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1992 J. Phys. A: Math. Gen. 25 5861

(http://iopscience.iop.org/0305-4470/25/22/014)

J. Phys. A: Math. Gen. 25 (1992) 5861-5865. Printed in the UK

The frustrated quantum spin-$\frac{1}{2}$ chain

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Received 22 April 1992

Abstract. The Trotter decomposition and transfer matrix methods have been used to study the frustrated quantum spin-$\frac{1}{2}$ chain. The random bond model in a uniform field and ferromagnetic models in a random field have been investigated. The results indicate the existence of non-zero entropy at zero temperature. The random bond model also exhibits non-analytic behaviour of the magnetization as a function of applied field.

1. Introduction

The interplay between quantum, thermal and frustration effects in many body systems is clearly one of some complexity. Frustration as an important determining factor in the behaviour of interacting systems has been appreciated for some time since Toulouse first introduced the concept [1]. This effect may arise due to randomness in sign of interpartical interactions such as in spin glasses or through the application of an external field. The effect of frustration in classical non-quantum systems has been well investigated particularly for the random bond case and spin glasses [2]. The study of frustration arising from random fields has mostly been confined to the random field Ising model and related classical models [3]. The effect of randomness and frustration on quantum models has been much less studied. Quantum spin glasses have been investigated from the quantum analogue of the Sherrington-Kirkpatrick model [4], and some exact diagonalization for small clusters has been done using the Lanczos method [5, 6].

The effect of frustration on quantum systems arising from external fields has not so far been investigated extensively. There are therefore many questions unanswered. In particular it is not known whether the interplay of quantum and thermal effects 'wash out' any of the behaviour evident in classical systems. Here two related models are investigated, these are:

1.1. *Model I*

The random bond non-isotropic spin-$\frac{1}{2}$ chain in a non-zero uniform magnetic field. The Hamiltonian for such a system is taken to be

$$\mathcal{H} = -\sum_{\langle ij\rangle} J_{ij}(S_i^z S_j^z + \Delta(S_i^x S_j^x + S_i^y S_j^y)) - H\sum_i S_i^z \tag{1}$$

where $\{S_i^x, S_i^y, S_i^z\}$ are Pauli spin-$\frac{1}{2}$ matrices and $\{J_{ij}\}$ are random variables taken to the $\pm J$ with equal probability, H is a uniform magnetic field, the summation is over nearest neighbours and Δ is the anisotropy parameter.

Model II

The isotropic spin-$\frac{1}{2}$ ferromagnetic chain in both a uniform and random magnetic field. The Hamiltonian for such a system is taken to be

$$\mathscr{H} = -J \sum_{\langle ij \rangle} (S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z) - H \sum_i S_i^z - \sum_i h_i S_i^z. \tag{2}$$

Here $\{h_i\}$ are external random fields. Two cases are considered:

case (a): $\{h_i\}$ distributed continuously according to a Gaussian distribution with mean 0 and standard deviation J.

case (b): $\{h_i\}$ distributed discretely taking $\pm J$ with equal probability.

The method used is the generalization of the Trotter decomposition as developed by Suzuki [7]. This method reduces a d dimensional quantum system to a $d+1$ dimensional Ising system using the result that

$$e^{\Sigma_i A_i} = \lim_{m \to \infty} \left(\prod_i e^{A_i/m} \right)^m \tag{3}$$

where A_i are non-commuting operators as in Hamiltonians 1 and 2. The way in which 3 is exploited to produce the required classical system is well explained in many places [8–10] and will not be repeated in detail here. The only approximation in the method arises through the replacement of the limit in (3) by some large but finite value of m. This reduces the original quantum problem to a $2m \times N$ Ising model where N is the length of the original chain and the Ising Hamiltonian contains four-spin interactions. The partition function of the analogue Ising model has been calculated using a development of the transfer matrix method of Morgenstern, Binder and Hornreich [11]. The transfer matrix is applied along the direction of the chain and the only difference from the original method is that at each iteration two spins are added instead of one. This is necessary because of the four-spin interactions in the Ising model. The calculation was done on a DAP which is a single instruction multiple data parallel processor capable of performing 4096 simultaneous operations. Using this machine it was possible to calculate the partition function for long chains. All thermodynamic quantities were then calculated by numerical differentiation.

Because of the approximation of truncating (3) at some finite value of m, errors are introduced, the first term of which is $(JS^2/mT)^2$. Because of this there are restrictions on the lowest temperature that can be reached. Since computer memory restricts m to a maximum value of $m=9$ only temperatures $T \geqslant 0.1J$ are accessible.

