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Path integrals, diffusion on $SU(2)$ and the fully frustrated antiferromagnetic spin cluster

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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 of geometrically frustrated spin systems. Using a Hubbard–Stratonovich transformation to decouple the interactions, the Boltzmann factor for the spin cluster is written in terms of the time-evolution operator for a single spin in a stochastically varying magnetic field. The time-evolution operator follows a random walk in $SU(2)$: by switching from a Langevin to a Fokker–Planck description of this walk and computing the probability distribution of its end-point, we arrive at an expression for the partition function as a finite sum of single integrals. The calculation provides an analytically tractable illustration of the auxiliary field approach, as used in quantum Monte Carlo calculations, and may potentially be extended to treat more complex frustrated spin systems.

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1. Introduction

In this paper we study the fully frustrated quantum antiferromagnetic spin cluster, consisting of an arbitrary number q of spins, each of magnitude S , with equal antiferromagnetic Heisenberg interactions of strength J between all pairs. The Hamiltonian for the cluster (dropping an additive constant) is

$$\hat{\mathcal{H}} = \frac{1}{2}J \left(\sum_{i=1}^q \hat{\mathbf{S}}_i \right)^2 \equiv \frac{1}{2}J \hat{\mathbf{S}}_i^2. \quad (1)$$

We focus on computation of the partition function. While there is an obvious and elementary way to do this, using addition of angular momentum to calculate the eigenvalues of $\hat{\mathbf{S}}_i^2$ and their degeneracies, our interest is instead to use the problem as a simple illustration of an

approach to frustrated spin systems which we believe is new and which we hope may be useful more generally. This approach is the quantum version of that used previously [1] to study order-by-disorder in the corresponding classical problem.

An outline of the paper is as follows. Our starting point, in section 2, is the coherent-state path integral for the partition function [2, 3]. We use a Hubbard–Stratonovich transformation to decouple the exchange interactions, obtaining a functional integral over the Hubbard–Stratonovich field. The integrand involves the time-evolution operator for a single spin, in which the Hubbard–Stratonovich field couples to the spin as a time-dependent magnetic field. In section 3 we show that this evolution operator follows a random walk on $SU(2)$. Averaging over configurations of the field, we derive Langevin and Fokker–Planck equations to describe this random walk. Since the eigenfunctions of the Laplacian on $SU(2)$ are known, the Fokker–Planck equation can be solved. From it, we obtain in section 4 an expression for the partition function of the spin cluster as a finite sum of single integrals. We check the results in special cases and examine asymptotics for large q .

Our approach differs from established treatments of quantum spin systems using Hubbard–Stratonovich fields [4–8] in the sense that the fields are associated not with individual spins but with each coupled set of spins—in our case, the entire cluster. In this sense, our calculation is an illustration of the auxiliary field method, developed in the context of quantum Monte Carlo simulations [9, 10]. While our hope is that the route we take will also be useful for studying geometrically frustrated antiferromagnets built from corner-sharing spin clusters [11, 12], such extensions are left for future work; we note that results for a single cluster have been used to develop mean field theories for frustrated antiferromagnets which reproduce some thermodynamic quantities quite successfully [13–15].

2. The partition function as a path integral

The partition function for the cluster is

$$\begin{aligned} Z &= \text{Tr} e^{-\beta \hat{\mathcal{H}}} \\ &= \left(\frac{2S+1}{4\pi} \right)^q \int d\Omega \langle \Omega | \exp \left\{ -\frac{1}{2} \beta J \hat{\mathbf{S}}_t^2 \right\} | \Omega \rangle, \end{aligned} \quad (2)$$

where the many-spin coherent state is given by the product of single-spin coherent states, $|\Omega\rangle = \prod_{i=1}^q |\Omega_i\rangle$. Making a Hubbard–Stratonovich transformation, the Boltzmann factor takes the form

$$\exp \left\{ -\frac{1}{2} \beta J \hat{\mathbf{S}}_t^2 \right\} = \int \mathcal{D}\mathbf{h}(\tau) \exp \left\{ -\int_0^\beta d\tau \left(\frac{1}{2J} \mathbf{h}^2(\tau) + i\mathbf{h}(\tau) \cdot \hat{\mathbf{S}}_t \right) \right\}. \quad (3)$$

