Ising and XY within the (Classical) Heisenberg Model

An intuitive and numerical analysis on the $O(3)$ model with an Anisotropic external field

by

Sebastián Nicolás Mendoza Vásconez

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Abstract

We analyse the classical Heisenberg Model (sometimes assimilated with the $O(3)$ model) with an anisotropic external coupling. We make an intuitive argument as to the governing structure of the different phases that arise at different regimes of the coupling constants, and proceed to numerically demonstrate this behaviour using Monte Carlo methods (a modified version of Wolff's clustering algorithm, to be precise). After reviewing the numerical results, we briefly touch on the quantum dual theory corresponding to our system, and then discuss further steps in investigating it.

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1 Introduction

1.1 Motivation

The Ising and XY models are among the most popular examples introduced to physics students as they begin learning about Statistical Field Theory. Both are special examples of an $O(n)$ system after being discretized, where the field's codomain is constrained to the hypersphere $\mathbf{S}^{n-1}$. In the case where $n = 1$, we have $\mathbf{S}^0 = \{-1, 1\}$, which are effectively the possible values any lattice point in the Ising system can take. Similarly, $n = 2$ corresponds to a lattice in which each point can take a value in a $r = 1$ circle. The Heisenberg model is a further example, being the case of $n = 3$; that is, each lattice point admits a value constrained to be in the sphere S^2. Here, we will examine a coupling (introduced below) which, depending on the value taken by the coupling constant, will either force the system to become either the Ising model or the XY model: quite a crossover indeed. The anisotropic Heisenberg model has been explored in different contexts before [5][3], but we have not been able to find extensive literature on this particular external coupling presented, (aside from [6], which presents it as an example to study further). Depending on the dimensionality of our lattice, the quantum dual theory will correspond to either a particle or a string (or a brane) moving within a sphere, and thus becomes quite an interesting example to be studied. We will come back to this in Section 4.

Nonetheless, performing the numerical analysis will turn out to not be as straightforward as it might initially seem. Applying the Metropolis or Wolff algorithm as is commonly done with the Ising model will not be possible because of two main complications: the fact that our output space has infinite cardinality (S^2 is a continuous object, as opposed to $\{-1, 1\}$), and the additional contribution coming from "sources" (our external coupling).

1.2 The Anisotropic Heisenberg System

We will proceed to more rigorously define the system we are dealing with. For a d-dimensional lattice, the field we are interested in is

$$s : \mathbf{Z}^d \to S^2$$

with $\mathbf{s}_i \equiv (s_i^x, s_i^y, s_i^z)^T \coloneqq s(i)$, and thus $\|\mathbf{s}_i\| = 1 \ \forall i$. In the general case, i is a multi-index $i \in \mathbf{Z}^d$, but we will be mostly dealing with the Heisenberg model on a chain $d = 1$ and briefly mention the case $d = 2$. We can then proceed to define our Energy function of interest:

$$E(s) = -J \sum_{\langle ij \rangle} \mathbf{s}_i \cdot \mathbf{s}_j + g \sum_i \left[(s_i^z)^2 - \frac{1}{2} \left((s_i^x)^2 + (s_i^y)^2 \right) \right] \tag{1}$$

where the sum over $\langle ij \rangle$ in Eq. (1) means summing over all (nearest) neighbors i, j in the lattice. This defines our classical anisotropic Heisenberg model, with the anisotropy clearly coming from the contribution corresponding to g.

