Approximate equivalence of quenched and annealed random systems in the effective Hamiltonian approximation

1980 J. Phys. A: Math. Gen. 13 2537

(http://iopscience.iop.org/0305-4470/13/7/037)

J. Phys. A: Math. Gen. **13** (1980) 2537–2540. Printed in Great Britain

COMMENT

Approximate equivalence of quenched and annealed random systems in the effective Hamiltonian approximation

M Ausloos† and A Pękalski‡

† Université de Liège, Institut de Physique B5, B-4000 Sart Tilman par Liège 1, Belgium
‡ University of Wrocław, Institute of Theoretical Physics, ul. Cybulskiego 36, 50205 Wrocław, Poland

Received 24 October 1979

Abstract. We show that in the effective Hamiltonian approximation and in a large volume of parameter space, quenched and annealed random locally anisotropic magnetic systems have the same critical temperature versus concentration behaviour.

The effective Hamiltonian approximation introduced by Oguchi and Ono (1966) has often been used to discuss the properties of spin models. It was first applied to the Heisenberg ferro- and antiferromagnetic models with (non random) varying anisotropy. Diluted ferro and antiferromagnets with site and bond disorder have been considered also by Oguchi and Obokata (1969) and Hattori (1977). Oguchi and Ueno (1977) and recently Tamariguchi and Takano (1978) used the same approximation to discuss the spin-glass phase in a random mixture of Ising ferro- and antiferromagnetic bonds.

The approximation is used as a first step beyond the molecular field approximation, and has found grace in many different problems (Corciovei *et al* 1972). It allows one to obtain, without much complicated algebra, a qualitative understanding of the variation of typical quantities like the critical temperature T_c, the specific heat, the susceptibility near the transition point. Along these lines, Ausloos and Pękalski (1978) have recently investigated such thermodynamic properties for a random system in which the local anisotropy is random, but is reflected in the spin–spin exchange integral: e.g., when an impurity sits between two spins, the character of the interaction changes from a Heisenberg-like to an anisotropic (Ising-like) interaction (Pękalski 1978). From the local anisotropy point of view such a model interpolates between the Ising and the Heisenberg case.

In this note, we would like to point out an interesting feature of the effective Hamiltonian approximation allowing us to discuss annealed and quenched systems on the same footing. For illustrative purposes we have taken a particular model at the numerical stage.

We will show an 'approximate equivalence' between quenched and annealed systems having *different* coordination numbers. Although the correspondence is only a mathematical one and does not seem to arise from a physical basis, the interest of the 'approximate equivalence' lies in the simplicity of the calculation of quenched system properties, and therefore in quickly obtaining results for the annealed cases in the effective Hamiltonian approximation.

0305-4470/80/072537+04$01.50

The effective Hamiltonian approximation consists in replacing the interaction between spins in a cluster by an effective exchange force. The size of the cluster to be considered (hence the number of interacting spins) primarily depends on the complexity of the problem. We have chosen to consider a two-spin cluster, describing exactly the interaction between two neighbouring spins S_1 and S_2 letting the effective exchange integral connect the remaining $2(z-1)$ nearest neighbours of S_1 and S_2.

The self consistency equation allowing us to determine $\beta_c J_{\text{eff}}$ consists in equating the density matrices for two clusters as

$$\hat{\rho}_1 = \mathrm{Tr}_{R+\delta}\, \hat{\rho}_2 \tag{1}$$

where $\tilde{\rho}_1$ and $\tilde{\rho}_2$ are density operators for the one-spin and two-spin Hamiltonian and $\boldsymbol{\delta}$ spans the coordinates of the neighbours of the central spin (say S_1). The trace is taken over the second spin states of the pair.

Consider first a *quenched* system. In the paramagnetic phase the exchange constant characterising the effective interaction of the $2(z-1)$ spins is $\Lambda_{\text{eff}} = 0$. Near T_c, Λ_{eff} is small, and equation (1) can be expanded and formally solved for Λ_{eff} whence one obtains an approximate density matrix. If we only wish to determine the critical temperature, then equation (1) as approximated is nothing else than an implicit equation for T_c. Taking into account the distribution of exchange integrals as given by a probability ($P(J)$, e.g.) we have

$$1-2/z = \int \mathrm{d}I \int \mathrm{d}J\, P(I)P(J) \exp(-\beta_c J_{\text{eff}}) \cosh(p\beta_c J) \tag{2}$$

where we have immediately chosen the general case of a random binary bond model interpolating between the Ising model when $p = 0$, and the isotropic Heisenberg case for $p = 1$. The exchange integrals are I and J respectively and are supposed to be positive, while $J_{\text{eff}} = pJ + (1-p)I$.

