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The fluctuating surface Hamiltonian for the classical Kagomé antiferromagnet

E F Shender†§ and P C W Holdsworth‡

† Department of Physics, University of California, Berkeley, CA 94720, USA
‡ Laboratoire de Physique Théorique ENSLAPP, URA 14-26 du CNRS, Ecole Normale Supérieure de Lyon, 69634 Lyon, France

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Abstract. Integrating over spin wave degrees of freedom, we derive the effective Hamiltonian to describe the problem of the classical Kagomé antiferromagnet in relevant variables. The intrinsically anharmonic character of this Hamiltonian, and the coupling between the continuous and discrete degrees of freedom contained within it, puts it into a completely new class of problem: that of highly fluctuating surfaces, for which the Hamiltonian gives a rigorous description of the thermodynamic properties at low T.

Heisenberg spin systems with non-trivial infinite degeneracy of the classical ground state have recently become fashionable. The classical ground states form a connected surface in phase space on which the system can move without crossing energy barriers. Correspondingly the harmonic excitation spectrum contains modes of zero frequency over and above the conventional Goldstone mode (for a recent review see [1]). Fluctuations can remove the degeneracy, at least partially: an effect known as 'order by disorder' [2, 3, 4]. The most interesting systems are those where the number of zero modes is macroscopic, that is proportional to the number of spins N [5, 6]. In this case perturbation theory in the fluctuations breaks down and we can expect to find a novel magnetic behaviour. The best studied experimental examples of such systems are the Kagomé [7] and pyrochlore [8] antiferromagnets. Experiments on these systems show no magnetic ordering transition down to temperatures much lower than the Curie–Weiss temperature θ justifying the term 'collective paramagnet' introduced by Villain [9]. At very low temperatures glassy behaviour is observed.

It has been shown [6] that thermal fluctuations in the classical Kagomé antiferromagnet preferentially select states with coplanar spin orientations. These states are the softest, in the sense that they have the maximum number of zero harmonic modes. The number of such coplanar states is proportional to $\exp(\alpha N)$, α being a numerical constant. The statistical weights of these planar states all have the same power law dependence on temperature [6] and they differ only in their numerical coefficients. Evidence from series expansions [5] and from simulations [6, 10, 11] suggests that a state with 3-sublattice Néel magnetic order, the so-called $\sqrt{3} \times \sqrt{3}$ state has the largest weight. However neither this state nor any finite number of states can be considered as selected. Typical snapshots of instantaneous configurations showed [11] that the system consists of domains of different $\sqrt{3} \times \sqrt{3}$ states. We interpreted this as follows: as the statistical weights of each coplanar state have the

§ Also at Institute of Nuclear Physics, St Petersburg, Russia.

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same temperature dependence, the free energy cost of creating a domain in the $\sqrt{3} \times \sqrt{3}$ state is simply given by $\Delta f \sim LT$, where L is the length of the domain boundary. Hence the probability of creating a particular domain is temperature independent and decreases exponentially with L for large L. However the number of possible domain boundaries (loops) of a given length increases, as a function of L, in an exponential manner, which in principle could compensate this small probability and lead to long loops, even at low temperature. Domains of other types of coplanar state are in principle possible, although they are not observed in the simulations. Thus, calculating any Gibbs average we need to sum over all coplanar states rather than only taking into account the contribution of the $\sqrt{3} \times \sqrt{3}$ state and those slightly distorted from it.

The zero modes are the decisive element leading to the novel thermodynamic behaviour; however there are also conventional acoustic spin wave excitations in the system. They play the role of 'fast motion' for this problem and there is a temptation to integrate over them, arriving at an effective Hamiltonian for the relevant variables only [12], i.e. for those variables associated with the zero modes. In doing this we do not make any assumption about the selection of specific coplanar states, rather the part of phase space where our effective Hamiltonian operates includes all coplanar states and those states slightly distorted from them. Strongly non-coplanar states are of no importance for the thermodynamics since their statistical weights are smaller in powers of T.

Following [6] we can expand the classical Hamiltonian in spin deviations from a coplanar state. At each site, i, we choose right-handed axes in spin space with $\hat{z}_i$ parallel to the unit vector S_i in the particular ground state, and all $\hat{y}_i$ perpendicular to the ground state spin plane and mutually parallel. With spin orientations parametrized by $S_i = (\epsilon_i^x, \epsilon_i^y, 1 - \alpha_i)$, and α_i determined from $|S_i| = 1$, the Hamiltonian becomes $H = H_0 + \sum_{n \geq 2} H_n$, where $H_n \sim O(\epsilon^n)$. Specifically we find

$$H_2 = (J/2)[(3\delta_{ij} - M_{ij})\epsilon_i^x \epsilon_j^x + 2M_{ij}\epsilon_i^y \epsilon_j^y] \tag{1}$$

where we use a summation convention and define the matrix $\mathbf{M}$ as $M_{ii} = 1$; $M_{ij} = \frac{1}{2}$ if i, j are nearest-neighbour sites; $M_{ij} = 0$ otherwise. J is the nearest-neighbour exchange constant.