We can derive this easily from the action of a continuous field $\vec{\phi} : \mathbf{R}^d \to \mathbf{S}^{n-1}$ (or $\phi^\alpha(x) \in \mathbf{R}$ with the constraint $\phi^\alpha \phi_\alpha = 1$ (using summation convention).

$$S[\phi] = \int \mathrm{d}^d x \left[-\frac{1}{2} \partial^\mu \phi^\alpha \partial_\mu \phi_\alpha + \lambda \left((\phi_3(x))^2 - \frac{(\phi_1(x))^2 + \phi_2(x))^2}{2} \right) \right] \tag{2}$$

In $d = 1$, we can discretize by

$$\begin{aligned} \sum_\alpha \left(\frac{d}{dx} \phi_\alpha \right)^2 &\to \sum_\alpha \left(\frac{\phi_\alpha(x + \Delta x) - \phi_\alpha(x)}{\Delta x} \right)^2 \\ &= \sum_\alpha \frac{1}{\Delta x^2} [\phi_\alpha(x + \Delta x)^2 + \phi_\alpha(x)^2 - 2\phi_\alpha(x + \Delta x)\phi_\alpha(x)] \\ &= \frac{1}{\Delta x^2} [2 - 2\vec{\phi}(x + \Delta x) \cdot \vec{\phi}(x)] \end{aligned}$$

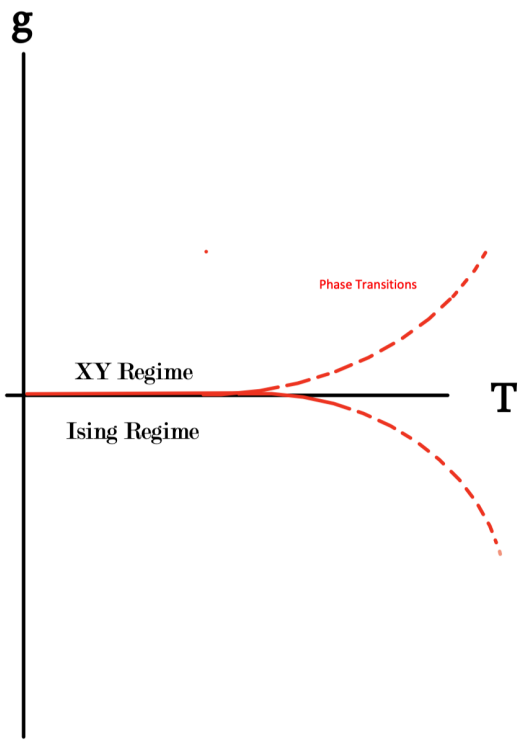

Figure 1: Phase Transition Diagram in different regimes of the coupling constant (and temperature)

Reabsorbing the constant energy shift and relabeling our coupling constants, we end up with the neighbor interaction term in (1) as desired.

2 A Physical Analysis

We begin with a very physical (intuitive) analysis of the system and examine its different regimes. Doing this, we can see that the situation is captured by the phase transition diagram in Fig. 1

How can we justify this claim? We see that, at low temperatures where the system sits on an ordered phase, there are two possible scenarios: g being positive or negative. If $g > 0$, we see that the contributions to the energy $E(s)$ coming from the external coupling are minimized when the vectors $\vec{s}_i$ lie on the circle described by $(s_i^x)^2 + (s_i^y) = 1$ (as the positive contributions come only from $g(s_i^z)^2$). Now that

the vectors are constrained to the circle in the x-y plane, we can clearly see that the system effectively becomes the XY-model. If $g < 0$, the positive contributions to the energy come from both the x and y components of the field vectors, while the values along the z direction will minimize the energy. Thus, the system becomes constrained to only take values $\mathbf{s}_i = \pm 1\hat{z}$, effectively becoming the Ising model. With a fixed g, we would then have the 'standard' phase transitions that would come form varying the temperature in the XY or Ising model.

3 Numerical Exploration

To perform the numerical analysis, we performed a Monte Carlo simulation using a modified version of the Wolff algorithm. Here, we will present the obstacles presented by working with the Heisenberg model (rather than Ising) and using external sources, but the full code can be found in this repository. Throughout the rest of this section, we will solely reffer to the case of the Heisenberg chain ($d = 1$) and with a lattice of size N with periodic boundary conditions.

