Topological Phase Transition in S=1/2 Spin Chains with Alternating Ferromagnetic (FM) and Antiferromagnetic (AFM) Couplings and Exchange Anisotropy

CMMP Summer Research Project Report
Appendix
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I. INTRODUCTION

This document serves as an extension of the one page report. It will show the steps of the derivations and computation in more detail, which are not sufficiently discussed in the one-page report.

II. MODEL DEFINITION

The model illustration is put here for convenience. We investigate the topological phase transistion of a model of 1D spin-1/2 chain of N lattice sites with alternating FM and AFM couplings in the regime of small magnetic exchange anisotropy (α), as illustrated in FIG 1 below:

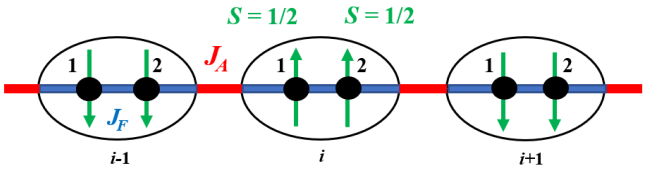

FIG. 1. An illustration depicting the model of interest. The green arrows represent the spin S of the electrons; the blue lines and red lines represent FM and AFM coupling respectively; J_F and J_A denote the FM and AFM spin coupling constants respectively.

We have chosen a nearest-neighbour Hamiltonian for our model which is given as:

$$\begin{aligned}\hat{H} =& -J_F N \sum_i (\underline{\hat{S}}_{i,1} \cdot \underline{\hat{S}}_{i,2} + \alpha \hat{S}^z_{i,1} \cdot \hat{S}^z_{i,2}) \\ &+ J_A N \sum_i (\underline{\hat{S}}_{i,2} \cdot \underline{\hat{S}}_{i+1,1} + \alpha \hat{S}^z_{i,2} \cdot \hat{S}^z_{i+1,1})\end{aligned} \tag{1}$$

where α denotes the magnetic exchange anisotropy, $\underline{\hat{S}}_{i,m}$ are spin operators: $\underline{\hat{S}}_{i,m} = (\hat{S}^x_{i,m}, \hat{S}^y_{i,m}, \hat{S}^z_{i,m})^\mathsf{T}$, with their subscripted indices i, m labelling the sites. i labels the unit cell and m labels the cite within that unit cell, where $m = 1, 2$, which are the numbers beside the green arrows.

III. DERIVATION

In this section, we detail the derivations of the main equations required to obtain the topological phase diagram of our model.

A. New Spin Operators

First, we perform a "spin flip", defining new spin operators:

$$\hat{T}^x_{i,m} = (-1)^i \hat{S}^x_{i,m} \tag{2}$$

$$\hat{T}^y_{i,m} = \hat{S}^i_{i,m} \tag{3}$$

$$\hat{T}^z_{i,m} = (-1)^i \hat{S}^z_{i,m} \tag{4}$$

These spin operators satisfy the commutator relationships:

$$\left[\hat{T}^f_{i,m}, \hat{T}^g_{i,m}\right] = i\hbar\epsilon_{fgh}\hat{T}^c_{i,m} \tag{5}$$

The raising and lowering spin operators are defined as:

$$\hat{T}^+_{i,m} = \hat{T}^x_{i,m} + i\hat{T}^y_{i,m} \tag{6}$$

$$\hat{T}^-_{i,m} = \hat{T}^x_{i,m} - i\hat{T}^y_{i,m} \tag{7}$$

We can write (2) and (3) in terms of these raising and lowering operators:

$$\hat{T}^x_{i,m} = \frac{1}{2}(\hat{T}^+_{i,m} + \hat{T}^-_{i,m}) \tag{8}$$

$$\hat{T}^y_{i,m} = \frac{1}{2}(\hat{T}^+_{i,m} - \hat{T}^-_{i,m}) \tag{9}$$

B. Jordan-Wigner Transformation

After rewriting (1) in terms of raising and lowering operators 8 and 9, we can then perform a Jordan-Wigner transformation (JWT) [1] to map the spin-1/2 operators to splinless fermions:

$$\hat{T}^z_{i,m} = \frac{1}{2} - c^\dagger_{i,m} c_{i,m} \tag{10}$$

$$\hat{T}^+_{i,m} = c_{i,m} D_{i,m} \tag{11}$$

$$\hat{T}^-_{i,m} = c^\dagger_{i,m} D_{i,m} \tag{12}$$

$c_{i,m}$, $D_{i,m}$ and their hermitian conjugates (h.c.) are proper fermionic operators which satisfy fermionic anticommutator relationships. Let us first discuss the string operators $D_{i,m}$. The idea of these operators is to conserve the quantum statistics of the spins and fermions, while mapping all the fermions on the left of the sub-sites:

$$D_{i,1} = \prod_{\ell<i} (1 - 2c^\dagger_{\ell,1} c_{\ell,1})(1 - 2c^\dagger_{\ell,2} c_{\ell,2}) \tag{13}$$

$$D_{i,2} = D_{i,1}(1 - 2c^\dagger_{i,1} c_{i,1}) \tag{14}$$

$$D_{i+1,1} = D_{i,2}(1 - 2c^\dagger_{i,2} c_{i,2}) \tag{15}$$

Applying all mentioned transformations, the Hamiltonian written in fermionic operators can be written as:

$$\begin{aligned}\hat{H} =& -\frac{J_F N}{2} \sum_i [c^\dagger_{i,1} c_{i,2} + c^\dagger_{i,2} c_{i,1} + \beta(c_{i+1,1} c_{i,2} + c^\dagger_{i,2} c^\dagger_{i+1,1}) \\ &- J_F N(1+\alpha) \sum_i (\frac{1}{2} - c^\dagger_{i,1} c_{i,1})(\frac{1}{2} - c^\dagger_{i,2} c_{i,2}) \\ &- J_F N \beta (1+\alpha) \sum_i (\frac{1}{2} - c^\dagger_{i,2} c_{i,2})(\frac{1}{2} - c^\dagger_{i+1,1} c_{i+1,1})]\end{aligned} \tag{16}$$

where we define $\beta := \frac{J_A}{J_F}$. After expanding the brackets, we will see 4 different terms appear in (16):

Hopping terms : $c^\dagger_{i,1}c_{i,2}, c^\dagger_{i,2}c_{i,1}$
Anomalous terms : $c_{i+1,1}c_{i,2}, c^\dagger_{i,2}c^\dagger_{i+1,1}$
Density terms : $c^\dagger_{i,m}c_{i,m} = n_{i,m}$
Interaction terms : $n_{i,m}n_{i+1,m}$

To solve the problem, we have to discard the density and interaction terms, which leads us to the mean-field approximation.

C. Mean-Field Approximation

There are several ways to solve this problem, including perturbation theory and variational methods. We have chosen to use the mean-field approximation (MFA), where we assume the interaction terms do not have significant contribution [2]. The MFA will break down as $\alpha \to 0$ because the interactions will start to dominate. Let A and B be two Hermitian operators. The mean-field approximation equation states that:

$$\langle A\rangle \cdot \langle B\rangle = \langle A\rangle B + \langle B\rangle A - \langle A\rangle\langle B\rangle \tag{17}$$

Henceforth, we apply (17) to the terms in (16). Using all possible decouplings, we have:

$$\begin{aligned} c^\dagger_{i,1}c_{i,1}c^\dagger_{i,2}c_{i,2} \simeq &- t(c^\dagger_{i,2}c_{i,1} + c^\dagger_{i,1}c_{i,2}) + t^2 \\ &+ \varrho(c^\dagger_{i,1}c_{i,1} + c^\dagger_{i,2}c_{i,2}) - \varrho^2 \end{aligned} \tag{18}$$

$$\begin{aligned} c^\dagger_{i,2}c_{i,2}c^\dagger_{i+1,1}c_{i+1,1} \simeq &\varrho(c^\dagger_{i,1}c_{i,1} + c^\dagger_{i,2}c_{i,2}) - \varrho^2 \\ &+ \lambda(c^\dagger_{i,2}c^\dagger_{i+1,1} + c_{i+1,1}c_{i,2}) - \lambda^2 \end{aligned} \tag{19}$$

