First- and second-order phase transitions in Potts models: Competing mechanisms (invited)[a]

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Many condensed matter systems, ranging from adsorbed surfaces to bulk magnets, are microscopically modelled by interacting q-state Potts spins, arrayed in d dimensions. A changeover from second-order phase transitions at $q \leq q_c(d)$ to first-order transitions at $q > q_c$ can be understood as a condensation of effect vacancies, which are patches of local disorder favored by entropy. Accordingly, the renormalization-group treatment of Potts models is within context of Potts-lattice-gas models, where critical and tricritical fixed points occur at low q, but merge and annihilate at q_c. This picture has led to exact tricritical exponents in two dimensions. It is also consistent with recent experimental results on intercalated systems in three dimensions. Effective vacancies in pure Potts models have also been studied by Monte Carlo simulation. Their effective chemical potential can be controlled by a four-point interaction, which proved useful in Monte Carlo renormalization-group studies.

Potts models[1] are simple generalized spin models, easily defined by the Hamiltonian

$$-\mathcal{H}/kT = J \sum_{<ij>} \delta_{s_i s_j} \quad , \tag{1}$$

where, at each site i of a lattice, a spin variable s_i can be in one of q states $\{s_i = a,$ or $s_i = b,$ etc.$\}$. The sum in Eq. (1) is over nearest-neighbor pairs of sites, and $\delta_{s_i s_j} = 0$ (1) for $s_i \neq s_j$ ($s_i = s_j$). Equation (1) defines the simplest form of such models. In fact, Hamiltonians can be written with combinations of many types of terms, e.g., further-neighbor and/or many-site interactions coupling Potts spins $\{s_i\}$. If the partition function

$$Z = \sum_{\{s_i\}} \exp(-\mathcal{H}/kT) \quad , \tag{2}$$

is invariant under any permutation[2] of the state labels $\{a,b,\ldots\}$, these systems share the so-called universal phase transition properties, such as the possible occurrence and critical exponents of second-order transitions. Thus, any system in which the energy of a spin configuration is fixed by groups of spins being in like or unlike states, that is without absolute but with relative reference to the labels of these states, is a Potts system. It is therefore not surprising that many physical systems are Potts systems. These include, in addition to the commonly studied Ising systems (q = 2), the q > 2 realizations such as cubic magnets in diagonal field,[3] epitaxially adsorbed systems on surfaces,[4] structural-transition systems under pressure,[5] intercalated systems,[6] and multicomponent liquid mixtures.[7] Formal extension to the limit q → 1 yields results for the percolation problem.[8] The phase transition of Potts systems involves a spontaneous breaking of the permutation symmetry manifest in the definition of the models: at low temperatures, one state is preferentially occupied by the spins.

For q > 2, Potts models admit a Landau free energy expansion with a third-order invariant, implying, according to classical approximations, that the phase transition is first order.[9] Thus, when Baxter[10] proved in 1973 that the latent heat in two dimensions vanishes as q → 4[+], a qualita-

tive shortcoming of classical theory was indicated. The same conclusion was independently reached by Straley and Fisher,[11] whose series expansion suggested a second-order transition for q = 3. On the other hand, whereas classical theory errs on the first-order side, modern renormalization-group theory[12] tends to err on the side of second-order phase transitions. This can be understood from Fig. 1. The simplest renormalization-group flow topology, for ordering at low temperatures, involves a single flow parameter, and an unstable fixed point at finite temperature, thereby implying a second-order phase transition (Fig. 1a). The simplest flow topology for a first-order transition is shown in Fig. 1b. The search for the second (elusive) flow parameter was thus the subject of several years of renormalization-group studies, when the Potts first- to second-order
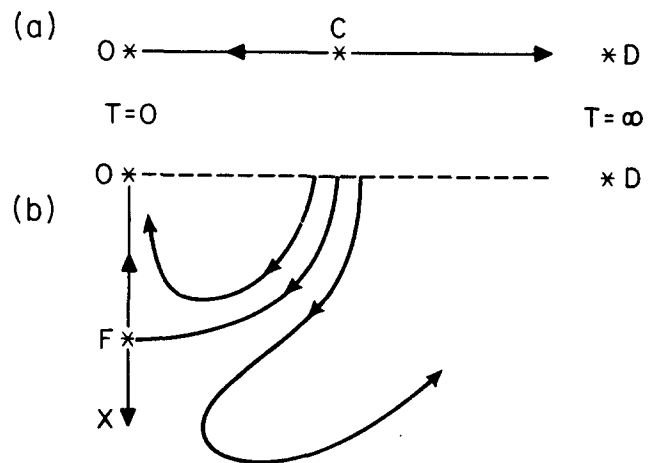

