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Tricritical Points with Different Universality Classes for Polymers in Two Dimensions.

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Abstract. – We report a numerical investigation of the tricritical behaviour of the dilute equilibrium polymerization model with annealed dilution on the square lattice using transfer matrix techniques. In general, the tricritical exponent ν_t is found to be compatible with the value for the tricritical $n = 1$ model. In the limit where the dilute model is equivalent to the interacting polymer model (whose tricritical point is known as the Θ -point), we observe a crossover of ν_t to the tricritical $n \rightarrow 0$ model value.

Equilibrium polymerization has been modelled on a lattice by self- and mutually avoiding walks [1, 2], and the equivalence of this model to the $n \rightarrow 0$ limit of the magnetic n -vector model [2, 3] is very useful for the investigations of the thermodynamic properties, particularly via renormalization group calculations. This model has been generalized for equilibrium polymerization in a solvent, and its magnetic counterpart turns out to be the $n \rightarrow 0$ vector model with annealed dilution [4]. Recently, it was shown that in a particular limit the diluted polymerization model is equivalent to the polymer model with attractive interactions between monomers on nearest-neighbour sites on the lattice which are not consecutive monomers of the same chain [5, 6]. This equivalence has been observed analytically in the solution of the models on the Bethe lattice [7]. Both the diluted polymerization model and the interacting polymer model exhibit tricritical points in their phase diagrams in two or more dimensions, which we will call the diluted tricritical point (DTP) [4, 7] and the Θ -point [7-10], respectively.

It has been discussed in the literature if the diluted polymerization model is an appropriate model for studying the Θ -point in two dimensions. On the one side [6, 11], it has

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been argued that, since the interacting polymer model is a particular limit of the diluted polymer model, the Θ -point should be described by the diluted polymer model. Another argument states that the tricritical exponents of the diluted polymer model should be determined by the embedding Ising lattice-gas (tricritical $n=1$ exponents), whereas different tricritical exponents ($n \rightarrow 0$) are to be expected for the Θ -point [12, 13].

In this paper, we study the locus of tricritical points of the diluted polymer model on the square lattice, paying particular attention to the exponent ν_t . We use transfer matrix calculations for strips of finite width together with finite size scaling methods [14]. These methods have been used before in similar systems with good results [9, 10]. All calculations were done directly, without using the analogy with the diluted $n \rightarrow 0$ vector model.

Let us consider a square lattice with N sites and periodic boundary conditions in one direction and fixed boundary conditions in the other one. On each site a variable ν is defined, denoting the presence of either a monomer ($\nu = 1$) or a solvent ($\nu = 0$). This monomer-solvent system interacts as an Ising lattice-gas. A self-avoiding walk, whose endpoints are confined to the boundary, is constrained to pass only through sites with monomers. The appropriate partition function for this system is given by [4]

$$Y_N(x, y, z) = \sum_{n=0}^{\infty} \sum_{\{\nu\}} x^n y^{l(\{\nu\})} z^{m(\{\nu\})} \Gamma_N(n, \{\nu\}), \quad (1)$$

where x is the statistical weight of a monomer incorporated into a polymer, y is the Boltzmann factor associated with a nearest-neighbour monomer-monomer pair, and z is the activity of a monomer. The number of monomers in the polymer chain is denoted by n . $l(\{\nu\})$ and $m(\{\nu\})$ stand for the numbers of nearest-neighbour monomer-monomer pairs and the number of monomers in the lattice configuration, respectively, and are given by

$$l(\{\nu\}) = \sum_{\langle i, j \rangle} \nu_i \nu_j; \quad m(\{\nu\}) = \sum_i \nu_i, \quad (2)$$

where the first sum is over nearest-neighbour pairs. The number of configurations described by n , and $\{\nu\}$ is $\Gamma_N(n, \{\nu\})$.

The partition function of the interacting polymer model may be obtained from the partition function of the diluted polymer model (1) in the limit $z \rightarrow 0$, $x \rightarrow \infty$, with x, z fixed [5-7]. In this limit all monomers on the lattice will be incorporated into the chain, and the partition function (1) is reduced to

$$Y_N(\tilde{x}, y) = \sum_{n=0}^{\infty} \sum_l \tilde{x}^n y^l \Gamma_N(n, l), \quad (3)$$

where $\tilde{x} = xyz$ and l is the number of nearest-neighbour monomers which are not consecutive on the polymer chain. The configurations in this partition function (3) are the possible configurations of a SAW on the lattice.