where we have defined expectation values λ, t and ϱ:

$$\lambda = \langle c_{i+1,1}c_{i,2}\rangle = \left\langle c^\dagger_{i,2}c^\dagger_{i+1,1}\right\rangle \in \mathbb{R} \tag{20}$$

$$t = \left\langle c^\dagger_{i,1}c_{i,2}\right\rangle = \left\langle c^\dagger_{i,2}c_{i,1}\right\rangle \in \mathbb{R} \tag{21}$$

$$\varrho = \left\langle c^\dagger_{i,1}c_{i,1}\right\rangle = \left\langle c^\dagger_{i,2}c_{i,2}\right\rangle \in \mathbb{R} \tag{22}$$

We can place constraints on ϱ, which are the expectation values of the occupation operators in the density terms. In the regime of $\alpha < 0$, magnetic moments will only develop in the xy-plane. Therefore, from (10), $\left\langle \hat{T}^z_{i,m}\right\rangle = 0 \Leftrightarrow \left\langle c^\dagger_{i,m}c_{i,m}\right\rangle = \varrho = \frac{1}{2}$. Under these approximations, the mean-field Hamiltonian can be obtained:

$$\begin{aligned} \hat{H}_{\mathrm{MF}} = &- \frac{J_F N}{2}\sum_i \Big[\gamma(c^\dagger_{i,1}c_{i,2} + c^\dagger_{i,2}c_{i,1}) \\ &+ \tilde{\beta}(c_{i+1,1}c_{i,1} + c^\dagger_{i,2}c^\dagger_{i+1,1})\Big] \\ &+ J_F N(1+\alpha)(\beta\lambda^2 - t^2) \end{aligned} \tag{23}$$

where we have defined:

$$\tilde{\beta} := \beta\big[1 + 2\lambda(1+\alpha)\big] \tag{24}$$

$$\gamma := 1 - 2t(1+\alpha) \tag{25}$$

D. Fourier Transform

To express (23) in k-space, we can perform Fourier transforms on the operators:

$$c^\dagger_{i,m}(x) = \int_0^{2\pi}\frac{dk}{2\pi}c^\dagger_i(k)e^{ikx} \tag{26}$$

$$c_{i,m}(x) = \int_0^{2\pi}\frac{dk}{2\pi}c_i(k)e^{-ikx} \tag{27}$$

where x is the position. Note that k is 2π periodic, therefore it is chosen that $k \in [0, 2\pi]$. For hopping and anomalous terms respectively, we relabel as follows:

$$\sum_i (c^\dagger_{i,1}c_{i,2} + c^\dagger_{i,2}c_{i,1}) \Leftrightarrow \sum_x (c^\dagger_1(x)c_2(x) + c_1(x)c^\dagger_2(x)) \tag{28}$$

$$\begin{aligned} \sum_i (c^\dagger_{i,2}c^\dagger_{i+1,1} + c_{i+1,1}c_{i,2}) \Leftrightarrow &\sum_x (c^\dagger_2(x)c^\dagger_1(x+a) \\ &+ c_1(x+a)c_2(x)) \end{aligned} \tag{29}$$

Here, a represents the distance between the unit cells. Evaluating the Fourier transforms, we get the Hamiltonian in k-space:

$$\begin{aligned} \hat{H}_{\mathrm{MF}}(k) = -\frac{J_F N}{2}\int_0^{2\pi}\frac{dk}{2\pi}\Big\{&\gamma\big[c^\dagger_2(k)c_1(k) - c_2(-k)c^\dagger_1(-k) \\ &+ c^\dagger_1(k)c_2(k) - c_1(-k)c^\dagger_2(-k)\big] \\ &+ \mu^*\big[c^\dagger_2(k)c^\dagger_1(-k) - c_2(-k)c_1(k)\big] \\ &+ \mu\big[c_1(-k)c_2(k) - c^\dagger_1(k)c^\dagger_2(-k)\big]\Big\} \\ &+ J_F N(1+\alpha)(\beta\lambda^2 - t^2) \end{aligned} \tag{30}$$

For simplification, we have defined $\mu := \tilde{\beta}e^{ika}$ and $\mu^* := \tilde{\beta}e^{-ika}$.