Now consider the time-evolution operator, $\hat{\mathcal{T}}(t)$, for a single spin of magnitude S in a time-dependent magnetic field $\mathbf{h}(t)$:

$$\hat{\mathcal{T}}(t) = \mathcal{T} \exp \left\{ -i \int_0^t d\tau \mathbf{h}(\tau) \cdot \hat{\mathbf{S}} \right\} \quad (4)$$

where \mathcal{T} is the time-ordering operator and \hbar has been set to unity. This evolution operator belongs to a $(2S+1)$ -dimensional representation of $SU(2)$, and is the solution to the Schrödinger equation

$$i\partial_t \hat{\mathcal{T}}(t) = [\mathbf{h}(t) \cdot \hat{\mathbf{S}}] \hat{\mathcal{T}}(t), \quad (5)$$

with the boundary condition $\hat{\mathcal{T}}(0) = \hat{\mathbb{1}}_{2S+1}$. The evolution operator appears as a factor in equation (3): combining ingredients, we have

$$Z = \int \mathcal{D}\mathbf{h}(\tau) \exp \left\{ -\int_0^\beta d\tau \frac{1}{2J} \mathbf{h}^2(\tau) \right\} \cdot \{\text{Tr} \hat{\mathcal{T}}(\beta)\}^q. \quad (6)$$

The path integral that is equation (6) can be interpreted as the average of $\{\text{Tr } \hat{T}(\beta)\}^q$ over stochastic fields $\mathbf{h}(\tau)$, which has a known, Gaussian, distribution. Writing

$$\langle \dots \rangle|_{t=\beta} \equiv \int \mathcal{D}\mathbf{h}(\tau) \dots e^{-\int_0^\beta d\tau \frac{1}{2J} \mathbf{h}^2(\tau)}, \tag{7}$$

we have

$$Z = \langle \{\text{Tr } \hat{T}(t)\}^q \rangle|_{t=\beta}. \tag{8a}$$

To evaluate equation (8a), we examine the variation of $\hat{T}(t)$ with t in more detail. The representation of $SU(2)$ to which $\hat{T}(t)$ belongs may be parametrized by three real coordinates. We initially denote these coordinates by \mathcal{Q} ; later we make use of two alternative specific choices: either Euler angles or a rotation axis and angle. Through equation (5), these coordinates evolve differently in time for each different realization of $\mathbf{h}(t)$, and so we may write them as functionals of these fields, $\mathcal{Q} = \mathcal{Q}([\mathbf{h}]; t)$. However, to evaluate the partition function using equation (6), only knowledge of the endpoint of this evolution, at time $t = \beta$, is required. Hence the functional integral in equation (8a) reduces to a triple integral over \mathcal{Q} , weighted by the probability density for paths on $SU(2)$ to arrive at \mathcal{Q} . We denote this probability density by $P(\mathcal{Q}; t)$. Translating in this way from a stochastic (Langevin) to a deterministic (Fokker–Planck) description allows us to rewrite the path-integral partition function simply as an integral over the group parameters \mathcal{Q} ,

$$Z = \int d\tau_{\mathcal{Q}} P(\mathcal{Q}; t) \{\text{Tr } \hat{T}(\mathcal{Q}; t)\}^q|_{t=\beta}, \tag{8b}$$

where now $\mathcal{Q} = \mathcal{Q}(t)$ only. It remains to find the probability distribution $P(\mathcal{Q}; t)$.

