Position space renormalization of 2D Ising model with Dzyaloshinskii-Moriya Interaction

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We study the quantum 2D anti-ferromagnetic Ising model with Dzyaloshinskii-Moriya (DM) interaction using position space renormalization group (PSRG). In particular, we find that there exist a quantum phase transition between the anti-ferromagnetic phase and the chiral phase, which is the phase dominated by large DM interaction, at a finite value of the DM coupling in both one and two dimensions.

I. INTRODUCTION

In spin systems without inversion symmetry, interaction terms other than the usual isotropic Heisenberg interaction can arise. In particular, Dzyaloshinskii [1] showed phenomenologically that interaction terms that are odd under inversion such as

\[ H_{DM} = D \cdot (s_i \times s_j) \]  

(1)

can occur, where \( s_i, s_j \) denote lattice spins. It was later shown by Moriya [2] that the microscopic origin of such interaction is due to spin-orbit coupling in inversion asymmetric systems, and hence such interaction is known as Dzyaloshinskii-Moriya interaction.

DM interaction has been found to be responsible for interesting magnetic ordering such as helical magnets in MnSi [3]. It has also garnered considerable interest in recent years due to its potential applications in magnetic memory [4]. In particular, it was found that DM interaction can stabilize topologically non-trivial structures such as magnetic skyrmions [5]. Quasi 2D systems such as a mono-layer of Fe on Pt [6] play important roles in such studies because inversion symmetry is broken at the interfaces, and DM interaction naturally arises. The vector \( \vec{D} \) can point in different directions for different material systems [4 and 7], which induces different forms of magnetic ordering.

It is thus of interest to investigate the phases of 2D systems with DM interaction to determine the presence of non-trivial magnetic orderings in order to contemplate their potential applications.

II. CHOICE OF SYSTEM

The 2D lattice Hamiltonian that we shall consider is:

\[ H = \frac{J}{4} \sum_{\langle i,j \rangle} \sigma_i^z \sigma_j^z + D(\sigma_i^x \sigma_j^y - \sigma_i^y \sigma_j^x) \]  

(2)

where \( \sigma_i^\alpha \) are the Pauli spin operators on the lattice sites, and we only consider nearest neighbour interactions. We consider \( J > 0 \), so that this describes a 2D anti-ferromagnetic Ising model with DM interaction where \( D \) is in the \( z \) direction. The sign of \( D \) determines the chirality of the system, which is the sense (either clockwise or anti-clockwise) that the spins would rotate in the \( xy \) plane.

This particular direction of \( D \) is chosen so that the renormalization scheme described below does not generate extra couplings that are not included in Eq. (2). We have tried several forms of \( D \), such as one in which the direction of \( D \) is parallel to \( \hat{z} \times \vec{r}_{ij} \), where \( \vec{r}_{ij} \) is the position vector between the interacting spins. These interactions generate extra couplings, such as \( \sigma_i^x \sigma_j^y \), under successive renormalization, rendering them unsuitable for RG analysis without some further approximations, such as truncation of the extra couplings. The symmetry of this Hamiltonian that precludes generation of extra interactions comes from the fact that the DM interaction causes the spins to orient in the \( xy \)-plane, and does not couple to the Ising anisotropy term. Other forms of DM interaction have some component of \( D \) in the \( xy \)-plane, and thus couples \( \sigma_i^z \) to \( \sigma_i^x, \sigma_i^y \).

III. QUANTUM POSITION SPACE RENORMALIZATION GROUP

In a RG scheme, successive coarse-graining steps are carried out, generating recursion relations for the renormalized couplings [8]. The existence of fixed points and the behaviour around the fixed points give us information about the phases of the system. Here we implement Kadanoff’s block scheme to do the coarse-graining, as it is particular suited for lattice systems [9]. We will first describe the method for the 1D chain, and then generalized to the 2D system. In this method, we divide the lattice into blocks in which the Hamiltonian can be exactly diagonalized [10]. The choice of such division is important as one needs to ensure that form of the Hamiltonian is preserved under RG. Hence we divide a 1D chain into blocks of three spins, i.e., \( b = 3 \), as illustrated in Fig. 1 . The Hamiltonian can then be written as the sum of all the intra-block and inter-block components,

\[ H_{intra,b} = \frac{J}{4} \left[ (\sigma_{1,1}^x \sigma_{2,1}^z + \sigma_{2,1}^x \sigma_{3,1}^z) + D(\sigma_{1,1}^x \sigma_{2,1}^y - \sigma_{1,1}^y \sigma_{2,1}^x) \right] \]