E. Bogoliubov Transformation

In momentum space, the mean-field Hamiltonian (23) can be rewritten as:

$$\begin{aligned} \hat{H}_{\mathrm{MF}}(k) = &- \frac{J_F N}{2}\int_0^{2\pi}\frac{dk}{2\pi}\Gamma^\dagger_k\underline{\Omega}_k\Gamma_k \\ &+ J_F N(1+\alpha)(\beta\lambda^2 - t^2) \end{aligned} \tag{31}$$

with $\Gamma^\dagger = \big(c^\dagger_1(k)\ \ c_1(-k)\ \ c^\dagger_2(k)\ \ c_2(-k)\big)$. $\underline{\Omega}_k$ is a 4x4 Hermitian matrix, given by:

$$\underline{\Omega}_k = \begin{pmatrix} 0 & 0 & \gamma & -\mu \\ 0 & 0 & \mu & -\gamma \\ \gamma & \mu^* & 0 & 0 \\ -\mu^* & -\gamma & 0 & 0 \end{pmatrix} \tag{32}$$

(32) can then be diagonalised and obtain the dispersion spectrum of Bogoliuibov quasiparticles [3]:

$$\epsilon^\pm(k) = \pm\frac{J_F N}{2}\sqrt{\tilde{\beta}^2 + \gamma^2 + 2\tilde{\beta}\gamma\cos(ka)} \tag{33}$$

It is useful to define a dimensionless quantity, the total energy density, $\varepsilon := \frac{E}{NJ_F}$, explicitly written as:

$$\begin{aligned} \varepsilon = -\frac{1}{4\pi}\int_0^{2\pi} dk\Big\{&\beta^2\big[1 + 2\lambda(1+\alpha)\big]^2 + \big[1 - 2t(1+\alpha)\big]^2 \\ &+ 2\beta\big[1 + 2\lambda(1+\alpha)\big]\big[1 - 2t(1+\alpha)\big]\cos(k)\Big\}^{\frac{1}{2}} \\ &+ (1+\alpha)(\beta\lambda^2 - t^2) \end{aligned} \tag{34}$$

For simplicity, $a = 1$.

IV. COMPUTATION

In this section, we explain the algorithms and steps required to obtain the topological phase transition diagram. All computations are performed using Python and Mathematica [4]. The main code used can be found here: `https://github.com/SavitarRL/CMMP-Research/blob/main/maincode.py`.

A. Integral Evaluation

We would first need to evaluate the integral in (34), which is done using Mathematica:

$$\varepsilon = -\frac{1}{\pi}\left|\tilde{\beta}+\gamma\right| E\left(\frac{4\tilde{\beta}\gamma}{\left|\tilde{\beta}+\gamma\right|}\right) + (1+\alpha)(\beta\lambda^2 - t^2) \quad (35)$$

where $E(\theta)$ is an Elliptic integral of the first kind. $\tilde{\beta}$ and γ are previously defined from (24) and (25).

B. Steepest Gradient Descent and Ascend

First, we need to self-consistently determine the expectation values λ and t for given parameters α and β. α and β are constrained to the following ranges: $\alpha \in [-1, 0]$; $\beta \in [0, 1]$. We begin with a random value between 0 and 1 for both quantities, with starting values: λ_0 and t_0 . Then, we implement a steepest gradient descent algorithm on λ_0 and a steepest gradient ascend algorithm on t_0, up to and until we reach the saddle point of $\varepsilon = \varepsilon(\lambda, t)$ with the parameters given:

$$\lambda_{\eta+1} = \lambda_\eta - r\frac{\partial\varepsilon}{\partial\lambda} \quad (36)$$

$$t_{\eta+1} = t_\eta + r\frac{\partial\varepsilon}{\partial t} \quad (37)$$

r is the rate of descending or ascending, which is set to 0.1, whereas η is the number of iterations performed, which is set to 1000. That is to say, the final values of λ and t should give us $\frac{\partial\varepsilon}{\partial\lambda} = 0$ and $\frac{\partial\varepsilon}{\partial t} = 0$. The derivatives are determined numerically using first principles:

$$\frac{\partial\varepsilon}{\partial\lambda} = \frac{\varepsilon(\lambda+h, t) - \varepsilon(\lambda, t)}{h} \quad (38)$$

$$\frac{\partial\varepsilon}{\partial t} = \frac{\varepsilon(\lambda, t+h) - \varepsilon(\lambda, t)}{h} \quad (39)$$

for sufficiently small h, which is set to $h = 0.00001$. FIG 2 shows the energy density surface plot when $\alpha = -0.6$ and $\beta = 0.2$, which has a saddle point, thus justifying our choice of using steepest gradient descent and ascend algorithms to reach such point.

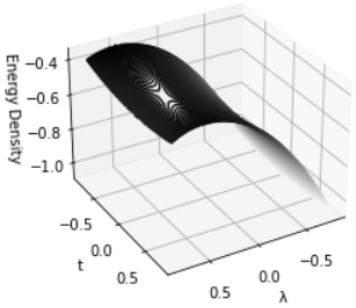

FIG. 2. An energy density surface plot against values of λ and t when $\alpha = -0.6$ and $\beta = 0.2$

C. The Bisection Method

To get the topological phase boundary, it is required to obtain the values of α and β where the magnetic excitation energy gap, Δ, closes ($\Delta = 0$). The gap occurs at $k = \pm\pi$. Since the spectra is symmetric along the x-axis, the gap calculated from the dispersion part of (34) can be expressed as:

$$\Delta = 2\Big\{\beta^2\big[1+2\lambda(1+\alpha)\big]^2 + \big[1-2t(1+\alpha)\big]^2 - 2\beta\big[1+2\lambda(1+\alpha)\big]\big[1-2t(1+\alpha)\big]\Big\}^{\frac{1}{2}} \quad (40)$$

We first initiate 200 evenly spaced points, each for α and β with their respective ranges: $\alpha \in [-0.99, 0.01]$; $\beta \in [0.01, 1]$. The values of Δ are evaluated for every pairs of α and β and saved into a CSV file for easier access. The gap data is converted into a 200×200 matrix, with the columns corresponding to values α and the rows corresponding to values of β. At $\Delta = 0$, there is a gradient change, thus a phase transition. Hence we first find the minimum value of Δ for every column, with their corresponding values of β. We look for the next "left" and "right" values of this particular value of β, which are β_l and β_r respectively. We then perform a simple mid-point search:

$$\beta_\mathrm{m} = \frac{\beta_\mathrm{l} + \beta_\mathrm{r}}{2} \quad (41)$$

We assume that this value of β_m in each column will give us $\Delta = 0$. For better accuracy, more initially set points can be used. These points will ultimately make up the topological phase boundary for our model (FIG 3), as shown in the report.

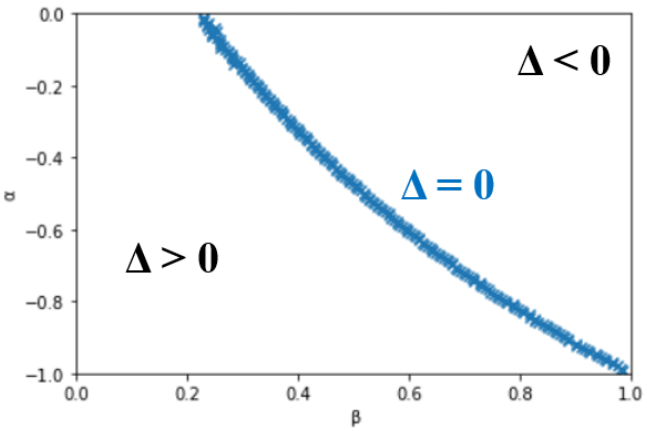

FIG. 3. The topological phase diagram of the model as a function of α and β in the regime of smaller anisotropies $\alpha \in [1, 0]$.

ACKNOWLEDGMENTS

I want to thank Dr. Frank Kruger for agreeing to be my supervisor and guiding me throughout the project. I would also like to thank the academic members of the UCL CMMP group who awarded me this summer studentship, which is an extremely invaluable opportunity.

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