3. Diffusion on $SU(2)$

We begin by describing the evolution of $\hat{T}(\mathcal{Q}; t)$ with t using the Euler-angle parametrization of $SU(2)$, $\mathcal{Q} \equiv (\alpha, \beta, \gamma)$. These coordinates are defined through

$$\hat{T}(\alpha, \beta, \gamma; t) = e^{-i\alpha(t)\hat{S}_3} e^{-i\beta(t)\hat{S}_2} e^{-i\gamma(t)\hat{S}_3}, \tag{9}$$

where the \hat{S}_i are the three $(2S+1)$ -dimensional generators of $SU(2)$, $0 \leq \alpha < 2\pi$, $0 \leq \beta \leq \pi$, $0 \leq \gamma < 4\pi$, and the angle β should not be confused with inverse temperature.

From equation (5) we extract Langevin equations describing the stochastic evolution of the three coordinates in terms of the components $h_i(t)$ of $\mathbf{h}(t)$:

$$\begin{aligned} \dot{\alpha} &= h_1(t)(-\cos \alpha \cot \beta) + h_2(t)(-\sin \alpha \cot \beta) + h_3(t) \\ \dot{\beta} &= h_1(t)(-\sin \alpha) + h_2(t)(\cos \alpha) \\ \dot{\gamma} &= h_1(t)(\cos \alpha \operatorname{cosec} \beta) + h_2(t)(\sin \alpha \operatorname{cosec} \beta). \end{aligned} \tag{10}$$

Using these equations we deduce [16] a Fokker–Planck equation, which describes the time evolution of the probability density $W(\alpha, \beta, \gamma; t)$ over the coordinates α, β and γ on $SU(2)$ (a quantity defined to include the measure, $\sqrt{g} = (16\pi^2)^{-1} \sin \beta$, so that the weight is $W(\alpha, \beta, \gamma; t) d\alpha d\beta d\gamma$):

$$\partial_t W(\alpha, \beta, \gamma; t) = \frac{1}{2} J \cdot \hat{L}_{FP} W(\alpha, \beta, \gamma; t) \tag{11a}$$

where

$$\hat{L}_{FP} = \partial_\beta \sin \beta \partial_\beta \operatorname{cosec} \beta + \operatorname{cosec}^2 \beta [\partial_\alpha^2 + \partial_\gamma^2 - 2 \cos \beta \partial_\alpha \partial_\gamma]. \tag{11b}$$

The corresponding equation satisfied by the scalar, coordinate-invariant probability density $P(\alpha, \beta, \gamma; t) = (\sqrt{g})^{-1} W(\alpha, \beta, \gamma; t)$ is

$$\partial_t P(\alpha, \beta, \gamma; t) = \frac{1}{2} J \cdot \hat{\Delta} P(\alpha, \beta, \gamma; t), \tag{11c}$$

where

$$\hat{\Delta} = \operatorname{cosec} \beta \partial_\beta \sin \beta \partial_\beta + \operatorname{cosec}^2 \beta [\partial_\alpha^2 + \partial_\gamma^2 - 2 \cos \beta \partial_\alpha \partial_\gamma] \quad (11d)$$

is the Laplace–Beltrami operator on $SU(2)$, describing a diffusion process resulting from free Brownian motion on the manifold [17].

The eigenfunctions and eigenvalues of $\hat{\Delta}$ are known [18]: they have the form

$$\hat{\Delta} \mathcal{U}_n = -\lambda_n \mathcal{U}_n, \quad (12)$$

where the $\mathcal{U}_n = D^j(\alpha, \beta, \gamma)_{m'}^m$ are the elements of the $(2j+1)$ -dimensional irreducible representation of $SU(2)$, with $m', m = -j, -(j-1), \dots, (j-1), j$; $\lambda_n = j(j+1)$ and $2j \in \mathbb{Z}_0^+$ (see the appendix for more detail). Thus, the general solution to the Fokker–Planck equation, equation (11), is

$$P(\alpha, \beta, \gamma; t) = \sum_n c_n \mathcal{U}_n e^{-\frac{1}{2} J \lambda_n t} \quad (13)$$

where the expansion coefficients c_n must be chosen to satisfy the initial condition, $\hat{\mathbb{T}}(0) = \hat{\mathbb{1}}_{2S+1}$. Making use of the completeness relation for the irreducible representations (see the appendix), we have

$$c_{jm'm} = (2j+1) \delta_{m'}^m \quad (14)$$

and hence

$$P(\alpha, \beta, \gamma; t) = \sum_j (2j+1) e^{-\frac{1}{2} j(j+1) J t} \sum_{m=-j}^{+j} D^j(\alpha, \beta, \gamma)_{m'}^m. \quad (15)$$