(3)

where \( \sigma_{i,j}^\alpha \) are the Pauli spin operators on the lattice sites.
where $\sigma^z$, refers to the z component of the first spin in the $I^{th}$ block. Then the full 1D Hamiltonian can be written as:

$$H = \sum_I (H_{\text{intra}, I} + H_{\text{inter}, I, I+1})$$

(5)

Each of the block can then be individually diagonalized to obtain the exact eight energy eigenvalues:

$$\epsilon_0 = -\frac{J}{4}(1 + k), \quad \epsilon_1 = \frac{J}{4}(1 - k), \quad \epsilon_2 = 0, \quad \epsilon_3 = \frac{J}{2}$$

(6)

where $k = \sqrt{1 + 8D^2}$, and the energies are all doubly degenerate.

To then project the Hamiltonian onto the two ground states, we define the projection operator

$$P = \bigotimes_{I=1}^{N/4} P_I$$

(7)

where $P_I$ is the projection operator for the $I^{th}$ block given by:

$$P_I = (| \uparrow \rangle \langle \psi_0 | + | \downarrow \rangle \langle \psi_1 |) I$$

(8)

where $| \uparrow \rangle \equiv | \psi_0 \rangle$, $| \downarrow \rangle \equiv | \psi_1 \rangle$ is just a relabelling of states for the new block.

The coarse-grained Hamiltonian is given by:

$$H^{c-g} = PHP$$

(9)

where we define $P_{I,I+1} \equiv P_I \otimes P_{I+1}$.

To compute the projection, we compute the transformation of the Pauli matrices, and for illustration purposes, we list an example of such transformation

$$P_I (1_{1,I} \otimes 1_{2,I} \otimes \sigma_{3,I}) P_I = \frac{1 + k}{2k} \sigma^z_{I}$$

(10)

where now $\sigma^z$ is the Pauli matrix corresponding to the new block spin.

The net result of these transformations is that we can write the coarse-grained Hamiltonian as

$$H^{c-g} = \frac{J'}{4} \left[ \sum_I \sigma^z_I \sigma^z_{I+1} + D' (\sigma^{\uparrow}_I \sigma^{\uparrow}_{I+1} - \sigma^{\uparrow}_I \sigma^{\uparrow}_{I+1}) \right]$$

(11)

with renormalized couplings $J'$ and $D'$. With our choice of Hamiltonian and the coarse-graining scheme, the form of the Hamiltonian is preserved under RG and we do not have to make further approximations. It shall be shown that this is the case for the 2D system as well.

IV. SUMMARY OF RESULTS IN ONE DIMENSION

The results for the 1D system was obtained by Jafari et al. [11], which despite a sign error in their derivation, agree with the summary presented here.

Under the block renormalization scheme, the coarse-graining of the intra-block Hamiltonian leads to an overall additive constant to the Hamiltonian that can be ignored:

$$P_I H_{\text{intra}, I} P_I = \frac{J}{4k^2} \left( \frac{16D^4}{k+1} - k - 1 \right)$$

(12)

Coarse-graining of the inter-block Hamiltonian leads to the renormalized coupling constants:

$$J' = J \left( \frac{1 + k}{2k} \right)^2, \quad D' = \frac{16D^3}{(1+k)^2}$$

(13)
The coupling $J$ flows to zero under RG, which is fine as it sets the overall energy scale for the system. The renormalization of $D$ determines the relative strength of the couplings between anti-ferromagnetism and DM interaction. There are two unstable fixed point occurring at $D = \pm 1$, and tiny variations around the fixed points flow under RG to the trivial stable fixed points at either zero or $\pm \infty$. This implies that at zero temperature, we expect a quantum phase transition between the anti-ferromagnetic Neel ground state and the DM state, across the $D = \pm 1$ fixed points. The sign of $D$ determines the sense of the chirality, i.e., whether the spin rotates clockwise (if $D$ is positive) or anti-clockwise (if $D$ is negative) around the $z$ axis.