The anharmonic parts of the Hamiltonian are

$$H_3 = \frac{J\sqrt{3}}{4} \sum_{\langle i,j \rangle} \sigma_{ij}((\epsilon_i^y)^2 \epsilon_j^x - (\epsilon_j^y)^2 \epsilon_i^x) \tag{2}$$

$$H_4 = \frac{J}{16} \sum_{\langle i,j \rangle} ((\epsilon_i^y)^2 - (\epsilon_j^y)^2)^2 \tag{3}$$

where σ_{ij} is the chirality

$$\sigma_{ij} = \frac{2}{\sqrt{3}} \hat{x}_i \cdot \hat{z}_j \tag{4}$$

and is defined as $+1$ (-1) if spin S_i must be rotated clockwise (anticlockwise) to lie in the direction of S_j. We omitted from H_4 terms proportional to $(\epsilon^x)^4$ and $(\epsilon^x)^2(\epsilon^y)^2$, as they give corrections to the thermodynamic functions that are of higher order in temperature. The Hamiltonian H_4, like H_2, is independent of the coplanar state being considered [6, 13]. H_3, which describes the coupling between the spin waves and the zero modes, does depend on the specific states through the variables σ_{ij}. There is no interaction in H_3 between the zero modes as no term proportional to $(\epsilon^y)^3$ is possible because of symmetry factors.

Once in Fourier space the part of H_2 concerning the in-plane spin deviations ϵ^x is diagonalized by the linear transformation from the ϵ^x variables to the normal mode variables $E^x_\alpha(k)$

$$\epsilon^x_\mu(k) = \sum_{\alpha=1}^{3} C_{\mu\alpha}(k) E^x_\alpha(k) \tag{5}$$

where indices $\mu = 1, 2, 3$ are for the three sites in the Kagomé lattice unit cell with coordinates $r_1 = (a, 0), r_2 = (a/2, -\sqrt{3a/2}), r_3 = (0, 0)$. Values of the eigenvalues and normalized eigenvectors may be easily obtained, as in [5, 6]

$$\lambda_1(k) = 3 \qquad \lambda_{2,3}(k) = \frac{3}{2} \pm \frac{1}{2}\sqrt{4(\cos^2(k_1) + \cos^2(k_2) + \cos^2(k_{12})) - 3} \tag{6}$$

$$C_{m\mu} = \begin{pmatrix} C_{\mu 1} \\ C_{\mu 2} \\ C_{\mu 3} \end{pmatrix} = \frac{1}{N_\mu} \begin{pmatrix} \cos(k_1)\cos(k_{12}) + (2 - \lambda_\mu)\cos(k_{12}) \\ (2 - \lambda_\mu)^2 + \cos^2(k_1) \\ \cos^2(k_1)\cos^2(k_{12}) + (2 - \lambda_\mu)\cos(k_2) \end{pmatrix} \tag{7}$$

where $k_1 = k_x a$, $k_2 = (k_x a - \sqrt{3}k_y a)/2$, $k_{12} = k_1 a - k_2 a$ and the normalizing factors N_μ are

$$\begin{aligned} N_1 &= \sin(k_1)\sqrt{2\ (1 - \cos(k_1)\cos(k_2)\cos(k_{12})} \\ N_2 &= \left(\lambda_3^2(k)(1 + \cos^2(k_{12}) + \cos^2(k_2)) - N_1^2\right)^{1/2} \\ N_3 &= \left(\lambda_2^2(k)(1 + \cos^2(k_{12}) + \cos^2(k_2)) - N_1^2\right)^{1/2}. \end{aligned} \tag{8}$$

The part of H_2 containing the out-of-plane spin deviations ϵ_y can be diagonalized by the same transformation by substituting $\lambda^y_\mu(k) = 2(3 - \lambda_\mu(k))$ for the $\lambda_\mu(k)$ defined in equation (6). One can see that $\lambda^y_1(k) = 0$ for all k, which gives the branch of zero modes in the harmonic spectrum.

Integrating $\exp(-\beta(H))$ over all $E^x_\alpha(k)$, and over $E^y_\alpha(k)$ with $\alpha = 2, 3$ we arrive at an effective Hamiltonian containing the slow degrees of freedom, $E^y_1(k)$, only. In performing these integrals we can neglect, to leading order in T, all the anharmonic terms in H which do not contain $E^y_1(k)$; we find

$$\begin{aligned} H_{\text{eff}} &= H_4 + \tilde{H}_{\text{eff}} \\ \tilde{H}_{\text{eff}} &= -\frac{J}{8} \sum_{\substack{R_\alpha, R'_{\alpha'} \\ \rho_\beta, \rho'_{\beta'}}} T^{\alpha'\beta'}\left(R'_{\alpha'} - \rho'_{\beta'}\right)\left(e^y_{R_\alpha}\right)^2 (e^y_{\rho_\beta})^2 \sigma_{(R_\alpha, R'_{\alpha'})} \sigma_{(\rho_\beta, \rho'_{\beta'})} \end{aligned} \tag{9}$$

where the tensor $T^{\alpha'\beta'}(r)$ is

$$T^{\alpha'\beta'}\left(R'_{\alpha'} - \rho'_{\beta'}\right) = \frac{3}{4} \sum_{\substack{\mu=1,2,3 \\ k}} \frac{1}{\lambda_\mu(k)} C_{\mu\alpha'}(k) C_{\mu\beta'}(k) \cos(k \cdot (R'_{\alpha'} - \rho'_{\beta'})). \tag{10}$$