3.1 Infinities of S^2

One of the factors that made the Metropolis algorithm possible in the Ising model is the fact that every Monte Carlo step consists of two main processes dealing with randomness:

1. We chose an index $i \in \{0, \dots N\}$ at random
2. We calculate the change in the action that would occur if the spin were flipped dS. Then, we chose a number $\chi \in [0, 1]$ and flip the spin if $\chi < e^{-dS}$

However, we cannot use this procedure anymore since flipping the elements $\mathbf{s}_i$ will not lead to any possible configuration (so it is clearly not ergodic).

Similarly, the Wolff algorithm also requires each spin in the lattice to either be or not be in the same 'spin' as the initial randomly selected index. This could even be extended to the Potts model easily to find clusters only belonging to the same category, but the sphere has uncountably many 'categories' and thus the same extension does not work.

Thus, we follow the approach outlined in [4] to be able to translate this method into our infinite dimensional system. The procedure begins by choosing a random $\vec{r} \in \mathbf{S}^2$, and then project our vectors over it. This then defines a variable that takes ± 1, namely $\epsilon_i \coloneqq \text{sgn}(\mathbf{s}_i \cdot \vec{r})$. With this variable in hand, we proceed to apply the Wolff procedure as usual.

3.2 External Source Contribution

The anisotropic contribution from the external coupling poses yet another challenge in the standard Wolff procedure. Essentially, the external sources will violate the condition of detailed balance.

In order to solve this, we apply the method outlined in [2]. Here, we apply a procedure mimicking the effect of the Metropolis Algorithm after applying the Wolff algorithm: after finding the cluster connected to the initial random index, we find the change in energy $dE_g = E_g(\tilde{s}) - E_g(s)$ and then apply the flipping of the cluster ($\epsilon_j \to -\epsilon_j \ \forall j \in$ cluster) if $\chi < e^{-\beta dE}$ for a randomly selected $\chi \in [0, 1]$ (Here $\tilde{s}$ is the flipped-cluster-configuration, and $E_g(\cdot)$ is the contribution coming solely from the external sources).

3.3 Results

The numerical exploration does indeed support the intuitive analysis presented in Section 2. First, we let the configurations thermalize as shown in Fig

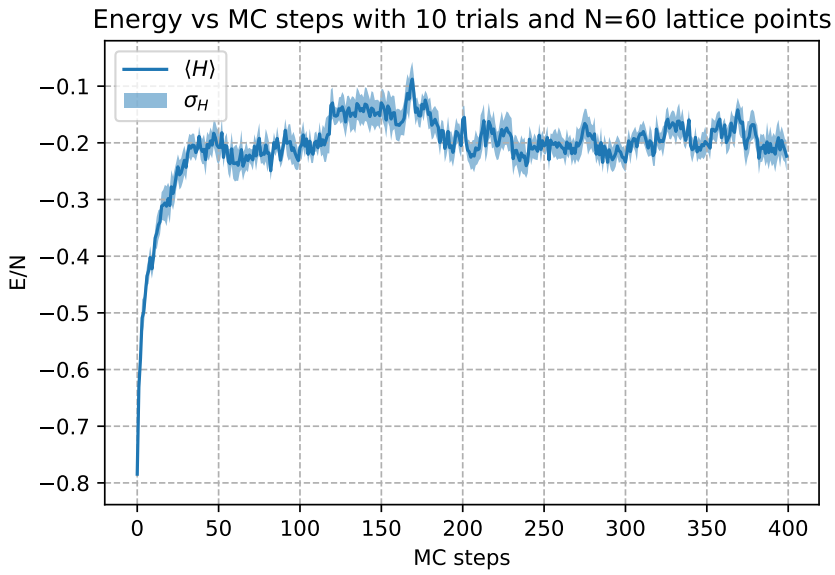

Figure 2: Thermalization of the Heisenberg Spin Configuration

2. We proceed to repeat this process for different coupling constants in order to observe the predicted changes in magnetization.