V. EXTENSION TO TWO DIMENSIONS

There are some technical difficulties if we try to directly apply the above prescription to the 2D system. Presumably we can use a block scheme that divides the 2D lattice into 2D blocks of size $b \times b$, and proceed to diagonalize each block as above. However, if we choose $b = 2$, we find that the eigenvalues are non-degenerate as before, and if we again choose $b = 3$, we have to diagonalize a $512 \times 512$ matrix just to obtain the two lowest lying states. The computational complexity increases exponentially with $b$.

Hence we shall employ another method following Miyazaki et al [12], in which we first do decimation in one direction, and then in the other direction. To preserve the Hamiltonian under RG, we first divide the lattice into horizontal blocks, and perform block decimation using the projection operator $P^{x}$ (see Fig. 2).

![Diagram of 2D decimation process](image)

**FIG. 2.** Illustration of the 2D decimation process for scheme A.

After this first step, we would generate renormalized couplings between the block spins which are different in the horizontal and vertical directions. This is because horizontal inter-block couplings are generated through interactions between the third spin of the left block and the first spin of the right block, while the vertical inter-block coupling are generated through interactions between all three spins of the bottom and top blocks. This asymmetry is a price we have to pay for carrying out the decimation process in two steps instead of one.

We now restore symmetry to the lattice by decimating in the vertical direction. This is done by dividing the lattice into blocks of three spins in the vertical direction, and carrying out the decimation procedure once again, this time with the projector $P^{y}$, which is constructed from the new ground states after the previous step, at the same time noting that the couplings are no longer symmetric in the vertical and horizontal directions. After this step, we would have completed a single coarse-graining step, and the recursion relations we obtain would be used to identify the fixed points and the phase diagram.

Since we will encounter anisotropic couplings during the renormalization process, we have to rewrite Eq. (2) to separate the horizontal and vertical couplings

$$H = \frac{J_x}{4} \left[ \sum_{<i,j>_{x}} \sigma_i^x \sigma_j^x + D_x(\sigma_i^z \sigma_j^z - \sigma_i^y \sigma_j^y) \right] + \frac{J_y}{4} \left[ \sum_{<i,j>_{y}} \sigma_i^y \sigma_j^y + D_y(\sigma_i^z \sigma_j^z - \sigma_i^y \sigma_j^y) \right]$$

where the notation $<i,j>_{\alpha}$ refers to nearest neighbors in the $\alpha$ direction.

Carrying out decimation in the horizontal direction, we find that the inter-block interactions are renormalized as

$$J^{(1)}_x = J_x f_1(D_x), \quad D^{(1)}_x = D_x f_2(D_x) \quad (15)$$
$$J^{(1)}_y = J_y f_3(D_y), \quad D^{(1)}_y = D_y f_4(D_y) \quad (16)$$

where the superscript (1) indicates that this is after the first step of decimation. The functions $f_1$ to $f_4$ are defined as

$$f_i(D) = \left( \frac{1 + k}{2k} \right)^{i}$$

where we have the usual notation that $k = \sqrt{1 + 8D^2}$. The functions $f_1$ to $f_4$ will be used again in the next step of decimation, as they are the basis of the recursion relations. The renormalization of the intra-block Hamiltonian again results in an overall additive constant to the Hamiltonian and hence can be ignored. The next step is to perform decimation in the vertical direction to recover a symmetric scaling of the lattice. The renormalized couplings after this step is given by

$$J^{(2)}_x = J^{(1)}_x f_3(D^{(1)}_y), \quad D^{(2)}_x = D^{(1)}_x f_4(D^{(1)}_y) \quad (18)$$
$$J^{(2)}_y = J^{(1)}_y f_1(D^{(1)}_y), \quad D^{(2)}_y = D^{(1)}_y f_2(D^{(1)}_y) \quad (19)$$

...
where the superscript (2) now indicates that this is the second step of decimation. At this stage, coarse graining is complete with $b = 3$, and by substituting Eq. (15) and (16) into Eq. (18) and (19), we obtain the renormalized couplings in terms of the original couplings. In general we do not get that the renormalized horizontal and vertical couplings to be the same.

