Path integrals, diffusion and the fully frustrated antiferromagnetic spin cluster

P.M. Hogan & J.T. Chalker

University of Oxford, United Kingdom

Abstract

We study the path integral treatment of the quantum mechanics of a fully frustrated cluster of spins: a cluster in which every pair of spins is coupled equally by antiferromagnetic Heisenberg interactions. Such clusters are interesting partly because they are the building blocks blocks of geometrically frustrated spin systems, such as the antiferromagnetic Heisenberg model on the kagomé or pyrochlore lattices. We consider the general case of clusters with an arbitrary number of arbitrary sized spins.

We first construct a coherent-state path integral for such a cluster's partition function, and through a Hubbard-Stratonovich transformation, we establish a relationship between it and the evolution of a single spin in a time-dependant, stochastic magnetic field.

We then translate the Langevin-type behaviour of this spin's evolution operator into the probabilistic diffusion of the SU(2) parameters which describe it. This process can be represented as a Fokker-Planck equation. As the corresponding eigenfunctions and eigenvalues are known, we may then readily rewrite the original cluster's partition function as a finite sum of a single integral, which gives results agreeing with those known for the few special cases treated using other methods.

It is hoped that by linking clusters approached in this way, we may be able to develop a new theoretical approach to quantum geometrically frustrated antiferromagnets. A more detailed exposition of the work in this poster can been found in *J. Phys. A: Math. Gen.* **37** (2004) 11751.

Geometrical Frustration

Introduction

Focus on spin systems

▷ Geometrical frustration occurs when spatial arrangement of spins on lattice results in the ground state of the system not minimizing the individual spin-spin interactions (see example, right).

Frustrated spin lattices (below) can display very rich and interesting behavior

▷ Much work done on classical systems

▷ Wish to gain better understanding of frustrated quantum systems

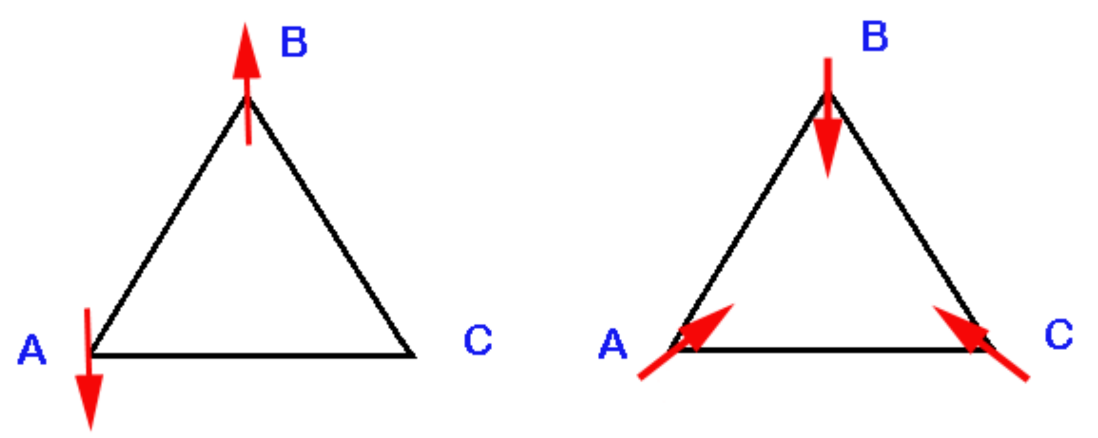
Present here an approach to understanding an individual quantum spin cluster

▷ Cluster can be used to build lattices

▷ Hope approach can help understand frustrated quantum systems

Example

A cluster of three classical spins, coupled equally by antiferromagnetic XY interactions:

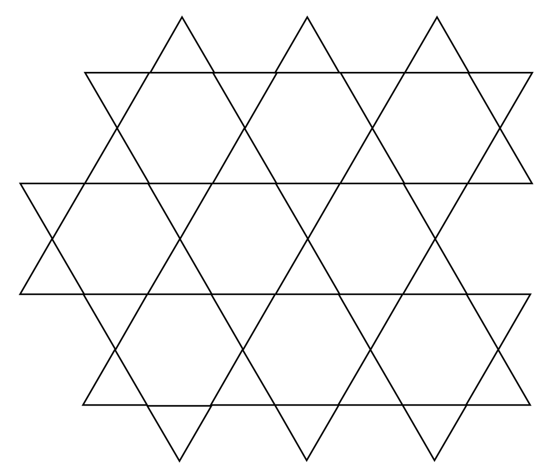


This interaction is satisfied - global and local energy minimum.

