CLRC

Technical Report
RAL-TR-96-058

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July 1996

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ISSN 1358-6254

Quantum Effects in two-dimensional Magnetic Systems

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Abstract

The main features of the application of the *pure-quantum self-consistent harmonic approximation* (PQSCHA) to the study of two-dimensional (2d) magnetic systems are briefly reviewed; particular attention is given to how the symmetry of the system affects the actual implementation of the method. Detailed results for the 2d Heisenberg antiferromagnet (HAF) are shown and compared with experimental data and theoretical results from different approaches.

1 Introduction

We consider the class of models described by the Hamiltonian

$$\hat{\mathcal{H}} = \tfrac{1}{2}\, J \sum\nolimits_{\langle ij\rangle} \left(\hat{S}^x_i\hat{S}^x_j + \hat{S}^y_i\hat{S}^y_j + \lambda\hat{S}^z_i\hat{S}^z_j\right) , \tag{1}$$

where i and j run over the sites of a two-dimensional square-lattice, and the sum is over nearest-neighbours. The quantum mechanical operators $\hat{\boldsymbol{S}}_i$ satisfy $[\hat{S}^\alpha_i, \hat{S}^\beta_j] = \delta_{ij}\epsilon^{\alpha\beta\gamma}\hat{S}^\gamma$ and $|\hat{\boldsymbol{S}}_i|^2 = S(S{+}1)$.

Eq. (1) describes systems whose behaviour can be utterly different depending on the value of the exchange anisotropy λ as well as on the sign of the exchange integral J. Both ferro- ($J{<}0$) and antiferromagnets ($J{>}0$) can be classified as *easy-plane* ($0{\le}\lambda{<}1$), *easy-axis* ($\lambda{>}1$) or *isotropic* ($\lambda{=}1$); models belonging to different classes, *i.e.* with different symmetries, may require a differentiated treatment even though studied by the same method. This is also the case of the PQSCHA method, as the spin-boson transformation which constitutes the first step towards the evaluation of the effective Hamiltonian (see Ref. [1]), must be carefully chosen in order to sensibly implement the method itself.

But where does this choice turn out to be fundamental? We know that, in order to carry out the complete PQSCHA renormalization of the Hamiltonian, the Weyl symbol of its bosonic form has to be a well behaved function in the whole phase-space. Spin-boson transformations, on the other hand, can introduce singularities (in the derivatives), as a straightforward consequence of the topological difficulties in mapping a spherical phase-space into a flat one. The choice of the transformation has then to be made trying to let the singularities to occur only when the system is in those configurations which are not thermodynamically relevant, so to make possible a physically sound approximation when using the transformation itself. Most of the methods for studying magnetic systems at finite temperature do in fact share this problem with the PQSCHA; what makes the difference is that by using the PQSCHA one separates the classical from the pure-quantum contribution to the thermal fluctuations, and the approximation only regards the latter, as the former is exactly considered as far as one can cast the effective Hamiltonian in the final form of a classical spin Hamiltonian. This is indeed a crucial point, as we will see in the specific application to the 2d-HAF.

2 Spin-boson transformations

Consider now the case $0\leq\lambda<1$: the easy-plane character of the model suggests to make use, for each spin operator, of the Villain transformation

$$\hat{S}^z = \hat{p}~, \qquad \hat{S}^+ = e^{i\hat{q}}\,\sqrt{\widetilde{S}^2 - (\hat{p}+\tfrac{1}{2})^2}~, \qquad \hat{S}^- = (\hat{S}^+)^\dagger~, \tag{2}$$

to canonically conjugate operators $[\,\hat{q},\hat{p}\,] = i$, with $\widetilde{S} \equiv S + \frac{1}{2}$; this transformation keeps the O(2) symmetry in the easy-plane, meanwhile allowing to deal with the square root in terms of a physically sensible small$-\hat{p}$ approximation.