Now the trace of the j th irreducible representation matrix of a group—such as the sum over m in the above probability density—is the character of that representation, $\chi^j(\alpha, \beta, \gamma)$ [18]. Moreover, the character depends only on the total angle of rotation and not on the orientation of the axis about which the rotation occurs. This fact motivates a coordinate transformation to a parametrization that describes a member of $SU(2)$ not by three Euler angles, but instead by the total angle of rotation ψ about an axis defined by a unit vector $\mathbf{n}(\theta, \phi)$. These two parametrizations are related by

$$e^{-i\alpha \hat{S}_3} e^{-i\beta \hat{S}_2} e^{-i\gamma \hat{S}_3} = e^{-i\psi \mathbf{n} \cdot \hat{\mathbf{S}}}, \quad (16a)$$

where the transformation is

$$\begin{aligned} \phi &= \frac{1}{2} (\pi + \alpha - \gamma) \\ \tan \theta &= \frac{\tan(\frac{1}{2}\beta)}{\sin[\frac{1}{2}(\alpha + \gamma)]} \\ \cos \psi &= 2 \cos^2\left(\frac{1}{2}\beta\right) \cos^2\left[\frac{1}{2}(\alpha + \gamma)\right] - 1, \end{aligned} \quad (16b)$$

with normalized measure $(4\pi^2)^{-1} \sin^2(\frac{1}{2}\psi) \sin \theta$, and $0 \leq \phi < 2\pi, 0 \leq \theta \leq \pi, 0 \leq \psi \leq 2\pi$.

As $\chi^j = \chi^j(\psi)$ only, an appropriate choice of axis allows us to write

$$\chi^j(\psi) = \sum_{m=-j}^{+j} e^{-im\psi} = \frac{\sin[(j + \frac{1}{2})\psi]}{\sin(\frac{1}{2}\psi)}. \quad (17)$$

Returning to the partition function, we see that the trace of the evolution operator, $\hat{\mathbb{T}}(Q; t)$, is also a character of $SU(2)$, and so we may write equation (8b) as

$$Z = \int d\tau_{(\psi, \mathbf{n})} \{\chi^S(\psi)\}^q \cdot \sum_j (2j+1) e^{-\frac{1}{2} j(j+1) \beta J} \chi^j(\psi). \quad (18)$$

We note here that Brownian diffusion on hyperspheres has been studied in [19]. Our equation (15) is in agreement with these results specialized to a 3-sphere, which is isomorphic to $SU(2)$.

4. Results

4.1. Integral form

Putting all the pieces together, the partition function for the general spin cluster may be written in a form which allows one to read off the degeneracies associated with each energy level of the system:

$$\begin{aligned}
 Z &= \sum_j e^{-\frac{1}{2}j(j+1)\beta J} \cdot (2j+1) \frac{2}{\pi} \int_0^\pi d\psi \left\{ \frac{\sin[(2S+1)\psi]}{\sin \psi} \right\}^q \sin[(2j+1)\psi] \sin \psi \\
 &\equiv \sum_j e^{-\beta E_j} \cdot g_j
 \end{aligned}
 \tag{19}$$

where, again, $2j \in \mathbb{Z}_0^+$.

Some of the terms in this sum are zero, for one of the two reasons. First, the total spin of the cluster has a maximum value, so that $\hat{\mathbf{S}}_t^2 \leq qS(S+1)$: by making use of the orthogonality relations of either the irreducible representations (see the appendix), or the trigonometric functions in the above integrand, one may deduce that $g_j = 0$ for $j > qS$. Second, the total spin of the cluster is half-integer if S is half-integer and q is odd; otherwise it is integer: by inspecting the symmetries of the integrand, we see that $g_n = 0$ if $(qS + j) \notin \mathbb{Z}_0$. The consequence of this second condition is that only every second term in the sum is non-zero.