Fig. 1: Simplest renormalization-group flow topologies for (a) second-order and (b) first-order phase transitions. The horizontal is the temperature direction. In (b), the vertical direction corresponds to an unspecified flow parameter.

changeover was considered one of the few short-comings of the generally successful renormalization-group approach. This article will consider the resolution of this search, which, it will be seen, turned out to be physically motivated and which led to novel information. Recent results from our Monte Carlo simulations and from inter-calation experiments will also be mentioned.

We shall proceed now by revealing the physical mechanism underlying the Potts changeover.[13] Consider the local configuration of spins of Fig. 2a. Under a length scale transformation (renormalization-group transformation), these four spins are replaced by a single spin variable reflecting the most important collective property of the four. In this case, the most important collective property is clearly majority occupation of state "a", so that the new spin variable should also be in state "a". Consider on the other hand Fig. 2b. The most important collective property of these spins is that they are thoroughly disordered. They cause no ordering tendency on neighboring localities. In fact, by carrying no ordering information, this locality effectively acts as a vacancy. Thus, the new spin variable should be in a new state, the vacant ("zero") state. The pure Potts system is thermodynamically equivalent, under length scale change, to a Potts-lattice-gas system containing annealed vacancies, previously introduced in the study of adsorbed systems.[14] In fact, this adsorption study had shown that straight-forward renormalization-group theory does yield first-order phase transitions for Potts models with vacancies. In the original pure Potts system, effective vacancies such as in Fig. 2b have a high multiplicity for large number of states q. Thus, effective vacancies are entropically favored for large q. Their condensation causes the first-order phase transition, preempting criticality. It is interesting to note that the basic tenet of a renormalization-group transformation is to project important collective properties, summing out unimportant details. The occurrence of the Fig. 2a configuration is energetically important, whereas the occurrence of Fig. 2b is entropically important, and therefore must be projected as well. Furthermore, we would like to stress the point of view that the effective vacancies of Potts models are real elementary excitations of the system, independent of the method of treatment (only originally the renormalization-group method). This will be illustrated below by our Monte Carlo results.
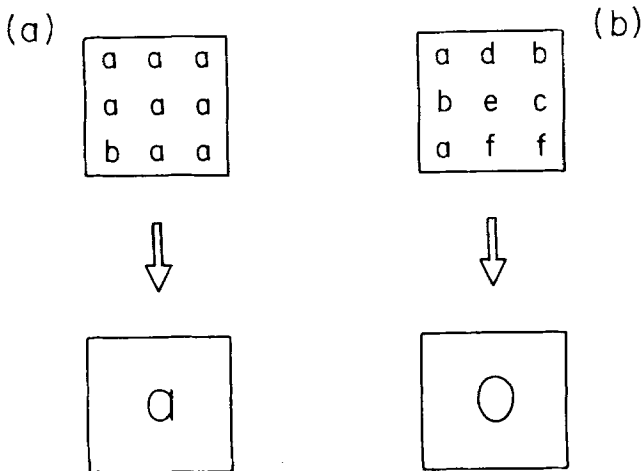

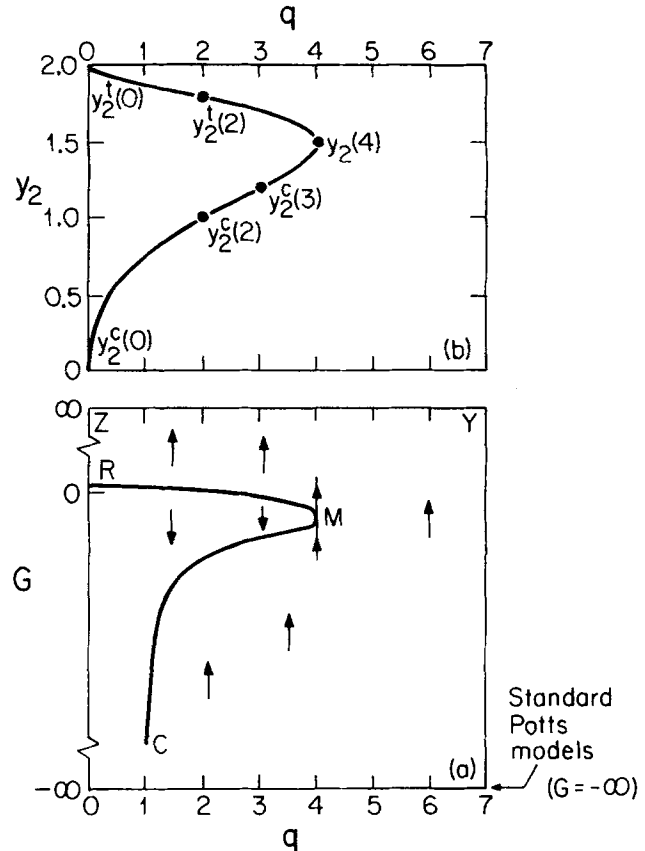Fig. 2: Renormalization-group mapping of (a) ordered and (b) effective-vacancy localities.