In the case of the *annealed* system, integrating equation (1) over the distribution of random exchange integrals and expanding with respect to Λ_{eff} (expected to be small again near T_c) leads to

$$\frac{z'}{2(z'-1)} = \iint \frac{P(I')P(J')\,\mathrm{d}I'\,\mathrm{d}J'}{1+\exp(-\beta_c J'_{\text{eff}})\cosh(p\beta_c J')} \tag{3}$$

with the same notation as in (2); the prime refers to the annealed case. The equivalence between annealed and quenched systems can be easily made after expanding the denominator in (3). This can be done if

$$\exp(-\beta_c J'_{\text{eff}})\cosh(\beta_c J' p) \ll 1 \tag{4}$$

and is obviously true in the case $p = 0$ (Ising) and $p = 1$ (Heisenberg).

Notice however that (4) is not *always* fulfilled but is restricted to a (nevertheless) large volume in the $(p\beta_c, I, J)$ space. One obtains

$$z'/2(z'-1) = \iint P(I')P(J')\,\mathrm{d}I'\,\mathrm{d}J' - \iint P(I')P(J')\cosh(\beta_c J' p)\exp(-\beta_c J'_{\text{eff}})\,\mathrm{d}I'\,\mathrm{d}J' + \ldots. \tag{5}$$

Comparison of (2) and (5) shows that mixed annealed and mixed quenched systems with different coordination number are equivalent as far as the determination of the critical