Before we discuss the phase diagram in the next section, we note that we could have chose to perform the coarse-graining first in the vertical direction, followed by the horizontal direction. Given the symmetry of the system, these two methods should yield the same results. However, there is actually an asymmetry in the two methods and we will need to compare the results from both. The procedure of first decimating in the horizontal direction, followed by in the vertical direction shall be denoted as $A$, and the reverse process by $B$. The renormalized couplings for $B$ are given as

$$J^{(1)}_x = J_z f_3 (D_y), \quad D^{(1)}_z = D_z f_4 (D_y) \quad (20)$$

$$J^{(1)}_y = J_y f_1 (D_y), \quad D^{(1)}_y = D_y f_2 (D_y) \quad (21)$$

$$J^{(2)}_x = J^{(1)}_x f_1 (D^{(1)}_y), \quad D^{(2)}_z = D^{(1)}_z f_3 (D^{(1)}_y) \quad (22)$$

$$J^{(2)}_y = J^{(1)}_y f_3 (D^{(1)}_x), \quad D^{(2)}_y = D^{(1)}_y f_4 (D^{(1)}_x) \quad (23)$$

Decimation in the horizontal and vertical directions are non-commutative, as evident by the fact that we do not obtain the same expressions for all the couplings for $A$ and $B$. If we started with the same value of $D$ in the horizontal and vertical direction, after a single step of $A$, we will end up with couplings $D^{(1)}_x$ and $D^{(1)}_y$; and it is clear that if we have carried out $B$ instead, we will have the values of $D^{(1)}_x$ and $D^{(1)}_y$ interchanged.

To further symmetrize the couplings, we can apply $A$ followed by $B$. In fact, in a successive renormalization procedure, it might be better to do successive RG in a symmetric sequence, such as $AB, ABAB, ABABABAAB$, and so on, such that the vertical and horizontal couplings converge to a single value as they should, since we started out with a symmetric square lattice.

**VI. PHASE DIAGRAM AND ORDER PARAMETER**

![FIG. 3. Phase diagram of the model. The phase diagram should be symmetric about $D=0$, with two unstable fixed points and three stable fixed points at zero and ±∞.](image)

We can solve for the fixed points of $D$ with the coupled recursion equations. For example, for $A$, we solve Eq. (18) and Eq. (19) together to obtain the fixed points for $D_x$ and $D_y$. The results are summarised in Table I.

We see that the fixed points obtained by processes $A$ and $B$ are indeed different, showing that the two processes are actually not equivalent. Carrying out coarse-graining with $A$ followed by $B$ converges the two values by a significant amount. The fixed points for $A$ and $B$ are listed only as negative values because the asymmetry in the decimation process for either one of them causes the positive fixed points to disappear. This asymmetric artifact is removed under the $AB$ process.

<table>
<thead>
<tr>
<th></th>
<th>$A$</th>
<th>$B$</th>
<th>$AB$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$D_x^{(2)}$</td>
<td>$-1.164$</td>
<td>$-0.981$</td>
<td>$±1.1445$</td>
</tr>
<tr>
<td>$D_y^{(2)}$</td>
<td>$-1.095$</td>
<td>$-1.168$</td>
<td>$±1.135$</td>
</tr>
</tbody>
</table>

**TABLE I. The critical values of the DM couplings under RG**

Similar to the case of 1D, the system exhibits quantum phase transition at a critical value of $D$, which we can assume to be the convergence of $D_x$ and $D_y$ with a symmetric RG procedure. The phase diagram is as illustrated in Fig. 3.