Fig. 3: (a) Renormalization-group flows within the phase transition surface of Potts-lattice-gas models. (b) The extended den Nijs conjecture for exact critical and tricritical exponents.

The renormalization-group flows,[13-17] within the phase transition surface of Potts models, is shown in Fig. 3a. The flow parameter G is the chemical potential of the vacancies (which thus turns out to be the mystery parameter of Fig. 1b). Schematically speaking, the temperature direction can be visualized as roughly orthogonal to the phase transition surface, i.e. out of the figure. Pure Potts models correspond to the initial conditions $G = -\infty$, and, for $q \leq q_c$, their transition points renormalize to the critical fixed line CM. For $q > q_c$, such flows miss CM, and renormalize to the first-order fixed line ZY. The line RM is a tricritical fixed line. The Potts changeover occurs by the merger and annihilation of the tricritical and critical fixed lines. Further, previously to the introduction of the effective vacancy mechanism, den Nijs[18] had conjectured a formula for the *exact critical exponents* $\nu = y_2^{-1}$ of Potts models in two dimensions. This is curve $y_2^c(0)y_2(4)$ in Fig. 3b, given by

$$(y_2 - 3) = 3/(y_B - 2) ,$$

where   (3)

$$y_B = (2/\pi)\cos^{-1}(\sqrt{q}/2) ,$$

is the critical exponent of the Baxter model at the map[10] of the transition point of the $(q \leq 4)$-state Potts model. The effective vacancy mechanism having revealed the tricritical fixed line as a smooth continuation of the critical fixed line, it was noted that Eq. (3) is double valued, the upper branch thus giving a conjecture[13] for the *exact*

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tricritical exponents of Potts models in two di-
mensions [$y_2^t(0)y_2(4)$ in Fig. 3b]. Subsequently,
such conjectures have been extended to other expo-
nents,[19] and, furthermore, the extended den Nijs
conjecture has been derived.[20]

    The role of effective vacancies can be noted,
visually, from snapshots of Monte Carlo simulations
on Potts models which are formally pure (no mani-
fest vacancies). In Figs. 4, we present examples
from two spatial dimensions. Figure 4a is a snap-
shot from a q = 3 system, 20% above the infinite
system transition temperature. Adjacent sites,
numbering at least twelve, and which are in the
same state, have been indicated. The remainder of
the system can be considered populated by effec-
tive vacancies. Note the large non-vacancy
regions, each aligned to one spin state. Such
regions have long boundaries of mutual contact,
the corresponding interfacial free energy presum-
ably having gone to zero, a signal for a second-
order phase transition. By contrast, in Fig. 4b
for q = 20, the system is overtaken by a "conden-
sation" of effective vacancies. Nonetheless, a
quasi-second-order behavior can be induced even
for q = 20 ($\gg q_c = 4$), by introducing a new inter-
action between Potts spins, which disfavors effec-
tive vacancies, as discussed below. The resulting
Fig. 4c should be compared with Fig. 4a.