3.3.1 Varying g

The first result we will discuss centers around the phase transition arising from varying g continuously from a negative number to a positive. We show the results in Fig. 3: the magnetization does indeed become mostly aligned towards the z direction for $g < 0$ (the average magnetization in the z direction squared $\langle (m_z)^2 \rangle$ is basically one, while the other components have no contribution), and then becomes almost entirely dominated by both the x and y direction when $g > 0$. This is precisely the scenario portrayed in Section 2

We can see a similar discontinuity in the average energy $\langle E \rangle$ (as shown in Fig. 4). Here, there is a clear maximum of energy when $g = 0$, which can also be intuitively explained: With $g \neq 0$, the fields are constrained to move either in a

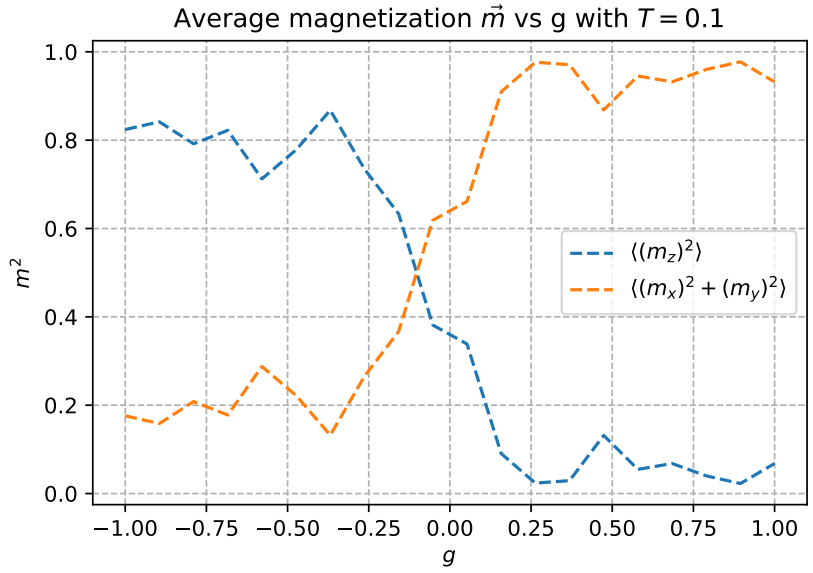

Figure 3: Magnetization as a function of the external coupling g at a fixed temperature $T = 0.1$

circle or in the poles, and thus it is easier for them to align in comparison to the entire sphere (thus decreasing their energy).

3.3.2 Varying T

We then proceed to analyse the change of the system by varying T with a fixed g. We will consider both positive and negative g, although the portrayal of the results will be a bit different for both cases. In both cases, however, the average energy of the system increases with T as was expected (shown in Fig. 5 for a reality check).

Most importantly, we now proceed to analyse how m changes as we vary T. The results for a positive g are shown in Fig. 6. Here, we plot once again the magnetization along the z axis squared vs the magnetization along the $x - y$ plane. We see that, as expected for $g > 0$, the magnetization is mostly aligned on the $x - y$ plane, but as temperature increases, it becomes more evenly distributed

