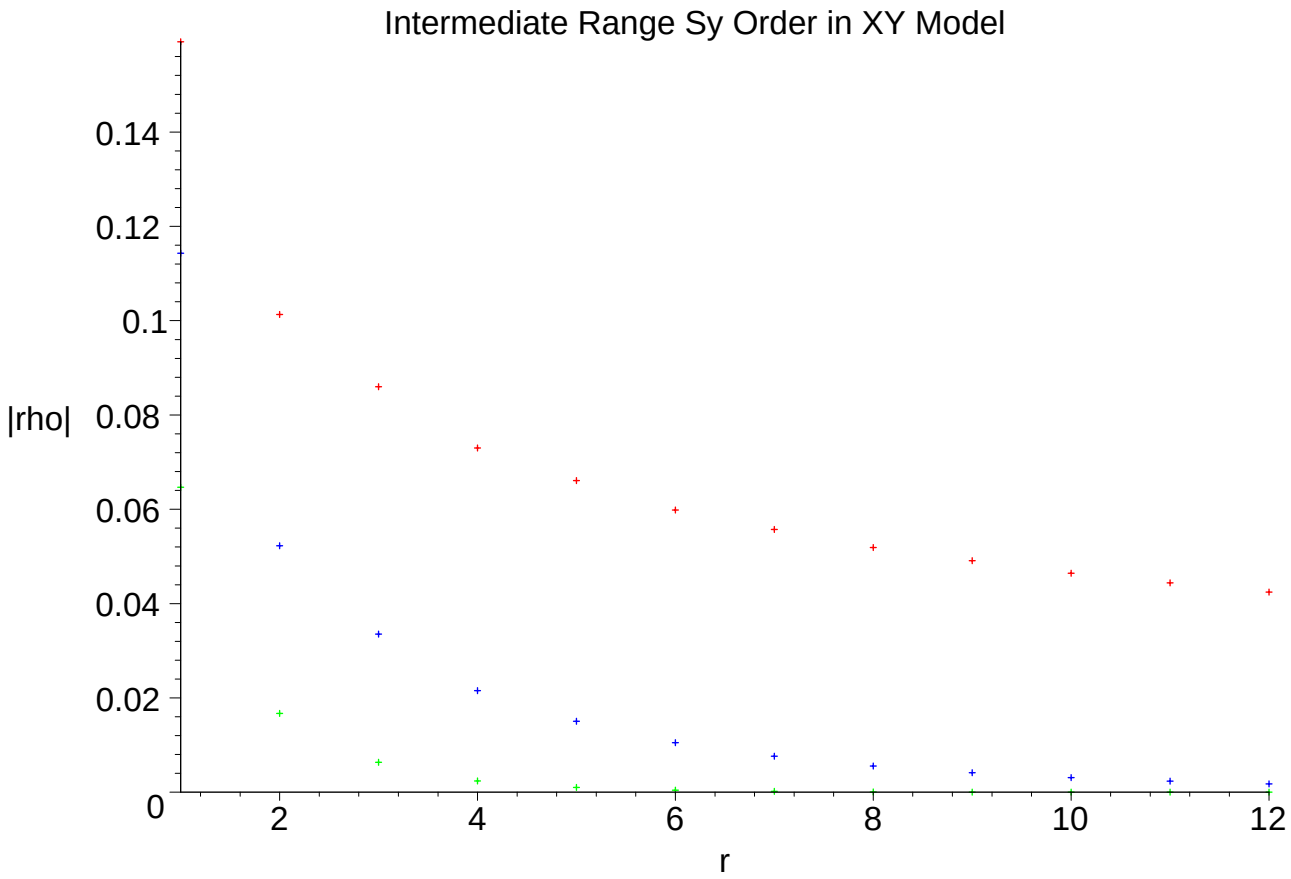

FIG. 4: In this figure we display correlations between y components of spins $(-1)^r \rho_r^y$ as a function of their separation r for several values of anisotropy γ. The red curve corresponds to $\gamma = 0$, the blue curve corresponds to $\gamma = 0.1$ and the green curve to $\gamma = 1/3$. We see that for all γ the correlator tends to 0.