$R_\alpha, R'_{\alpha'}, \rho_\beta, \rho'_{\beta'}$ run over all the sites of the Kagomé lattice, $R_\alpha = R + r_\alpha$, where R is the coordinate of the unit cell, and r_α the coordinate of the site within the cell. Pairs of coordinates for the chirality (for example $\left(R_\alpha, R'_{\alpha'}\right)$ are nearest neighbours. The $e^y_{R_\alpha}$ are the parts of the ϵ^y variables associated with the zero modes only:

$$e^y_{R_\alpha} = \frac{1}{\sqrt{N}} \sum_k e^y_\alpha(k) e^{-i(k \cdot R_\alpha)} \qquad e^y_\alpha(k) = C_{\alpha 1}(k) E^y_1(k). \tag{11}$$

Correspondingly, one should retain only the terms stemming from the $e^y_{R_\alpha}$ variables in the H_4 appearing in equation (9). The calculation of the partition function from the

effective Hamiltonian for zero modes presented above implies integrating over all continuous variables $E_1^{\gamma}(k)$ and summing over all allowed sets of chiral variables σ.

The principal feature of H_{eff} is the absence of an 'elastic' quadratic term, with leading terms being quartic. There are two kinds of quartic term in H_{eff}. The first, appearing in H_4 only, is independent of the chiralities and therefore identical for each coplanar state. The second type includes a coupling between the $(e^{\gamma})^4$ and products of chiralities, and is therefore different for each coplanar state. It is this kind of term that leads to unequal statistical weights for different coplanar states.

The matrix elements $T^{\alpha'\beta'}(r)$, which come from this second type of term, are long ranged and oscillate in sign leading to highly frustrated couplings between the σ variables. At large distance between two bonds the leading contribution to $T^{\alpha'\beta'}(r)$ comes from the term with $\mu = 3$, as $\lambda_3(k) \sim k^2$ for small k, and provides a Coulomb-like fall in $T^{\alpha'\beta'}(r)$ with distance. The long-range, frustrated couplings are consistent with a system that remains strongly fluctuating in the limit of T going to zero, and for which no single long-range ordered state is preferred. That is, a model with short-range coupling between the chirality variables would lead to long-range order in the limit of T going to zero. In the simplest case, where the interaction is limited to nearest neighbours, either the $\sqrt{3} \times \sqrt{3}$, or a second Néel ordered state, the $q = 0$ state [5] would be selected, depending on the sign of the coupling. With the present H_{eff} no such such conclusion can be reached, and a consistent treatment represents a formidable problem.

Together with Cherepenov and Berlinsky we recently presented a way of visualizing the ground state manifold, by mapping the plane formed by the spins in each triangle of the Kagomé lattice onto a rigid equilateral triangle [14]. The triangles form a membrane surface, and each ground state can be represented by a configuration of the triangulated surface in a three-dimensional phase space. The effective Hamiltonian (9,10) can be considered as a generalization of this mapping. Order by disorder selection of the coplanar spin states means that we are principally concerned with the coplanar configurations of the membrane, and with small fluctuations away from these states. The intrinsically anharmonic character of H_{eff}, and the coupling between the continuous and discrete degrees of freedom contained within it puts the classical Kagomé antiferromagnetic into a completely new class of problems; that of highly fluctuating surfaces, for which the Hamiltonian H_{eff} gives a rigorous description of the thermodynamic properties at low T.

The summation over different sets of σ, that is over different coplanar states, is a vital ingredient in the calculation of the partition function. From simulations [6, 11] and the qualitative arguments presented above it is therefore clear that we cannot restrict ourselves to fluctuations around a single coplanar state. The latter procedure is exactly that of a mean-field theory [13] for our Hamiltonian H_{eff}: the integration over the continuous variables is done for a fixed set of chiralities, that is, a local partition function is calculated for fluctuations around a single coplanar state. In this approximation the free energy is then the sum of the logarithms of such states. Such a procedure completely ignores the possibility of large fluctuations between different coplanar states, with the result that in the limit of $T \to 0$ the state with the lowest local free energy would be uniquely accepted. To perform the integration the product of four continuous e_{γ} variables is decoupled, with one pair of variables being replaced by its thermal average.

Within the mean-field formalism the anharmonicity gives rise to a linear dispersion with the spin wave velocity proportional to a power of temperature. The result means that anharmonicity effectively restores a non-zero elasticity for spin motion corresponding to the zero mode. This leaves an extremely interesting problem, as we see no reason why the result should hold in a rigorous theory. As is usually the case in strongly fluctuating non-

perturbative systems, the self-energy should be renormalized into a non-analytic function of variables, leading to overdamped excitations and a non-analytic dispersion for the zero modes.

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