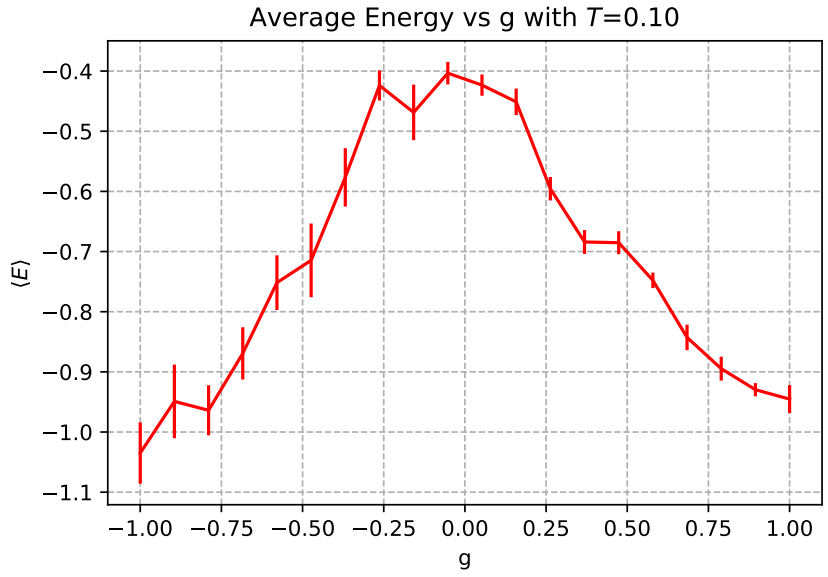

Figure 4: $\langle E \rangle$ vs g at a fixed temperature $T = 0.1$

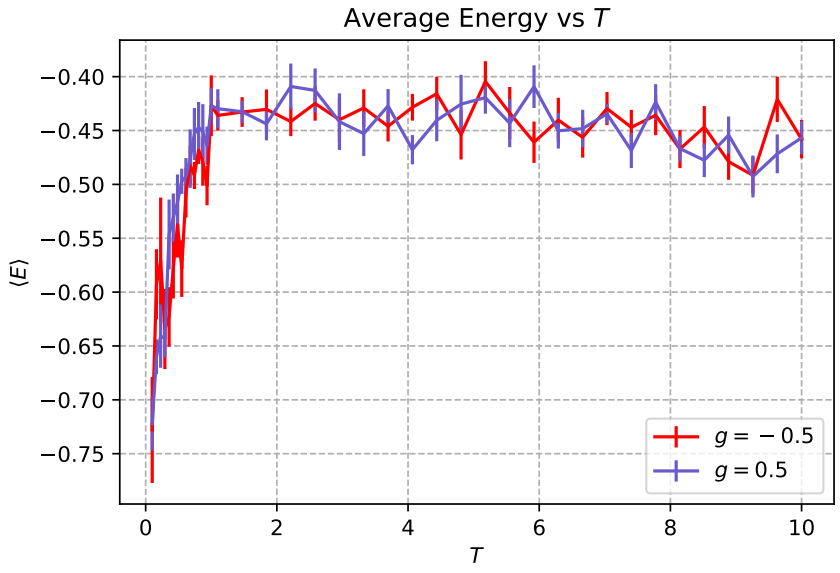

Figure 5: $\langle E \rangle$ vs T with fixed $g = \pm 0.5$

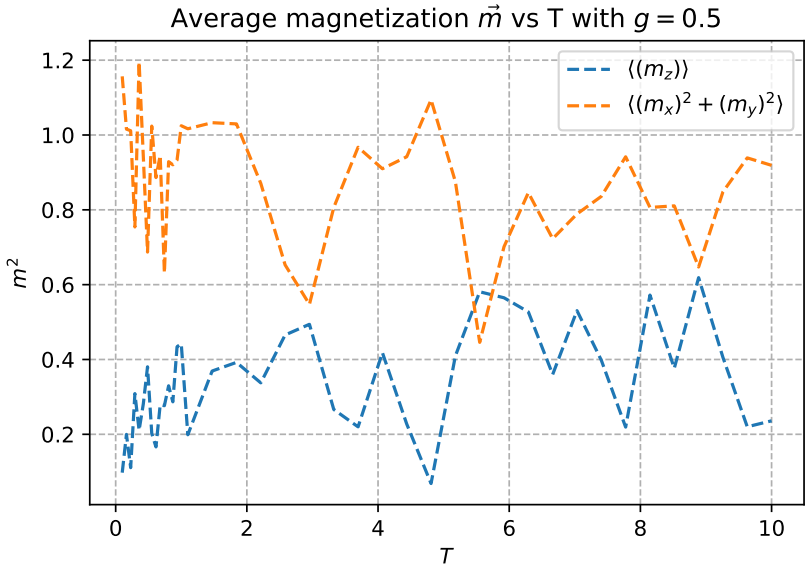

Figure 6: Magnetization m^2 over a varying T with a fixed positive $g = 0.5$

around the entire sphere (with m_z occupying roughly a third of the contribution as expected).