The transfer matrix for the diluted polymer model on strips of width L and periodic boundary conditions may be constructed through a simple generalization of the appropriate transfer matrix for the model without dilution [15]. In one dimension, the diluted polymer model exhibits a first-order phase transition [16, 17], expected to occur for any finite width L . The study of the density of sites incorporated into the polymer,

$$\rho(x, y, z) = \lim_{N \rightarrow \infty} \frac{x}{N} \frac{\partial}{\partial x} \ln[Y_N(x, y, z)], \quad (4)$$

at the first-order transition allows us to draw conclusions about the behaviour of the $L \rightarrow \infty$ two-dimensional model [18]. For a finite strip, the first-order transition occurs when the activity reaches its transition value, $x_L(y, z)$, such that the largest eigenvalue of the transfer matrix is equal to the largest eigenvalue of the lattice-gas transfer matrix. The density ρ will be given by

$$\rho_L(x, y, z) = \begin{cases} 0, & x < x_L, \\ \frac{x}{L\lambda_L} \frac{\partial \lambda_L}{\partial x}, & x > x_L. \end{cases} \quad (5)$$

Following the arguments of Derrida and Saleur [9] and Saleur [10], we define

$$\beta = \ln(y) \quad \text{and} \quad \zeta = \frac{z}{1+z},$$

and study the behaviour of the quantity

$$X_L(\beta, \zeta) = \left[\frac{\ln[\rho_{L+2}(x_{L+2}, \beta, \zeta)/\rho_L(x_L, \beta, \zeta)]}{\ln[(L+2)/L]} + 2 \right]^{-1} \quad (6)$$

for increasing values of L . At the tricritical point, X_L should be independent of L , and therefore the intersection of the curves $X_L(\beta, \zeta_0)$ for different values of L gives an estimate for the tricritical point $\beta_t^{(L)}(\zeta_0)$. The estimate for the tricritical exponent will be

$$\nu_t^{(L)} = X_L(\beta_t^{(L)}, \zeta_0).$$

Since parity effects are observed, as described in ref. [9, 10], it was necessary to use widths L and $L+2$ in the calculation of X_L . In fig. 1, five curves of $X_L(\beta, \zeta_0)$ for $\zeta_0 = 0.05$ and

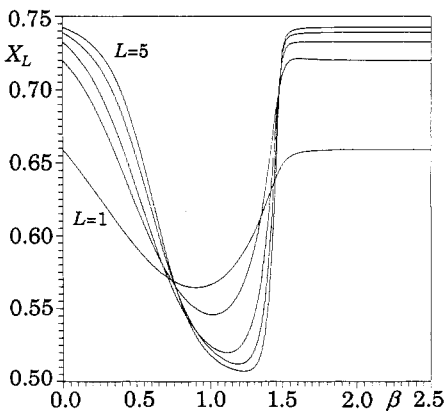


Fig. 1.

Fig. 1. – Curves of X_L vs. β for $\zeta = 0.05$ and $L = 1, \dots, 5$. The estimated location of the tricritical points correspond to the intersection of the curves.

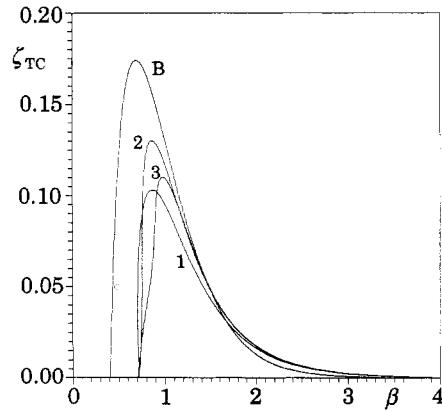


Fig. 2.

Fig. 2. – ζ_{TC} as a function of β . The curves labelled by a number i were obtained from calculations for strips of width $L = i, i+2$ and $i+4$. Curve B corresponds to Bethe lattice results for coordination number $q = 4$.

$L = 1, \dots, 5$ are depicted. From the intersections of the curves it is clear that two tricritical points are observed, with different values for the estimates of the tricritical exponent ν_t . Also, we found that for very small values of ζ ($\zeta \cong 10^{-5}$) the curves are graphically indistinguishable from fig. 7a of ref. [10] for the interacting polymer model, thus confirming numerically the relation between this model and the diluted-polymer model in the $\zeta \rightarrow 0$ limit.

Each pair of consecutive curves in fig. 1 defines two tricritical points. Repeating those calculations for a variety of values for ζ , we obtain the tricritical curves ζ_{TC} vs. β shown in fig. 2. For comparison, we included in this figure the result for a Bethe lattice calculation [7] with coordination number $q = 4$, showing the correct qualitative behaviour.