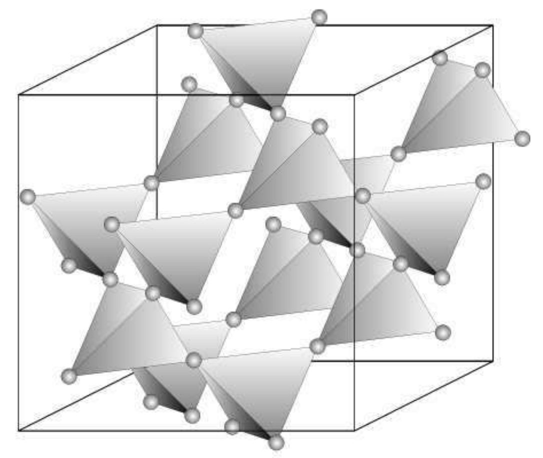
No individual interation satisfied, but global energy minima - frustration.

Lattices

Frustrated clusters can be the building blocks of frustrated lattices:



Triangles in 2D - kagomé lattice



Tetrahedra in 3D - pyrochlore lattice

The Single Cluster

Generalize quantum cluster to q Heisenberg spins:

$$\hat{\mathcal{H}}_0 = J\sum_{i,j=1}^{q}\hat{\mathsf{S}}_i\cdot\hat{\mathsf{S}}_j = \tfrac{1}{2}J\left(\sum_{i=1}^{q}\hat{\mathsf{S}}_i\right)^2 - \tfrac{1}{2}J\sum_{i=1}^{q}\hat{\mathsf{S}}_i^2 \equiv \hat{\mathcal{H}} - \tfrac{1}{2}JS(S+1)$$

Would like partition function:

- Quantum addition of angular momentum possible
  - ▷ Only an implicit general scheme
  - ▷ Rapidly becomes extensive and intractable
- Explicit closed form for arbitrary q, S and T preferred

Partition Function

Hubbard-Stratonovich Transformation

Begin by constructing an 'imaginary time' coherent state path integral:

▷ Time-slice the exponential operator ($\epsilon = \beta/N$)

▷ Insert resolutions of the identity

$$Z = \mathrm{Tr}\, e^{-\beta\hat{\mathcal{H}}}$$
$$= \int\left(\prod_{n=1}^{N} d\mathbf{\Omega}_n\right)\prod_{m=1}^{N}\langle\mathbf{\Omega}_m|\; e^{-\epsilon\hat{\mathcal{H}}}\;|\mathbf{\Omega}_{m-1}\rangle \qquad |\mathbf{\Omega}\rangle = \prod_{i=1}^{q}|\mathbf{\Omega}_i\rangle$$

Hubbard-Stratonovich

$$e^{-\epsilon\hat{\mathcal{H}}} = \left(\frac{\epsilon}{2\pi J}\right)^{3/2}\int_{-\infty}^{+\infty} d^3\boldsymbol{h}\;\exp\left\{-\epsilon\left[\frac{1}{2J}\boldsymbol{h}^2 + i\boldsymbol{h}\cdot\hat{\mathsf{S}}_t\right]\right\} + O\left(\epsilon^2\right)$$

$$\xrightarrow[N\to\infty]{} \int\mathcal{D}\boldsymbol{h}(\tau)\;\exp\left\{-\int_0^\beta d\tau\,\frac{1}{2J}\boldsymbol{h}^2\right\}\cdot\left\{\mathrm{Tr}\,\mathsf{T}(\hbar\beta)\right\}^q$$

Single spin path-integral

A Single Spin

Now take a step back:

▷ Consider the Schrödinger Equation for a *single* spin in a time-dependent, stochastic magnetic field $\boldsymbol{h}(t)$:

$$i\hbar\,\partial_t\,|\psi(t)\rangle = \boldsymbol{h}(t)\cdot\hat{\mathsf{S}}\quad|\psi(t)\rangle$$
$$\equiv \boldsymbol{h}(t)\cdot\hat{\mathsf{S}}\quad\hat{\mathsf{T}}(t;0)\;\;|\psi(0)\rangle\cdot\Theta(t)$$