We now portray the case of $g > 0$ a bit differently, shown in Fig. 7. Here, we stop plotting m^z (we did not do this before because we needed to display the dominance of the $x - y$ plane components of the magnetization m, rather than along a particular direction). We now clearly visualize the spins aligned along the z-direction dominate for low temperature, but then rapidly drop to a third of the contribution (on average). The increase in temperature certainly randomizes the magnetization, as expected from an analysis from both XY and Ising model.

4 The Quantum Dual

We proceed to analyze the quantum dual to the theory. We do this by Wick rotating one of the spatial dimensions, and then treating the output of the fields as a setting for the Hilbert Space of the quantum dual theory. However, we will begin with a simpler example to make the idea more clear.

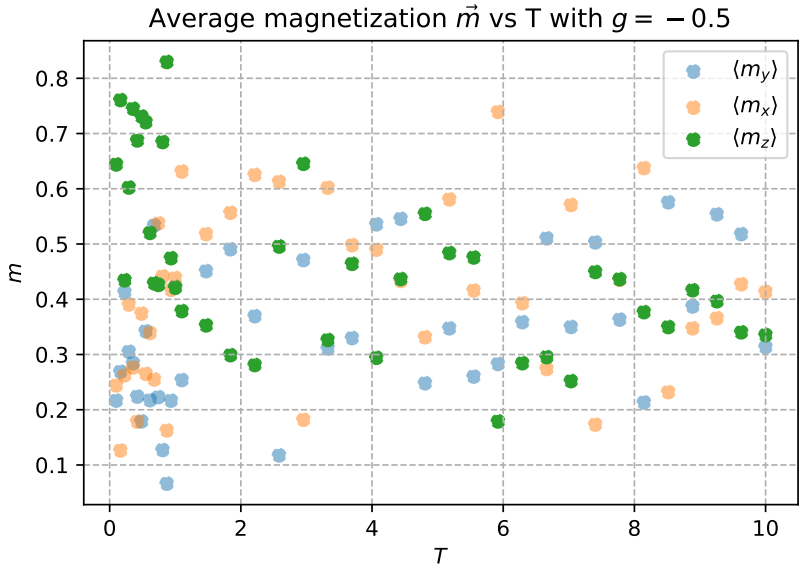

Figure 7: Magnetization $\vec{m}$ over a varying T with a fixed negative $g = -0.5$

A Simpler Example: The Ising Model on a 1D lattice

As a brief example, we consider the Ising model on a chain. The values that can be taken by the fields on each lattice point are $\{-1, 1\}$, or alternatively, we can represent them with the (isomorphic) set $\mathcal{A} \coloneqq \{\downarrow, \uparrow\}$. We then represent our Hilbert space with linear combinations of elements in $\mathcal{A}$. In particular, we can think about this Hilbert space as

$$\mathcal{H} = \left\{ \psi : \mathcal{A} \to \mathbf{C} \,\middle|\, \sum_{a \in \mathcal{A}} |\psi(a)|^2 < \infty \right\} \tag{3}$$

which, in this case, is basically isomorphic to $\mathbf{C}^2$.

Using Dirac notation, we can represent $\psi(a) \equiv \langle \psi | a \rangle$, which helps us express our states as $|\psi\rangle = \sum_a \psi(a) |a\rangle$. Then, we define the evolution of our states as follows: given an initial state $|\varphi_i\rangle$ and a final state $|\varphi_f\rangle$, (for simplicity, we take $|\varphi_i\rangle, |\varphi_f\rangle \in \{|\uparrow\rangle, |\downarrow\rangle\}$, but this result can be extended by linearity), we calculate the probability amplitude between the time evolution of the initial state over the

final state by summing over all configurations with the boundary conditions being given by the initial and final state. Mathematically connecting the classical theory and its quantum dual: if we have a lattice with N points and length scale Δx, and the time elapsed is given by $T = N\Delta x$, then we have

$$\langle \varphi_f | \, U(T) \, | \varphi_i \rangle = \sum_{s \in \mathcal{S}_{\varphi_i}^{\varphi_f}} e^{-\beta E(s)} \quad \text{with } \mathcal{S}_{\varphi_i}^{\varphi_f} = \{ s \mid s(0) = \varphi_i, s(N) = \varphi_f \} \tag{4}$$