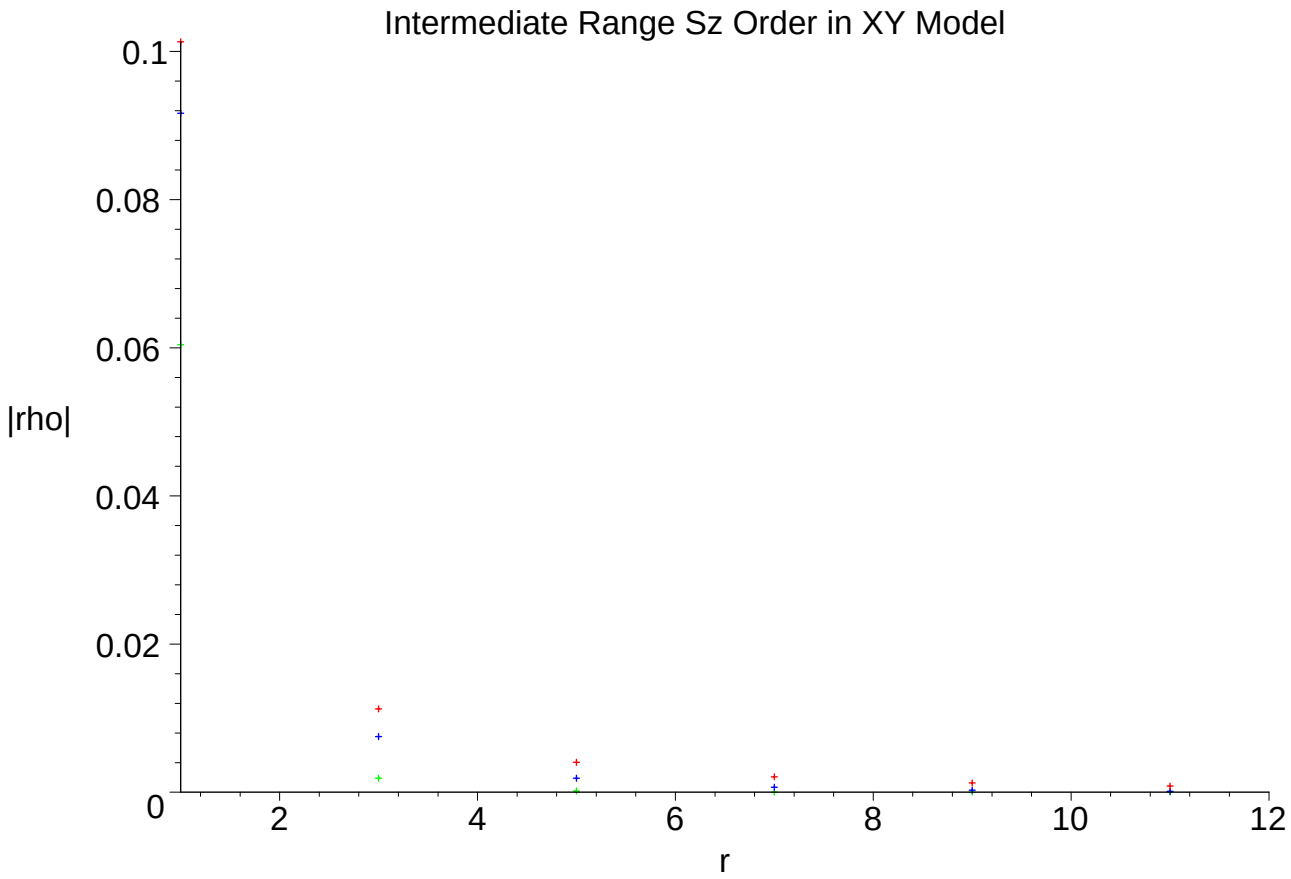

FIG. 5: In this figure we display correlations between z components of spins $-\rho_r^z$ as a function of their separation r for several values of anisotropy γ. The red curve corresponds to $\gamma = 0$, the blue curve corresponds to $\gamma = 0.1$ and the green curve to $\gamma = 1/3$. We see that for all γ the correlator tends to 0.