The partition function may of course also be computed in an elementary way. To do this one needs the degeneracies g_{S_t} of the eigenstates of $\hat{\mathbf{S}}_t^2$. These degeneracies can be written in terms of the degeneracies $g_{S_t^z}$ of the eigenstates of S_t^z , as $g_{S_t=k} = g_{S_t^z=k} - g_{S_t^z=k+1}$ (see, for example, van Vleck [20]). For the cluster, $g_{S_t^z=k}$ is given by the appropriate coefficient in the expansion of

$$\left\{ \sum_{m=-S}^{+S} e^{im\varphi} \right\}^q = \sum_{k=-qS}^{+qS} g_{S_t^z=k} e^{ik\varphi},
 \tag{20}$$

which can be picked out by multiplying the above expression by $e^{-ik\varphi}$ and integrating over the range $0 \leq \varphi < 2\pi$. The resultant expression for $g_k = (2k+1) \cdot g_{S_t=k}$ is exactly that in equation (19).

4.2. Computation of degeneracies

The integral in equation (19) can be reduced to a sum of residues:

$$g_j = \sum_{\substack{k=0 \\ p \geq 0}}^q \frac{(2j+1)q!(-1)^{k+1}}{2 \cdot k!(q-k)!} \cdot \frac{1}{p!} \frac{d^p}{dz^p} \frac{z^{4j+2} - 1}{(z^2 - 1)^{q-1}} \Big|_{z=0}
 \tag{21}$$

where $p = 2j + 2k(2S + 1) - 2q(S + 1) + 2$. This form has the advantage of being computationally much more efficient to evaluate than equation (19).

For some specific instances further simplification is possible—for example, for $q = 2r$, where r is integer, and $S = \frac{1}{2}$ the zero-energy state has degeneracy $g_0 = 2^r(2r-1)!/(r+1)!$. Further specific cases provide checks of equation (19), including the ground-state degeneracies

deduced by the quantum addition of angular momentum for $q \leq 6$; and results in the literature tabulated for particular q and S [14, 15].

4.3. Asymptotics

The behaviour of the partition function for large q at fixed j and S may be found from equation (19) using steepest descents

$$g_j = (2S + 1)^q (2j + 1)^2 3\sqrt{3} [2\sqrt{3}\pi S(S + 1)]^{-3/2} q^{-3/2} + O(q^{-5/2}). \quad (22)$$

This result may be interpreted by considering the addition of q classical vectors of length $\sqrt{S(S + 1)}$, as follows. First, examining terms on the right-hand side of equation (22), we note that since the total number of states for the quantum system is $(2S + 1)^q$, the remaining factor is the normalized fraction of states having a given value of j . To compute the equivalent from addition of classical vectors, we should evaluate

$$P(\mathbf{r}) = [4\pi S(S + 1)]^{-q} \prod_{i=1}^q \int d^3 \mathbf{S}_i \delta(|\mathbf{S}_i| - \sqrt{S(S + 1)}) \delta\left(\mathbf{r} - \sum_{j=1}^q \mathbf{S}_j\right). \quad (23a)$$

At large q , this gives

$$P(\mathbf{r}) = 3\sqrt{3} [2\pi S(S + 1)]^{-3/2} q^{-3/2} \exp\left\{-\frac{3r^2}{2qS(S + 1)}\right\} + O(q^{-5/2}). \quad (23b)$$

With the replacement $r = j + \frac{1}{2}$, the value of $P(\mathbf{r}) \cdot 4\pi r^2$ for large q at fixed j and S is in exact agreement with the expression for $(2S + 1)^{-q} g_j$ from equation (22). We note that similar distributions of numbers of states arise in work on the statistical distribution of angular momentum states in systems of interacting fermions [21–23].