In the easy-axis case ($\lambda > 1$) it makes no sense to use Eqs. (2), as the expectation value of the z-component of each spin is now substantially different from zero. On the other hand, the Holstein-Primakoff (HP),

$$\hat{S}^z = \widetilde{S} - \hat{z}^2~, \qquad \sqrt{2}\,\hat{S}^+ = \sqrt{S+\widetilde{S}-\hat{z}^2}\,(\hat{q}+i\hat{p})~, \qquad \hat{S}^- = (\hat{S}^+)^\dagger~, \tag{3}$$

and Dyson-Maleev (DM),

$$\hat{S}^z = \widetilde{S} - \hat{z}^2~, \qquad \sqrt{2}\,\hat{S}^+ = \hat{q}+i\hat{p}~, \qquad \sqrt{2}\,\hat{S}^- = (\hat{q}-i\hat{p})\,(S+\widetilde{S}-\hat{z}^2)~, \tag{4}$$

with $\hat{z}^2 \equiv (\hat{q}^2+\hat{p}^2)/2$, do both suggest the z-component to be privileged for alignment, thus fitting nicely to the easy-axis case. A few words have to be spent to clarify the relation between the HP and the DM transformation before considering the isotropic case, where both of them can be used. Eqs. (3) contains a square root that we cannot deal with unless introducing an approximation of small $\hat{z}^2$. After having checked whether or not such an approximation is reasonable (which is the case for the easy-axis models), we still have to face ordering problems so to find the explicit expression of the Weyl symbol of the Hamiltonian, as requested by the

PQSCHA according to Ref. [1]. The Dyson-Maleev transformation seems much simpler, as it is normally ordered and does not contain square roots; as a counterpart to these nice properties, however, Eqs. (4) do not represent a hermitean transformation and do not take into account the kinematic interaction, allowing $\hat{S}^z$ to be smaller than $-S$. To avoid considering unphysical states, one can make use of a proper projection operator [4] whose insertion does actually bring back, though in a slightly different form, the very same problems affecting the HP.

3 Isotropic model

When λ=1 Eq. (1) can be written in the isotropic form of the two-dimensional Heisenberg model

$$\hat{\mathcal{H}} = \tfrac{1}{2} J \sum_{\langle ij \rangle} \hat{\boldsymbol{S}}_i \cdot \hat{\boldsymbol{S}}_j \; . \tag{5}$$

Like in the easy axis case, it makes no sense to use the Villain transformation for an isotropic model; at variance with the easy-axis case, however, also the HP and DM transformations seem to be unsuitable now, as they both break the full $\mathcal{SU}(2)$ symmetry of Eq. (5). At T=0 this is not a problem, as the ground state is ordered by spontaneous symmetry breaking (though the case $S=\frac{1}{2}$, $J>0$ is not yet fully understood). At finite temperature the ordered ground state is unstable against low-wavevector thermal excitations which are indeed responsible for the symmetry restoration, *i.e.* the vanishing of the (staggered) magnetization of the 2d Heisenberg (anti)ferromagnet. As T increases, these excitations' character becomes more and more classical, which means, as pointed out in the previous section, that the PQSCHA takes them into account more and more accurately, no matter what transformation has been used or what further approximation introduced to deal with the transformation itself. This means, as we eventually reconstruct the effective Hamiltonian in the form of a spin-Hamiltonian, that we can safely use the HP or DM transformations for any value of temperature.

Making use of the DM transformation and following the procedure described in [1] and [2], we find the effective Hamiltonian to be

$$\mathcal{H}_{\rm eff} = \tfrac{1}{2} J\widetilde{S}^2\theta^4 \sum_{\langle ij \rangle} \boldsymbol{s}_i \cdot \boldsymbol{s}_j + NJ\widetilde{S}^2\mathcal{G}(t) \; . \tag{6}$$

where $\widetilde{S} \equiv S + \frac{1}{2}$ is the 'classical spin length' [1] and $\boldsymbol{s}_i$ are unit vectors; the term $\mathcal{G}(t) = tN^{-1}\sum_k \ln[\sinh f_k/(\theta^2 f_k)] - 2\theta^2\mathcal{D}$ only depends upon the dimensionless temperature $t \equiv T/J\widetilde{S}^2$, and $\theta^2 \equiv 1 - \mathcal{D}/2$ embodies the effect of pure-quantum fluctuations through the parameter