    The choice of such appropriate new interac-
tion is dictated by the desire to disfavor effec-
tive vacancies, the mechanism for the first-order
phase transition, without simultaneously disfavor-
ing interfaces between locally ordered regions, the
mechanism for a second-order transition. One
choice[21] is a four-site term which is non-zero (and
unfavorably energetic) only when all four bonds in
an elementary square connect unlike states. The
corresponding term in the Hamiltonian $-\mathcal{H}/kT$ is

$$F \sum_{<ijk\ell>} (1-\delta_{s_i s_j})(1-\delta_{s_j s_k})(1-\delta_{s_k s_\ell})(1-\delta_{s_\ell s_i}) \quad , \tag{4}$$
$$F < 0 \quad .$$

Alternatively, F could be made positive, to favor
effective vacancies, still without introducing mani-
fest vacancies. Thus, using a pure Potts q = 4
system and varying F, the fixed point M of Fig. 3
was probed[21] in a Monte Carlo renormalization-group
study, to obtain quantitatively the special proper-
ties of this changeover point. Quantitatively
improved results for q = 3 have also been obtained
similarly.[22] Most recently, the use of similar
interactions have yielded novel phenomena as well
as high accuracy for the XY spin models in two and
three dimensions.[23]

    Finally, it should be noted that even when the
critical fixed line CM (Fig. 3) is missed by the
renormalization-group flow for q somewhat greater
than q_c, the presence of the fixed line at $q \leq q_c$
is felt. This is because, by the analytic nature of
renormalization-group transformations, flows to the
left of M slow down about the G value of M, that is
to say, a given length rescaling causes a smaller
change in the value of G. Many renormalization-
group iterations in this neighborhood cause the
accumulation of pseudo-critical "singularities" in
the statistical properties of the system. This is
presumably what happens in stage-one lithium inter-
calated in graphite[24] which is a realization of
q = 3, since in three dimensions q_c is believed[17]
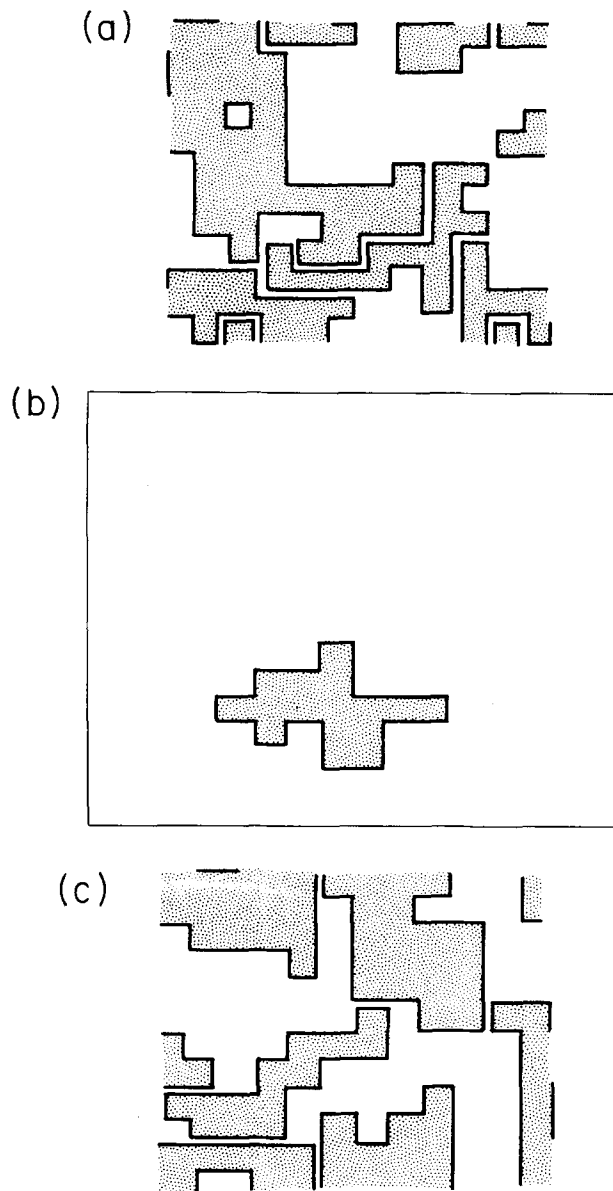to be between 2 and 3.

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Fig. 4: Monte Carlo snapshots of finite, pure
Potts systems[Eqs. (1) and (4)] with
periodic boundary conditions, taken
after 1,500 Monte Carlo steps per site.
Shaded are groups of twelve or more ad-
jacent sites in the same state. The
boundary of each group is shown with dark
lines. The remainder of the system can
be considered occupied by effective
vacancies. (a) q = 3, F = 0, 12 x 12
system, 20% above the infinite system
transition temperature; (b) q = 20, F = 0,
16 x 16 system, 10% above the infinite
system transition temperature; (c) q = 20,
F = 5J, 12 x 12 system, 25% above the
infinite (F = 0) system transition
temperature.

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