5. Discussion

We have presented here a new approach for studying a fully frustrated quantum antiferromagnetic spin cluster, and have used it to calculate an explicit, closed and general expression for the cluster's partition function as a finite sum of single integrals. While, as indicated above, the results can also be obtained by elementary means, we believe that the approach is of interest in its own right, for several reasons. It provides a tractable illustration of the use of auxiliary fields in a path-integral calculation, complementing numerical applications [9, 10]. Here the correspondence is that a distribution equivalent to our $P(\mathcal{Q}; t)$ is generated using Monte Carlo sampling, and weighted with an equivalent to the factor $\{\text{Tr} \hat{T}(\mathcal{Q}; t)\}^q$ that appears in equation (8b). The sign problem in quantum Monte Carlo calculations is demonstrated by the fact that our weighting function is oscillatory for odd q . Our approach is, at least formally, straightforwardly generalized to deal with a geometrically frustrated spin system consisting of many corner-sharing clusters. In this case a Hubbard–Stratonovich field is associated with each cluster and the time-evolution operators for different spins are not identical, as in our treatment of a single cluster, but have partial correlations. The price, of course, is that the Fokker–Planck operator is much more complicated in this case than for a single cluster, and can presumably only be studied approximately. A striking feature is that the size S of spins enters the calculations only at a later stage, when evaluating the integrals on \mathcal{Q}_i for each spin i in the analogue of equation (8b), while the Fokker–Planck operator \hat{L} itself is independent of S . A consequence of this is that, for a given lattice, all eigenvalues of the spin Hamiltonian, taken for every S , must belong to the spectrum of \hat{L} . Fixing S and integrating on \mathcal{Q}_i projects out the relevant subset.

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Appendix. Properties of the irreducible representations of $SU(2)$

In this appendix, we summarize some standard results (see, for example, [18]) that we use in this paper.

The matrix elements $D^j(\alpha, \beta, \gamma)_{m'}^m$ of the j th irreducible representation of $SU(2)$ —which is of dimension $(2j + 1)$, with $2j \in \mathbb{Z}_0^+$ —are written in various ways, following many different conventions. We adopt the widely used Condon–Shortley convention, and in the Euler-angle parametrization we write

$$D^j(\alpha, \beta, \gamma)_{m'}^m = e^{-i\alpha m'} d^j(\beta)_{m'}^m e^{-i\gamma m}, \quad (\text{A.1a})$$

where

$$d^j(\beta)_{m'}^m = \left[\frac{(j+m')!(j-m')!}{(j+m)!(j-m)!} \right]^{\frac{1}{2}} \cos^{m+m'} \left(\frac{1}{2}\beta \right) \sin^{m-m'} \left(\frac{1}{2}\beta \right) P_{j-m'}^{m'-m, m'+m}(\cos \beta), \quad (\text{A.1b})$$

and $P_l^{a,b}(x)$ are the Jacobi polynomials, with $m', m = -j, -(j-1), \dots, (j-1), j$.

On the $SU(2)$ group manifold, for a given parametrization \mathcal{Q} and an invariant integration measure $d\tau_{\mathcal{Q}}$, these irreducible representations are orthogonal,

$$(2j+1) \int d\tau_{\mathcal{Q}} D_j^\dagger(\mathcal{Q})_{m'}^m D_j^j(\mathcal{Q})_{m'}^n = \delta_j^{j'} \delta_{m'}^m \delta_n^{n'}, \quad (\text{A.2})$$

and complete,

$$\sum_{jmn} (2j+1) D_j^j(\mathcal{Q})_{m'}^m D_j^\dagger(\mathcal{Q}')_{m'}^n = \delta(\mathcal{Q} - \mathcal{Q}'), \quad (\text{A.3})$$

where $D_j^\dagger(\mathcal{Q})_{m'}^m = [D_j^j(\mathcal{Q})_{m'}^m]^*$. The above Dirac-delta function must be suitably defined on the manifold—for example, in the Euler-angle parametrization,

$$\delta(\mathcal{Q} - \mathcal{Q}') = 16\pi^2 \delta(\alpha - \alpha') \delta(\cos \beta - \cos \beta') \delta(\gamma - \gamma'). \quad (\text{A.4})$$

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