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A success of the Martinelli–Parisi expansion: The crossover to first-order transition in the 2D Potts model

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Abstract. We show that an instability for $q > q_c$ of the Migdal–Kadanoff recursion relations for the two-dimensional Potts model is related to the appearance of a discontinuity fixed point in the Martinelli–Parisi expansion. Consequently, at first order in this expansion, we can evidence a crossover to discontinuous transition, without explicit introduction of vacancies. Through numerical derivation of the free energy, we simulate remarkably well the discontinuous jump in the internal energies.

At first sight it seems difficult to get a satisfactory description of first-order phase transitions in the context of the renormalisation group approach to critical phenomena.

Nonetheless, some time ago Nienhuis and Nauemberg (1975) gave sufficient conditions to observe this kind of behaviour in terms of a 'discontinuity fixed point'.

A challenging problem is naturally provided by the well known two-dimensional Potts model (Potts 1952). Indeed it has been rigorously proved (Baxter 1973) that, in the presence of only nearest-neighbour interactions, when the number of states q is greater than four a latent heat appears at the transition temperature.

Anyhow, the first attempt to study the model using Kadanoff variational real space renormalisation group failed to detect any drastic change in the behaviour of the recursion relations for different q's (Dasgupta 1977).

Such a disturbing feature has been overcome through the extension of the space of renormalised Hamiltonians with the inclusion of vacant sites (Nienhuis *et al* 1979).

If on the one hand this picture confirms the expectations of Nienhuis and Nauemberg (1975) about the role of a discontinuity fixed point, on the other hand the introduction of vacancies may seem an *ad hoc* procedure since this fixed point is located at the extreme condition of a completely unoccupied lattice.

In this spirit we consider it of some interest to look for a renormalisation procedure which singles out automatically the important couplings and at the same time manages to show the expected crossover to a first-order transition.

We applied the Migdal–Kadanoff potential moving procedure (Migdal 1976, Kadanoff 1976) to the model defined on a triangular lattice by the effective Hamiltonians

$$-(kT)^{-1}\mathscr{H} \equiv \beta \sum_{\langle ij\rangle} \delta_{\sigma_i\sigma_j} \tag{1}$$

where the spins σ take q different values‖. The recursive relation for the variable

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‖ The Migdal-Kadanoff procedure had first been considered for the Potts model by Stephen (1976).

$y = e^{\beta}$ when the lattice spacing is scaled by a factor two is

$$y' = (y^4 + q - 1)/(2y^2 + q - 2) \tag{2}$$

which has one non-trivial ferromagnetic fixed point for any positive q at y^* given by the equation

$$(y^* - 1)^2(y^* + 1) = q. \tag{3}$$

Only in the limit $q \to \infty$ does this approximation show evidence of a first-order transition. There the fixed point given by (3) plays the role of the discontinuity fixed point.

We interpreted this failure as a due consequence of the restriction to a single-parameter space of interactions. As a matter of fact the introduction of a small three-body interaction $\delta_{\sigma_i\sigma_j\sigma_k}$ for the spins located on elementary triangles reveals that for $q > q_c \simeq 5.025$ the fixed point given by (3) becomes unstable also in this new direction. At q_c this operator is marginal. The connection of the occurrence of a marginality for q_c has been advocated by many authors (den Nijs 1979, Solyom and Pfeuty 1981†, Rebbi and Swendsen 1981).

The role of this interaction in determining the first-order transition can be consistently analysed by using the Martinelli–Parisi expansion (Martinelli and Parisi 1981). This consists in multiplying the potential moving operator by a factor $(1 - \varepsilon)$ and in formally developing the recursion relations in powers of ε. In this way the Migdal–Kadanoff results, which represent the zeroth order in the expansion, can be systematically improved in the extrapolation to the exact results which should appear in the limit $\varepsilon \to 1$, relying on the good behaviour of the perturbative series.

At first order in ε the only new interaction which is generated is the three-spin interaction previously described. Denoting its decoupling by γ, the improved relations have the structure

$$\beta' = f^{(0)}(\beta, \gamma) + \varepsilon f^{(1)}(\beta, \gamma), \qquad \gamma' = g^{(0)}(\beta, \gamma) + \varepsilon g^{(1)}(\beta, \gamma) \tag{4}$$

where by putting $\varepsilon = 0$ and $\gamma = 0$ we get the Migdal–Kadanoff formula (2); indeed the following relation holds

$$0 = g^{(0)}(\beta, 0) \tag{5}$$

which expresses the fact that γ is not generated at zeroth order, as it should be.