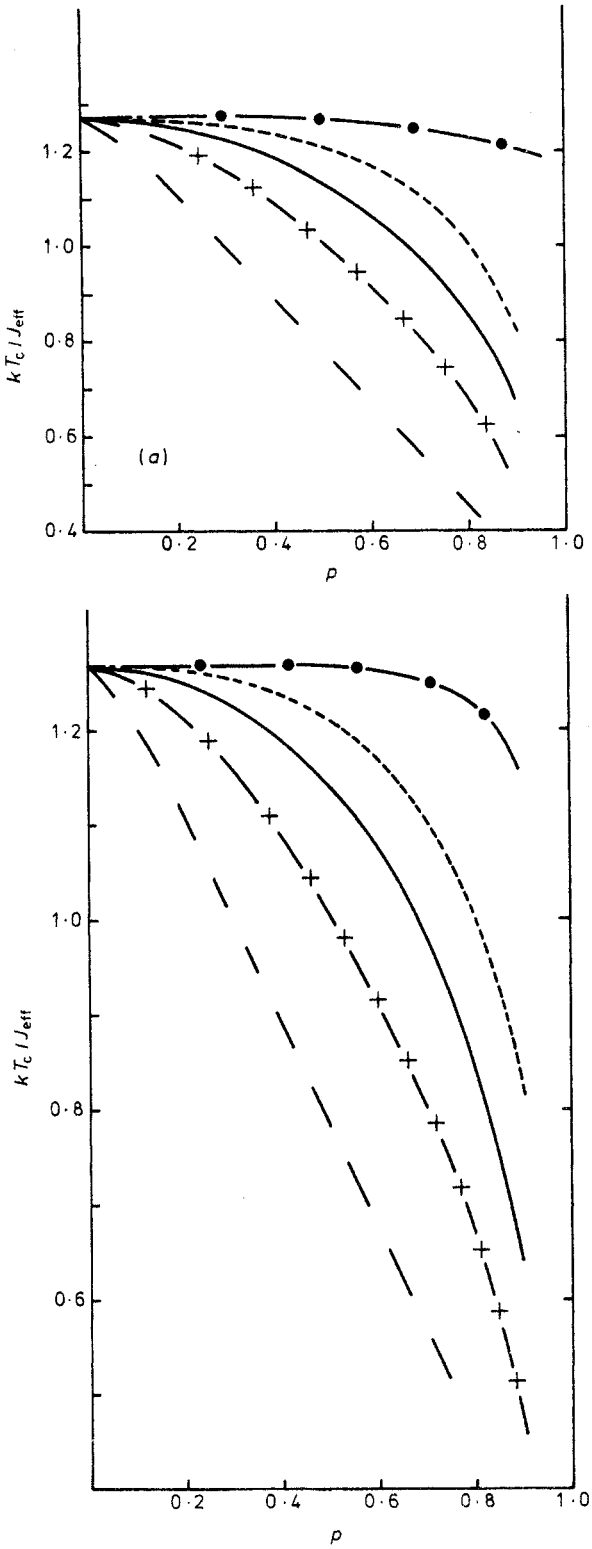

Figure 1. Reduced critical temperature of the quenched random Heisenberg–Ising mixture Hamiltonian with coordination number $z = 11/3$ in the cases: (*a*) $a = d = 10$; (*b*) $a = 40$, $d = 10$; for various ratios $y = I_0/J_0$ as a function of the concentration p of Heisenberg bonds.

y	I_0/J_0
0·2	— — — — —
0·5	—×—×—×—
1·0	———
5·0	- - - - - - - - -
10·0	—•—•—•—•

temperature is concerned (when the exchange integrals obey (4)) if

$$z' = 4/(4-z). \tag{6}$$

As expected both systems are strictly equivalent for the (trivial) case $z = z' = 2$. A table of corresponding systems can be made e.g. $z' = 4 \Leftrightarrow z = 3$; $z' = 8 \Leftrightarrow z = 3{\cdot}5$; $z' = 12 \Leftrightarrow z = 11/3$. Non-integer coordination numbers although surprising are not to be scorned since this is the usual case for amorphous crystals. We have shown the variation of kT_c/J_{eff} when the widths of the (Gaussian) distributions

$$P(I) = (a/\sqrt{\pi}I_0)\exp[-a^2(1-I/I_0)^2] \tag{7a}$$

and

$$P(J) = (d/\sqrt{\pi}J_0)\exp[-d^2(1-J/J_0)^2] \tag{7b}$$

are equal, $a = d = 10$, (figure 1(a)), and when $a = 40$, $d = 10$ (figure 1(b)).

Notice as a conclusion the very quick drop of T_c towards zero when p approaches 1, which corresponds to the Heisenberg case. It is indeed well known that the planar Heisenberg magnet ($z = 4$) has no transition at finite temperature (Mermin and Wagner 1966). Finally the stronger I_0, the longer T_c remains close to the exact Ising value when p increases.

It might be a little puzzling that the annealed FCC Heisenberg model with no admixture of Ising bonds cannot remain ordered. However, the cases considered here are for rather wide Heisenberg bond distributions. The long tail extending on the J negative axis can thus bring enough negative (i.e. antiferromagnetic) bonds into play so that T_c as a result goes to zero. This effect is of course visible on the side of the 'pure' (in the sense that the ground state is well defined) Heisenberg systems only, since in the absence of an external magnetic field, a pure Ising system is not sensitive to the presence of negative coupling constants. Unfortunately we have not been able to calculate $T_c(p)$ up to $p = 1$ since such a limit corresponds to a singular point. However it is clearly seen on the figures that for stronger Ising forces the system remains longer in the ordered state.

The authors gratefully acknowledge Dr J M Kowalski and Dr P Clippe for their interest and comments.

References

Ausloos M and Pękalski A 1978 *Solid St. Commun.* **26** 977
Corciovei A, Costache G and Vamanu D 1972 *Solid St. Phys.* **27** 237
Hattori K 1977 *J. Phys. Soc. Japan* **42** 1525
Mermin N D and Wagner H 1966 *Phys. Rev. Lett.* **17** 1133
Oguchi T and Obokata T 1969 *J. Phys. Soc. Japan* **27** 1111
Oguchi T and Ono I 1966 *J. Phys. Soc. Japan* **21** 2178
Oguchi T and Ueno Y 1977 *Prog. Theor. Phys.* **57** 683
Pękalski A 1978 *Acta Phys. Polon.* A**54** 641
Tamariguchi T and Takano F 1978 *Prog. Theor. Phys.* **60** 31