$(2S+1)$-spinor

$\hat{\mathsf{T}}(0;0) = \mathbb{I}_{2S+1}$

▷ Construct 'real time' path integral solution for $\hat{\mathsf{T}}(t)$

▷ Relate it to our partition function:

$$Z = \int\mathcal{D}\boldsymbol{h}(\tau)\;\exp\left\{-\int_0^\beta d\tau\,\frac{1}{2J}\boldsymbol{h}^2\right\}\cdot\left\{\mathrm{Tr}\,\mathsf{T}(\hbar\beta)\right\}^q$$

Underlying Idea

$$Z = \int\mathcal{D}\boldsymbol{h}(\tau)\;e^{-\int_0^\beta d\tau\,\frac{1}{2J}\boldsymbol{h}^2}\quad\left\{\mathrm{Tr}\,\mathsf{T}(\hbar\beta)\right\}^q$$

Gaussian average

$$= \left\langle\left\{\mathrm{Tr}\,\mathsf{T}(\mathcal{P};t)\right\}^q\right\rangle\Big|_{t=\hbar\beta} \qquad \mathcal{P} = \mathcal{P}([\boldsymbol{h}],t) = \text{Parameters describing integrand}$$

$$= \int d\tau_{\mathcal{P}}\;P(\mathcal{P};t)\quad\left\{\mathrm{Tr}\,\mathsf{T}(\mathcal{P};t)\right\}^q\Big|_{t=\hbar\beta} \qquad \mathcal{P} = \mathcal{P}(t)$$

Stochastic (Langevin) ⟶ Deterministic (Fokker-Planck)

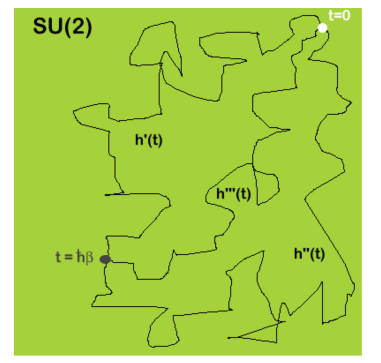
▷ Path integral can be viewed as Gaussian average over stochastic $\boldsymbol{h}(t)$, whose distribution is known.

▷ Parameters $\mathcal{P}$ evolve differently in time for each $\boldsymbol{h}(t)$ - but we are only interested in their end-point, at $t = \hbar\beta$.

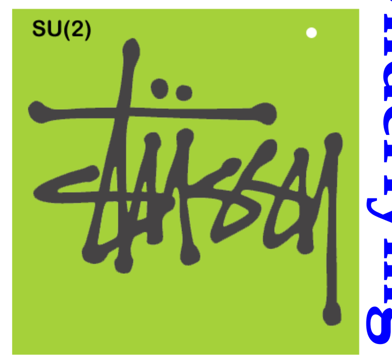
Hence we may instead integrate over the probability, due to all possible $\boldsymbol{h}(t)$'s, of arriving at that endpoint.

This may perhaps be visualized with the aid of the diagrams to the right, and PMH's T-shirt.

Visualization



Paths due to different $\boldsymbol{h}(t)$ on SU(2)



Resultant $P(\mathcal{P};\hbar\beta)$

Paths on $SU(2)$

Stochastic Evolution

$$i\partial_t\,\mathsf{T}(\mathcal{P};t) = \left[\boldsymbol{h}\cdot\mathsf{S}\right]\mathsf{T}(\mathcal{P};t)$$

$(2S+1)$-dimensional representation of SU(2)

Choose Euler-angle parametrization: $\mathcal{P}\to\mathcal{E} = \alpha,\beta,\gamma$

$$\mathsf{T}(\alpha,\beta,\gamma;t) = e^{-i\alpha(t)\mathsf{J}_3}e^{-i\beta(t)\mathsf{J}_2}e^{-i\gamma(t)\mathsf{J}_3} \qquad 0\le\alpha<2\pi,\; 0\le\beta\le\pi,\; 0\le\gamma<4\pi$$

Langevin equations for (α,β,γ)

with initial conditions $\hat{\mathsf{T}}(0) = \mathbb{I}_{2S+1}$

Deterministic Diffusion

Langevin equations for (α,β,γ)

Gaussian average over stochastic fluctuations: $\langle h_i(t)\rangle = 0$, $\langle h_i(t)h_j(t')\rangle = J\,\delta_{ij}\,\delta(t-t')$

$$\partial_t\,P(\mathcal{E};t) = \tfrac{1}{2}J\;\hat{L}_{FP}\;P(\mathcal{E};t)$$

$$\hat{L}_{FP} = \mathrm{cosec}\beta\partial_\beta\sin\beta\partial_\beta + \mathrm{cosec}^2\beta\left[\partial_\alpha^2 + \partial_\gamma^2 - 2\cos\beta\partial_\alpha\partial_\gamma\right]$$