In the same way, estimates for the exponent ν_t may be found and the results are shown in fig. 3. There we notice that the estimated values for ν_t are small for small values of β (which correspond to the interacting polymer limit) and increase rapidly with β , stabilizing at higher values of β . Furthermore, it is apparent that these small values of ν_t are compatible with the value $\nu_t = 4/7$ supposed to be exact for the Θ -point [19]. Also, the larger values for the estimates of ν_t are close to the tricritical Ising value $\nu_t = 8/11$ [13].

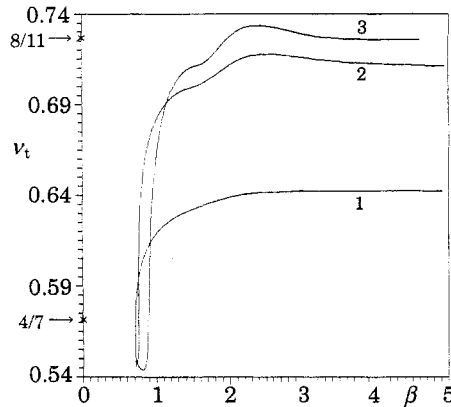


Fig. 3. – Estimates for the tricritical exponent ν_t plotted against β corresponding to curves 1, 2, and 3 in fig. 2. The values considered to be exact discussed in the text are indicated by arrows.

In conclusion, our results indicate that a crossover occurs in the tricritical behaviour of the diluted polymer model (1). In general, in agreement with the arguments by Duplantier and Saleur [13], Ising tricritical exponents are obtained. However, in the limit $\zeta \rightarrow 0$, $x \rightarrow \infty$, when the model is equivalent to the interacting polymer model, a crossover to the $n \rightarrow 0$ tricritical behaviour is found. As a matter of fact, the argument by Duplantier and Saleur [13] that the thermodynamics of the diluted polymer model should be dominated by the embedding Ising lattice-gas model, since the lattice-gas is not sensitive to the presence of the polymer, breaks down in the limit $\zeta \rightarrow 0$, $x \rightarrow \infty$. In this limit the locations of the monomers are completely determined by the polymer chain.

We also have performed phenomenological renormalization group calculations [14] to study the tricritical behaviour of the diluted polymer model (1). Although in general the results obtained by this technique are poorer than the ones via the first-order transition method presented above, they corroborate our conjecture regarding the crossover in the tricritical behaviour. These calculations, together with an analysis of the conformal invariance properties of the model, will be the subject of a forthcoming paper.

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REFERENCES

- [1] DE GENNES P. G., *Scaling Concepts in Polymer Physics* (Cornell University Press, New York, N.Y.) 1979.
- [2] WHEELER J. C. and PFEUTY P. M., *Phys. Rev. A*, **24** (1981) 1050.
- [3] DE GENNES P. G., *Phys. Rev. A*, **38** (1972) 339.
- [4] WHEELER J. C. and PFEUTY P. M., *J. Chem. Phys.*, **74** (1981) 6415.
- [5] VANDERZANDE C., *Phys. Rev. B*, **38** (1988) 2865.
- [6] MAES D. and VANDERZANDE C., *Phys. Rev. A*, **41** (1990) 3074.
- [7] SERRA P. and STILCK J. F., *J. Phys. A*, **23** (1990) 5351.
- [8] DE GENNES P. G., *J. Phys. (Paris)*, **36** (1975) L-55.
- [9] DERRIDA B. and SALEUR H., *J. Phys. A*, **18** (1985) L-1075.
- [10] SALEUR H., *J. Stat. Phys.*, **45** (1986) 419.
- [11] SENO F., STELLA A. L. and VANDERZANDE C., *Phys. Rev. Lett.*, **61** (1988) 1520.
- [12] DUPLANTIER B. and SALEUR H., *Phys. Rev. Lett.*, **61** (1988) 1521.
- [13] DUPLANTIER B. and SALEUR H., *Phys. Rev. Lett.*, **62** (1989) 1368.
- [14] BARBER M. N., *Finite-Size Scaling, Phase Transitions and Critical Phenomena*, edited by C. DOMB and J. L. LEBOWITZ, Vol. 8 (Academic Press, London) 1983.
- [15] DERRIDA B., *J. Phys. A*, **14** (1981) L-5.
- [16] PFEUTY P. M. and WHEELER J. C., *Phys. Rev. A*, **27** (1983) 2178.
- [17] STILCK J. F. and WHEELER J. C., *J. Stat. Phys.*, **46** (1987) 1.
- [18] DERRIDA B. and HERRMANN H. J., *J. Phys. (Paris)*, **44** (1983) 1365.
- [19] DUPLANTIER B. and SALEUR H., *Phys. Rev. Lett.*, **59** (1987) 539.