Under the quantum renormalization group scheme, we can calculate expectation values of operators by deriving a recursion relation for the expectation values. To illustrate this process, we define the staggered magnetization, which can be used as an order parameter, as

$$S_M = \frac{1}{N} \sum_{i,j} \langle 0 | (-1)^{i+j} \sigma^z_{i,j} | 0 \rangle \quad (24)$$

where $| 0 \rangle$ denotes the ground state of the system, and $N$ the number of sites. The recursion relation for the expectation value is calculated by noting that the coarse-grained ground state, $| 0' \rangle$, is related to the original one for process $A$ by

$$P^x P^y | 0' \rangle = | 0 \rangle \quad (25)$$

We can then show that

$$S_M^{(1)} = \frac{1}{9} \left( \frac{2 + k_x}{k_x} \right) \left( \frac{2 + k_y^{(1)}}{k_y^{(1)}} \right) S_M^{(1)} \quad (26)$$

where $S_M^{(1)}$ is the expectation value calculated in the coarse-grained ground state, $k_x = \sqrt{1 + 8 D_x^{(2)}}$, and similarly for $k_y^{(1)}$, except that we use the renormalized value of $D_y$ after horizontal decimation. We can calculate $S_M$ for a fixed value of $D$ by iterating this equation, and noting that after sufficient iterations, the staggered magnetization should renormalize to either zero or one depending on the initial value of $D$.

We can also define another quantity of interest that we shall call the chiral order [13], as

$$C = \frac{1}{2N} \sum_{<i,j>} \langle 0 | \sigma^x_i \sigma^y_j - \sigma^y_i \sigma^x_j | 0 \rangle \quad (27)$$
and we have the recursion relation for the case of scheme $A$

$$C = \frac{1}{12} \left( g_1(D_x) + \frac{1}{3} g_1(D_y^{(1)}) g_2(D_x) \right) + \frac{1}{9} g_2(D_x) g_2(D_y^{(1)}) \mathcal{C}^{(1)}$$

(28)

$$g_1(D) = \frac{16D^3}{k^2(1+k)}, \quad g_2(D) = \left( \frac{2D}{q} \right)^2$$

(29)

From the form of Eq. (27), we can see that the chiral order asymptotes to one in the classical limit when $D$ is infinite, as each bond contributes one to the sum (see Fig. 5). A plot of $S_M$ and $C$ against $D$ for negative values of $D$ is shown in Fig. 4. We see that $S_M$ is a suitable order parameter as it is zero in the chiral phase, and increases monotonically in the anti-ferromagnetic phase. It is possible to fit the curve close to the critical value of $D$ to find that $S_M \propto \sqrt{D-D^*}$. Chiral order increases with the strength of $D$, and is finite for any finite value of $D$. We can also calculate the eigenvalues of $D_x$ and $D_y$ to obtain $y_{D_x} = 2.40$ and $y_{D_y} = 2.07$ with the $AB$ scheme.

![FIG. 4. The variation of the order parameter $S_M$ and chiral order $C$ with $D$, for coarse-graining scheme A. If a successive symmetric RG scheme is used, the figure should be symmetric about $D = 0$.](image)

VII. CONCLUSION

We have reviewed the method of quantum PSRG and how it can be applied to a particular Hamiltonian. Using PSRG we find that there are indeed two distinct phases for the Hamiltonian described by Eq (2), and we have found approximate values for the critical fixed points at which quantum phase transition occurs. While we can expect the qualitative results of PSRG to be accurate, it would be useful to compare the quantitative predictions with other methods. Monte Carlo methods employed to classical spin system with DM interaction indeed shows a rich phase diagram [14] with multiple chiral phases. In order to compare to experimental data, it would be necessary to include other forms of interactions such as crystalline anisotropy and Zeeman energy, rendering the RG process considerably harder as one would need to deal with the generation of additional couplings.

VIII. ACKNOWLEDGMENT

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