Results

Model I

All results are obtained from a single long chain containing 1000 spins. The partition function was obtained for a single external field strength of $H=J$ and two values of the anisotropy parameter. These were $\Delta=1$ (isotropic) and $\Delta=0.2$ (easy axis).

Results for the entropy are shown in figure 1. The implication from these results is that for $\Delta=1$ there is zero entropy at $T=0$ while there is finite entropy for $\Delta=0.2$. The approach of the $\Delta=1$ curve to zero has been investigated. It is not possible to fit the results to a power low approach of the form T^x. Figure 2 shows the data on a log-linear plot. For $\Delta=1$ the results are clearly consistent with an exponential approach

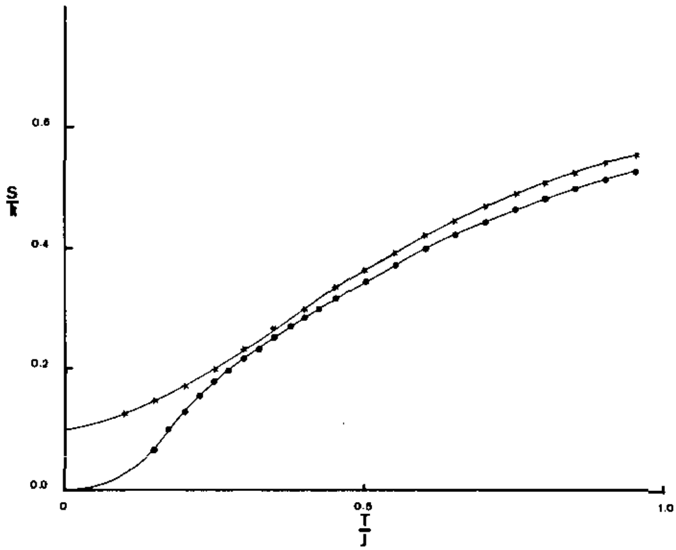

Figure 1. Entropy S against temperature T for model I: ● is for $\Delta=1$ and ★ is for $\Delta=0.2$. Lines are only visual guides.

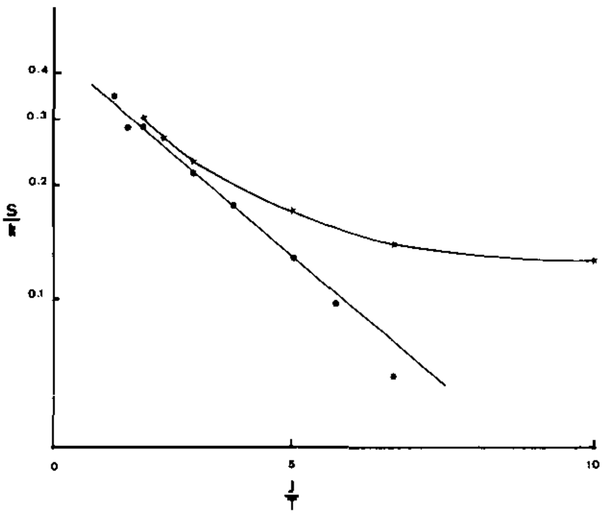

Figure 2. Log-linear plot of entropy S against reciprocal of temperature T, for model I: ● is for $\Delta=1$ and ★ is for $\Delta=0.2$. Lines are only visual guides.

to zero of the form

$$s \sim \mathrm{e}^{-(c/T)}.$$

However the data at the lowest temperature is seen to pull away from linearity indicating the possibility of crossover to even more rapid approach to zero. The result for $\Delta=0.2$ are also shown on figure 2 confirming the approach to a non-zero value already indicated in figure 1. This result should be compared with that of Puma and Fernandez [12] for the random field Ising model. Their result for the $T=0$ entropy for that model was $0.125k$ compared with $0.1k$ for the present case, k being the Boltzmann constant. Thus quantum effects seems to have suppressed but not eliminated $T=0$ entropy.

Figure 3 shows plots of the magnetization for varying applied field H. For $\Delta=0.2$ distinct discontinuities of slope are apparent, particularly if comparison is made with $\Delta=1$ case which is also shown.

To try to interpret this result consideration can be given to the analogous result for the one dimensional random field Ising model. Here exact calculation at $T=0$ shows that the magnetization is a devil's staircase [13–15]. Even though the results here are not given at $T=0$ but at $T=0.1J$, the lowest temperature accessible, the indications are of similar structure to the magnetization for the quantum case. That is the magnetization is not everywhere an analytic function of external field. It is at present a matter of speculation as to whether the non-analyticities are of the same nature in both the quantum and Ising cases.