We see that the quantum theory corresponds to a two level system: the lattice of spins up and down became a single particle with spin up or down evolving through time! In fact, the *rhs* of Eq. (4) is very similar to a partition function, except that it has fixed boundary conditions. We could also represent this as

$$\langle \varphi_f | \, U(T) \, | \varphi_i \rangle = \mathcal{Z}[\varphi_i, \varphi_f]$$

A very important factorization happens in this system because the interactions between each pair of neighbors are the same and only depend on the nearest neighbors (namely, the fact that we can express our system as a product of transfer matrices): We end up having $U(N\Delta x) = (U(\Delta x))^N$. Using the definition for the Hamiltonian (generator of time translations), we can then find an equation for the Hamiltonian of the dual theory:

$$e^{-T\hat{H}} = U(T) \Rightarrow e^{-N\Delta x \hat{H}} = U(N\Delta x) \Rightarrow (e^{-\Delta x \hat{H}})^N = (U(\Delta x))^N$$

Thus, we see precisely that $e^{-\Delta x \hat{H}} = U(\Delta x)$, or equivalently:

$$\hat{H} = -\frac{d}{d\Delta x} U(\Delta x) \Big|_{\Delta x = 0} \tag{5}$$

The Particle on a Sphere

The same procedure can be applied to the system of interest: the classical Heisenberg model with an anisotropic external source. Instead of having a finite dimensional Hilbert Space, we will have something more complicated. The setting is not a simply finite set like $\{-1, 1\}$, but it is S^2. Thus, our Hilbert space is

$$\mathcal{H} = \left\{ \Psi : S^2 \to \mathbf{C} \;\middle|\; \int_{S^2} \mathrm{d}\varphi |\Psi(\varphi)|^2 < \infty \right\} \equiv L^2(S^2) \tag{6}$$

which is simply the space of square integrable functions on a sphere! Thus, we see that the quantum dual to the classical Heisenberg Model (or $O(3)$) will be a particle on a sphere. Since the interactions described by the energy function in (1) can also be decomposed into a product of transfer 'matrices' (although now they are no longer matrices but operators acting on infinite dimensional spaces), we can analogously find the exact Hamiltonian corresponding to our classical Heisenberg model with an external anisotropic interaction. While we will not explicitly derive this result here, it is certainly an area of interest and further work should be done in the future. Nonetheless, we can have some intuition as to what the Hamiltonian will be: it will consist of the classical Laplacian constrained to the sphere (due to the kinetic term in the classical theory) and it will have some an anisotropic term in the shape of some external field (coming from the external source). How will this external field behave? For low temperatures, it will constrain the particle to either be on one of the poles along the z axis ($g < 0$) or on the $x - y$ plane ($g > 0$). For higher temperatures, this field will not pick a particular direction, but still be strong enough to cause wild oscillations in our system. Thus, the field will therefore likely be time dependent, with the rate of change of direction proportional to the temperature.

5 Discussion

As we saw, this modification of the Heisenberg model (with the anisotropic source) provides a very interesting setting: both encapsulating the Ising and XY models for different regimes of the coupling constants. The numerical results were quite successful, and future work would incorporate more trials (only 10 were used in this study due to the inner workings of Python and NumPy), which might require a different paradigm (such as switching the algorithms to Jax and Lax [1]). This was briefly attempted, but the amount of conditionals and ambiguous structures required in the Wolff algorithm make jitting the code overly complicated.

The quantum dual is quite an interesting theory indeed (particle moving on a sphere) and the corresponding Hamiltonian should be explored more in the future. Even more interestingly, the analysis we did for the 1D chain can be similarly made for higher dimensional lattices. In particular, a 2D lattice would be of interest, as the quantum dual would become a quantum string moving in a sphere and the external source might become some sort of interaction with an external time-dependent field. This would be of direct relevance to modern quantum gravitational theories.

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