$$\mathcal{D} = (N\widetilde{S})^{-1} \sum_k \sqrt{1-\gamma_k^2}\, (\coth f_k - f_k^{-1}) \; , \tag{7}$$

with $\gamma_k = (\cos k_x + \cos k_y)/2$, and $f_k = \omega_k/(2\widetilde{S}t)$. Our last step is now to evaluate the frequencies ω_k; we recall that, as we are dealing with a system with many degrees of freedom, in order to solve the self-consistent equations eventually leading to the renormalization coefficients, we have to introduce a further Low Coupling

Approximation (LCA) to avoid the PQSCHA frequencies $\omega_k(\boldsymbol{p},\boldsymbol{q})$ to depend on $(\boldsymbol{p},\boldsymbol{q})$ [1]; the usual LCA is obtained by assuming $\omega_k \simeq \omega_k(\boldsymbol{p}_0,\boldsymbol{q}_0)$ where $(\boldsymbol{p}_0,\boldsymbol{q}_0)$ is the minimum configuration of $\mathcal{H}_{\rm eff}$, *i.e.* the configuration of (anti)aligned spins. In the specific case of the isotropic model, however, low energy excitations destabilize the minimum as soon as the temperature is switched on, so that a more refined LCA can be essential for a better description of the low and intermediate temperature regime. As suggested in [3], one could take $\omega_k \simeq \langle\omega_k(\boldsymbol{p},\boldsymbol{q})\rangle_{\rm eff}$, where $\langle\cdots\rangle_{\rm eff}$ is the classical-like average defined by the effective Hamiltonian, but, whenever an analytical expression for $\langle\omega_k(\boldsymbol{p},\boldsymbol{q})\rangle_{\rm eff}$ is not available, the solution of the self-consistent equations prescribed by the PQSCHA remains an almost impossible task. Nevertheless, we can evaluate $\langle\omega_k(\boldsymbol{p},\boldsymbol{q})\rangle_{\rm eff}$ in the framework of a classical SCHA, and, as we know that the classical SCHA on a system whose hamiltonian is $\mathcal{H}_{\rm eff}$ is nothing but the full quantum SCHA on the original system [3], we obtain, in the HAF case we are interested in,

$$\omega_k = 4\,\kappa^2\,\sqrt{1-\gamma_k^2}\;, \qquad \kappa^2 = 1-(2N\widetilde{S})^{-1}\textstyle\sum_k \sqrt{1-\gamma_k^2}\;\coth[\omega_k/(2\widetilde{S}t)]\;, \qquad (8)$$

where κ^2 is the well-known SCHA renormalization coefficient. In the ferromagnetic case $\sqrt{1-\gamma_k^2}$ should be replaced by $(1-\gamma_k)$, also in Eq. (7). Eqs. (8) can be self-consistently solved for κ^2 and the frequencies, and hence the pure-quantum renormalization coefficient θ^2 is calculated via Eq. (7).

Though giving much better results at low and intermediate temperatures, this type of LCA transfers to the PQSCHA an instability at $t=\theta^4$, which is indeed typical of the SCHA, where the self-consistent solution becomes complex. This comes from having considered all possible spin-waves, including those with wavelength $\lambda > 2\xi$ (ξ is the spin correlation length) which do not actually survive in the system because of the lack of long-range-order. The instability is then avoided by not taking into account the unphysical spin-waves, i.e. introducing a cut off $|k| \geq \pi/\xi$ over the (antiferromagnetic) Brillouin zone. Furthermore, by writing κ^2 as

$$\kappa^2 = 1-(\mathcal{D}+\mathcal{D}_{\rm cl})/2\;, \qquad \mathcal{D}_{\rm cl} = (N\widetilde{S})^{-1}\textstyle\sum_k \sqrt{1-\gamma_k^2}\; f_k^{-1}\;,$$

we see that the above mentioned instability comes from the classical component $\mathcal{D}_{\rm cl}$ of κ^2, as the pure-quantum $\mathcal{D}$ is decreasing with t and takes contributions from the highest frequencies (as a consequence of representing only the short-ranged pure-quantum fluctuations). This suggests to insert the cut-off just in the evaluation of $\mathcal{D}_{\rm cl}$, so that for $t\to\infty$, $\mathcal{D}_{\rm cl}$ vanishes as $\xi\to 0$ and we find the very same results that would have been obtained by the usual LCA.