Laplace-Beltrami operator

Eigenfunctions $D_j(\mathcal{E})^{m'}{}_m$ and eigenvalues λ_j known.

$$P(\mathcal{E};t) = \sum_j(2j+1)e^{-\frac{1}{2}j(j+1)Jt}\sum_m D_j(\mathcal{E})^m{}_m \qquad \lambda_j = j(j+1),\quad m',m = -j...j$$

j^{th} character of SU(2)

But $\{\mathrm{Tr}\,\mathsf{T}(\mathcal{P};t)\}$ is also the S^{th} character of SU(2)

▷ Depends *only* on total angle of rotation

Take advantage of this:

▷ Coordinate transformation from $\mathcal{E}$ to $(\psi,\hat{\boldsymbol{n}})$ parametrization, describing same rotation but with the total angle of rotation about required axis.

$$k^{\mathrm{th}}\text{ character of SU(2)} = \frac{\sin\left(k+\frac{1}{2}\right)\psi}{\sin\left(\frac{1}{2}\psi\right)} \qquad 0\le\psi\le2\pi$$

Final Result

Integral Form

Putting all the pieces together:

$$Z = \sum_{j=0}^{qS}e^{-\frac{1}{2}j(j+1)J\beta}\cdot\frac{1}{\pi}(2j+1)\int_0^{2\pi}d\psi\left\{\frac{\sin\left(S+\frac{1}{2}\right)\psi}{\sin\left(\frac{1}{2}\psi\right)}\right\}^q\sin\left[\left(j+\tfrac{1}{2}\right)\psi\right]\sin\left(\tfrac{1}{2}\psi\right)$$
$$= \sum_n e^{-E_n\beta}\cdot g_n \qquad 2j\in\mathbb{Z}_0^+$$

▷ May immediately deduce that $g_n = 0$ if $(qS+j)\notin\mathbb{Z}_0$

Residue Form

Evaluating this as a contour integral:

$$Z = \sum_{j=0}^{qS}e^{-\frac{1}{2}j(j+1)J\beta}\cdot\sum_{\substack{k=0\\ \Delta>-1}}^{q}\frac{(2j+1)\,q!\,(-1)^{k+1}}{2\cdot k!(q-k)!}\cdot\frac{1}{\Delta!}\frac{d^\Delta}{dz^\Delta}\frac{z^{4j+2}-1}{(z^2-1)^{q-1}}\Bigg|_{z=0}$$

$\Delta = 2j + 2k(2j+1) - 2q(S+1) + 2$

▷ Computationally at least two orders of magnitude more efficient

Asymptotics

Behaviour of the partition function for large q may be deduced by applying a saddle-point approximation to the dominant maxima of the above integrand:

$$Z = \sum_{j=0}^{qS}e^{-\frac{1}{2}j(j+1)J\beta}\cdot\left\{q^{-3/2}(2S+1)^q(2j+1)^2\left(3/2S(S+1)\sqrt[3]{\pi}\right)^{3/2} + O\left(q^{-5/2}\right)\right\}$$

▷ Can interpret dependence of summand on q and j via addition of q classical vectors

Conclusions

Discussion

Agrees with known results

▷ Simple $q=2$, $S=\frac{1}{2}$ case: $\quad Z = 1 + 3e^{-\beta J}$

▷ Quantum addition of angular momentum - up to $q=6$

▷ Tabulated literature results

▷ Highly degenerate ground state for large q

e.g. $g_0 = 9\;694\;845$ for $q=30$, $S=\frac{1}{2}$

Have sidestepped spin path integral problem of significant contribution from discontinuous and non-differentiable paths

Further work:

▷ Applying technique to a lattice

Overview

Frustrated cluster - q identical spins

↓ Hubbard-Stratonovich transformation

Evolution of single spin in stochastic magnetic field

(Langevin equations)

↓ Gaussian average

Deterministic evolution of probability on SU(2)

(Fokker-Planck equations)

↓ Solution known

Explicit form for partition function - arbitrary q, S and T

Address for correspondence: Rudolf Peierls Centre for Theoretical Physics, 1 Keble Road, Oxford, OX1 3NP, United Kingdom. Email: `patrick dot hogan at physics dot org`