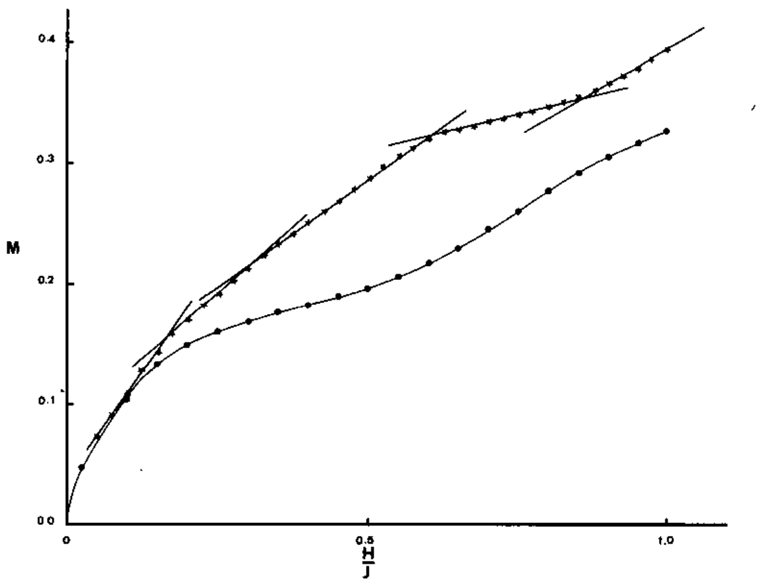

Figure 3. Magnetization M against external magnetic field H at temperature $T=0.1J$ for model I: ● is for $\Delta=1$ and ● is for $\Delta=0.2$. Lines are only visual guides.

1.2. Model II

A single chain containing 250 spins has been studied. Results for the entropy for the case external field $H=J$ and continuous random fields (case (a)) and discrete random fields (case (b)) are shown in figure 4. The results for discrete random fields indicate clearly a non-zero entropy at $T=0$. For continuous Gaussian fields the implication is less clear but a zero entropy is indicated from the present data through a small but finite entropy cannot be excluded.

Results have also been obtained for other values of the uniform external field. The data here is rather weak and it will be necessary to access even lower temperatures before any definite prediction can be made. The tentative conclusion so far which is put forward only as a speculation is that for the Gaussian field the entropy is always

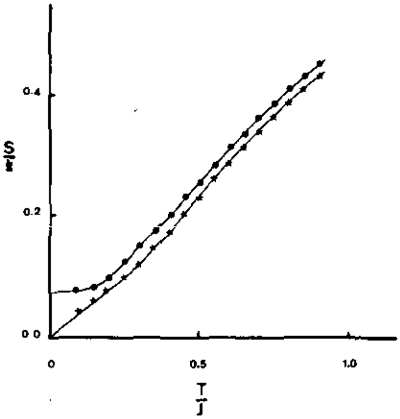

Figure 4. Entropy S against temperature T for model II and external field $H = J$: ● is for case (a) and ★ is for case (b).

zero for all $H \leqslant J$. However for the discrete case there maybe a crossover to zero entropy at lower field strengths. The precise resolution of these possibilities will have to await further investigation.

Acknowledgments

I thank the SERC for support and John Steel and the staff at the centre for Parallel Computing, University of London for all their assistance.

References

[1] Toulouse G 1977 *Commun. Phys.* **2** 115
[2] Binder K and Young A P 1986 *Rev. Mod. Phys.* **58** 1801
[3] Fisher D S 1984 *Phys. Rev.* **B 31** 7233
[4] Bray A J and Moore M A 1980 *J. Phys. C: Solid State Phys.* **13** L655
[5] Marland L G and Betts D D 1979 *Phys. Rev. Lett.* **43** 1618
[6] Dagotta E and Morea A 1989 *Phys. Rev. Lett.* **63** 2148; *Phys. Rev.* **B 39** 4744
[7] Suzuki M 1976 *Prog. Theor. Phys.* **56** 1454
[8] Suzuki M (ed) 1987 *Quantum Monte Carlo Methods* (Berlin: Springer)
[9] Cullen J J and Landau D P 1983 *Phys. Rev.* **B 27** 297
[10] Barma M and Shastry B S *Phys. Rev.* **B 18** 3351
[11] Morgenstern I, Binder K and Hornreich R M 1981 *Phys. Rev.* **B 23** 1981
[12] Puma M and Fernandez J F 1978 *Phys. Rev.* **B 18** 1391
[13] Derrida B, Vannimenus J and Pomeau Y 1978 *J. Phys. C: Solid State Phys.* **11** 4749
[14] Nieuwenhuizen T M and Luck J M 1986 *J. Phys. A: Math. Gen.* **19** 1207
[15] Bruinsma R and Aeppli G 1983 *Phys. Rev. Lett.* **50** 1494