As for the correlation functions, they can be easily evaluated, as shown in Refs. [1] and [2]; their expressions, together with the form of the effective Hamiltonian Eq. (6), tell us that the quantum correlation length ξ at temperature t takes the same value that the classical $\xi_{\rm cl}$ has at a higher temperature $t_{\rm cl}=t/\theta^4(t)$, being $\xi(t)=\xi_{\rm cl}(t/\theta^4(t))$. In this way, by knowing the classical $\xi_{\rm cl}(t)$, we can obtain the quantum results for any value of the spin.

In Fig. 1 we show $\xi(t)$ for a $S=\frac{1}{2}$ 2d-HAF as obtained by the PQSCHA (lines), compared with experimental data, quantum Monte Carlo (QMC) and high-T expansion results. The continuous lines are the low- and high-T results of our theory, *i.e.* those obtained by the refined LCA described above and the usual one, respectively; the dashed line, which is obtained by applying the cut-off, smoothly connects them. The classical ($S = \infty$) correlation length is also shown and the open circles are new results from classical Monte Carlo simulations that we have performed (the dash-dotted line is a fit to the classical data). Remarkably, such a good agreement is obtained without any best-fit parameter; this really gives us confidence to draw out conclusions about the physics of the 2d-HAF out of the PQSCHA results.

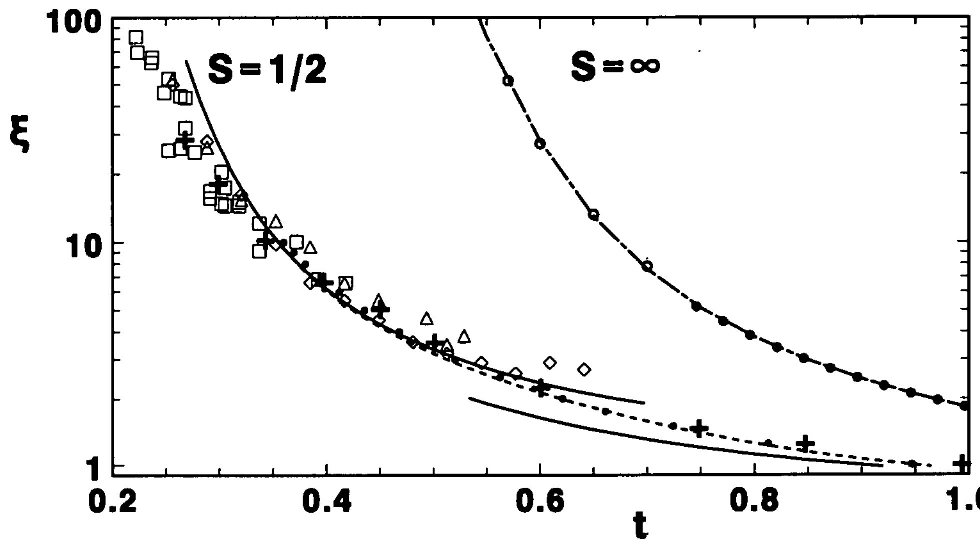

Figure 1: $\xi(t)$ as a function of $t = T/(J\widetilde{S}^2)$ (see text). Squares, triangles (neutron scattering for $Sr_2CuO_2Cl_2$ and La_2CuO_4), diamonds (NQR relaxation for La_2CuO_4), crosses (QMC) and filled circles (high-T expansion), in the order, from Refs. [5].

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