We now introduce in (4) the formal expansion of couplings

$$\beta = \beta_0 + \varepsilon\beta_1, \qquad \gamma = \varepsilon\gamma_1 \tag{6}$$

as $\gamma_0 = 0$ for (5), and obtain for the first-order contributions

$$\begin{pmatrix} \beta_1' \\ \gamma_1' \end{pmatrix} = \begin{pmatrix} f^{(1)}(\beta_0, 0) \\ g^{(1)}(\beta_0, 0) \end{pmatrix} + \begin{pmatrix} f_\beta^{(0)}(\beta_0, 0) & f_\gamma^{(0)}(\beta_0, 0) \\ 0 & g_\gamma^{(0)}(\beta_0, 0) \end{pmatrix} \begin{pmatrix} \beta_1 \\ \gamma_1 \end{pmatrix} \tag{7}$$

where subscripts denote partial derivatives.

In figure 1 we plot the fixed point value γ^* as a function of q. This coupling diverges when in the matrix in (7) (which at the fixed point is but the linearised transformation of the zeroth order) the eigenvalue $g_\gamma^{(0)}(\beta_0^*, 0)$ becomes one, that is, as we have seen previously, at $q = q_c$.

† Curiously we find $q_c \simeq 6.82$ in agreement with this paper if we restrict the three-body interaction only to up-pointed triangles.

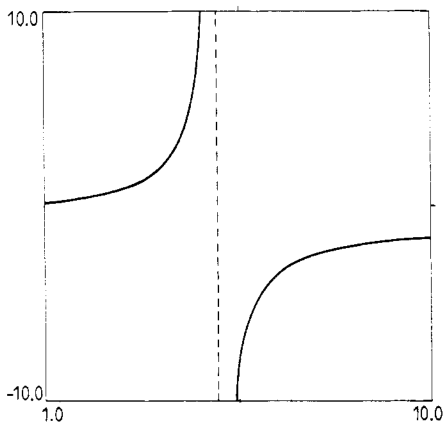

Figure 1. Fixed-point value of the three-spin coupling $\delta_{\sigma_i\sigma_j\sigma_k}$ as a function of the number of states q.

For $q > q_c$ γ_1^* is negative and repulsive; this means that the critical point on the canonical trajectory $\gamma = 0$ is mapped by iteration towards $\gamma_1^* = \infty$ which plays the role of the desired discontinuity fixed point.

In table 1 we list the improved results on the critical temperatures. As is usual in this expansion the first-order contribution goes in the right direction but is too large. In order to improve the extrapolations we exploited the fact that the error on the free energy is of order $(1-\varepsilon)^2$. This leads to reorder the series in such a way that the condition of zero derivative in ε at $\varepsilon = 1$ is fulfilled order by order (Martinelli and Parisi 1981, Caracciolo 1981, Martinelli and Menotti 1981, Belforte and Menotti 1982). For instance we extrapolated the values for the inverse critical temperatures using $\beta_0^* + \varepsilon(1-\frac{1}{2}\varepsilon)\beta_1^*$, so that $\beta_0^* + \frac{1}{2}\beta_1^*$ appears in table 1. The error of this evaluation is of the same order as at zeroth order. Otherwise $\beta_0^* + \frac{1}{4}\beta_1^*$ is in excellent agreement with the exact results.

Table 1. Inverse critical temperatures for some values of q: comparison among[(a)] exact determination, [(b)] Migdal–Kadanoff approximation and [(c)] first-order Martinelli–Parisi expansion

q	β_{cr} (a)	β_{cr} (b)	β_{cr} (c)
2	0.5493	0.6094	0.4782
3	0.6309	0.6931	0.5650
4	0.6931	0.7563	0.6285
10	0.9131	0.9762	0.8634

More striking are the plots of the reduced internal energies: we have never seen such a clear signal of the onset of a discontinuous transition in approximate recursion relations of the real space renormalisation group (see figure 2).

The internal energy has been obtained as the derivative of the free energy which has been computed, as usual, by integrating numerically the renormalisation group equation for the constant term in the partition function. The inverse temperature is parametrised as $\lambda(\beta_0^* + \varepsilon\beta_1^*)$.

