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
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I. MODEL DEFINITION

We investigate the topological phase transistion of a 1D model of spin-1/2 chain with alternating FM and AFM couplings (see FIG 1), consisting of N lattice sites in the limit of small magnetic exchange anisotropy (α).

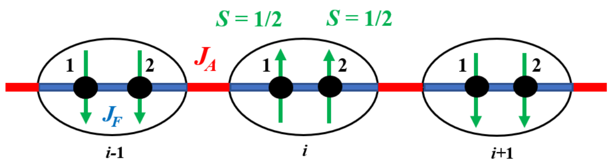

FIG. 1. An illustration depicting the model of interest. The green arrows represent the spin S of the electrons; the blue lines and red lines represent FM and AFM coupling respectively; J_F and J_A denotes the FM and AFM spin coupling constants respectively; i labels the unit cell and the numbers 1 and 2 beside the green arrows label the site within that unit cell.

II. DERIVATION

We perform a Jordan-Wigner transformation (JWT) on the Hamiltonian of the model [1] to map the spin-1/2 operators to splinless fermions, with non-local string operators being introduced to conserve the quantum statistics of the spins and fermions. Assuming the interaction terms do not have significant contribution, a mean-field approximation (MFA) is applied [2]. We define λ and t being non-zero expectation values of the anomalous and hopping terms respectively. The expectation value of the occupation operators are set to $\frac{1}{2}$ as a result of the JW, since magnetic moments will only develop in the xy-plane when $\alpha < 0$. Then, a Fourier transform is performed on the rewritten Hamiltonian, followed by a Bogoliubov transformation, getting a dispersion spectrum of Bogoliubov quasiparticles in k-space [3]:

$$\begin{aligned}\epsilon^{\pm}(k) = \pm\frac{J_F}{2}\{&\beta^2[1+2\lambda(1+\alpha)]^2 + [1-2t(1+\alpha)]^2 \\ &+2\beta[1+2\lambda(1+\alpha)][1-2t(1+\alpha)]\cos(k)\}^{\frac{1}{2}}\end{aligned} \tag{1}$$

The total energy density can also be acquired:

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

where we have defined $\beta := \frac{J_A}{J_F}$.

III. COMPUTATION

We first determine λ and t self-consistently using steepest gradient descent (for λ) and ascend (for t) algorithms for given parameters α and β, which are constrained to the following ranges: $\alpha \in [-1, 0]$; $= \beta \in [0, 1]$. The energy gap, Δ, can then be calculated from the dispersion spectrum discussed in section II. To get the topological phase boundary, we require the values of α and β with corresponding values of λ and t where the gap closes ($\Delta = 0$), which occurs at $k = \pm\pi$. All computations are performed using Python and Mathematica [4].

IV. RESULTS AND DISCUSSION

For $\alpha = -1$ (xy case), the z-components of the spins do not contribute and the model is exactly solvable [5], with a topological phase transition at $J_A = J_F$ [3]. For large β, the fermions will become non-interacting and pairs of $S = 1/2$ spins (dimers) form effective $S = 1$ moments. The model will be equivalent to the Haldane spin chain with AFM coupled, effective $S = 1$ spins [6], with topologically protected edge states at both ends of the chain [7]. Due to its topological protection, the topological phase will extend to smaller values of the FM coupling and be stable against anisotropy α.

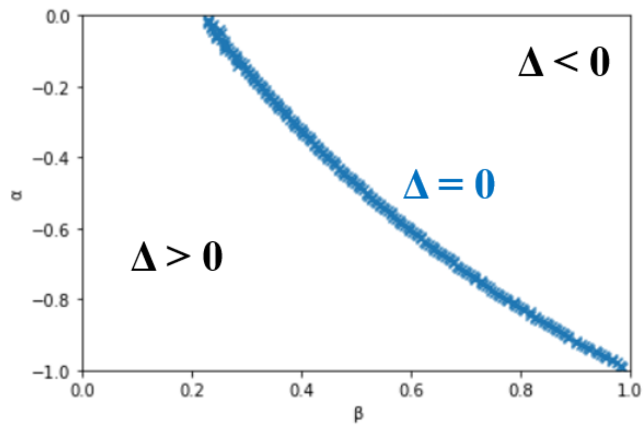

FIG. 2. The topological phase diagram of the model as a function of α and β in the regime of smaller anisotropies ($\alpha \in [-1, 0]$).

FIG 2 above shows the topological phase diagram of the investigated model. 200 points on the topological phase transition line (blue) are found numerically, using a bisection method. The region where $\Delta > 0$ is topological where magnetic excitations are gapped. The region where $\Delta < 0$ is not topological.

V. CONCLUSION

In the regime of $\alpha \in [-1, 0]$, it is shown that topological order is extended and the topological phase boundary is found for our model (see FIG 1). Alternative methods can be implemented, such as perturbation theory or variational methods. Future experimental studies on materials with similar configuration to our model could be compared with the theoretical model to make further corrections to the theory, as the MFA will start to break down when $\alpha \to 0$.

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