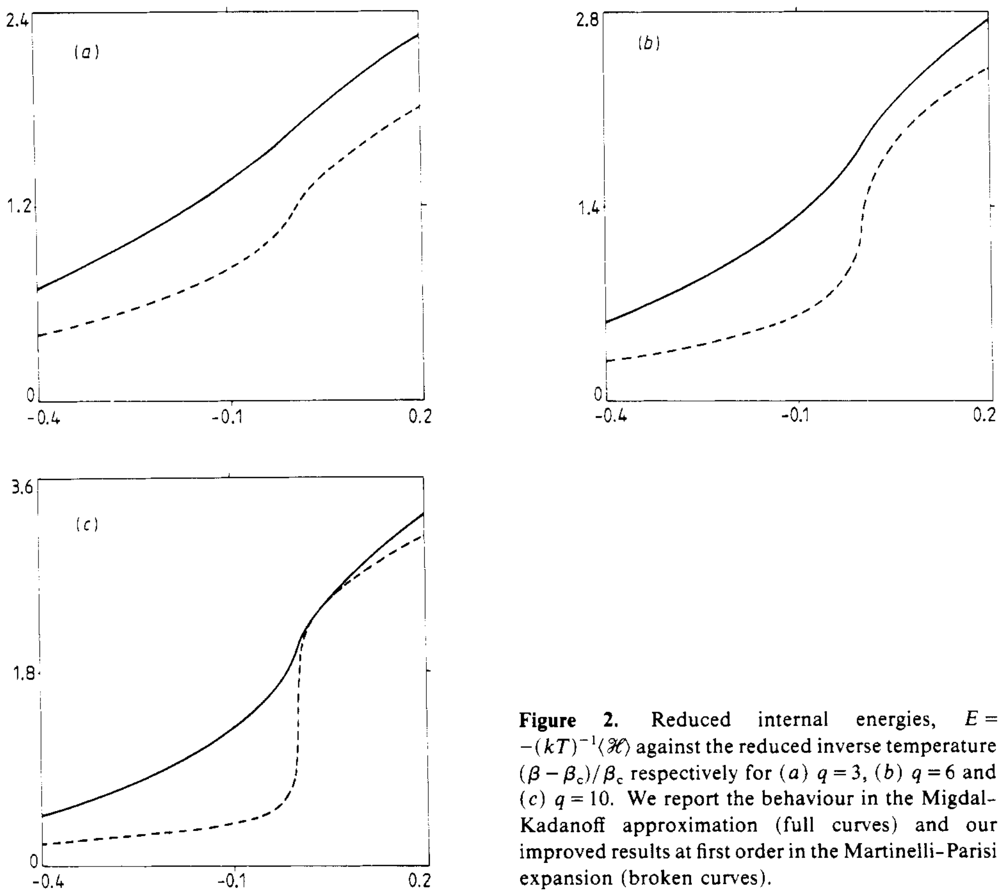

Figure 2. Reduced internal energies, $E = -(kT)^{-1}\langle \mathscr{H} \rangle$ against the reduced inverse temperature $(\beta - \beta_c)/\beta_c$ respectively for (a) $q = 3$, (b) $q = 6$ and (c) $q = 10$. We report the behaviour in the Migdal-Kadanoff approximation (full curves) and our improved results at first order in the Martinelli-Parisi expansion (broken curves).

In order to understand the connection of these results with those of Nienhuis *et al* (1979) we observe that the effective Hamiltonians can be written as

$$-(kT)^{-1}\mathscr{H} \equiv \tilde{\beta} \sum_{\langle ij \rangle} \delta_{\sigma_i\sigma_j} + \tfrac{1}{2}\gamma \sum_{\langle ijk \rangle} (2\delta_{\sigma_i\sigma_j\sigma_k} + 1 - \delta_{\sigma_i\sigma_j} - \delta_{\sigma_j\sigma_k} - \delta_{\sigma_k\sigma_i}) \tag{8}$$

where γ appears as the coupling distinguishing configurations with spins in three different states on elementary triangles. This interaction governs effective vacancies, that is disorder, on the lattice. In this perspective our scenario is quite consistent with the picture proposed in a paper by Swendsen *et al* (1982) where a Monte Carlo renormalisation group calculation is performed at q_c without the explicit introduction of vacancies, but in the presence of a multi-spin interaction controlling disorder which is shown to be responsible of marginality.

Eventually, we observe that our first-order calculations indicate a new non-trivial fixed point for $q > q_c$ with negative γ^*. This feature is so interesting as to suggest an investigation also with different techniques. Anyhow, higher-order calculations in the Martinelli–Parisi expansion could give stronger indications about the existence of these possible new universality classes as well as a more precise evaluation of q_c which is, at first order, somewhat larger than the expected one (i.e. $q_c = 4$). We would also like to point out that this expansion has such character of generality that its success in this case opens the possibility of obtaining reliable information on a wide class of systems in which one suspects first-order behaviour, as for instance lattice gauge theories.

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