Physica A 206 (1994) 283–288
North-Holland

PHYSICA A

SSDI 0378-4371(93)E0591-2

Crossover in smart kinetic growth walks

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Received 13 December 1993

By extending the study of smart kinetic growth walks on the honeycomb lattice we are able to extract a value for the crossover exponent, 0.44 ± 0.02, which is consistent with the conjectured value of $\frac{3}{7} \approx 0.428$ for interacting walks at the θ-temperature. This work corroborates similar results on the oriented Manhattan lattice.

The sharp change of the conformational properties a polymer undergoes in a dilute solution as the temperature or solvent quality is lowered is seen as a critical phenomenon [1–3]. The study of this system in lattice statistical mechanics [1–3] is based upon the self-avoiding walk which possesses the excluded volume interaction important in physical polymers. The complex monomer–solvent interactions that cause the collapse transition are modelled by associating an energy with (non-consecutive) nearest neighbour sites on the walk.

This collapse transition, known as the θ-point in polymer physics, has been argued to be described by the standard ϕ^6 tricritical behaviour of an $O(n)$ field theory in the limit $n \to 0$ [4]. In two dimensions, where many exact solutions [5] exist for lattice models and the sophisticated techniques of conformal invariance [6] and the Coulomb gas [7] can be used to predict the critical properties of these models, the θ-point has been the subject of intense debate. Much of this debate [8–16] has centred on a model of loops on the honeycomb lattice with annealed vacancies put forward by Duplantier and Saleur (DS) [17]. When considered as a model of collapse it possesses a particular subset of next-nearest neighbour interactions as well as the canonical nearest neighbour monomer–monomer attraction. This has led to doubts over the relevance, in

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the renormalisation group sense, of these unusual interactions. While it is generally accepted that the values of the radius of gyration exponent, ν_t, and the partition function exponent γ_t most likely take on their DS values, which are $\frac{4}{7}$ and $\frac{8}{7}$ respectively, in interacting self-avoiding walks with only nearest neighbour attraction (ISAW), the crossover exponent has been more controversial. Numerical estimates [18–20,16,21] of the crossover exponent, ϕ, have consistently failed to be close to the exact conjecture of $\frac{3}{7} \approx 0.428$ and have ranged from 0.48 to 0.90 [22,20]. It is usually acknowledged that this exponent is the most difficult to estimate [23]. The collapse transition in the DS model is connected to the percolation of the vacancies. The loops of the DS model at the critical temperature are indistinguishable from the hulls of the percolating vacancies [17]. The temperature of the more standard ISAW system is argued to map to the percolation probability of the vacancies. This mapping is important in identifying the crossover exponent and has been questioned as the possible source of the crossover exponent discrepancies [15]. In this paper we shall present numerical evidence that confirms the predicted value of the crossover exponent, $\phi = \frac{3}{7}$, for the closely related θ'-model of Coniglio *et al.* [24].

An intimate relationship between θ-point-like walks and percolation had already been noticed [24] prior to the description of the DS model and involved models of dynamic polymerisation as intermediaries. These models are *smart* kinetic growth walks [25–27], because they are constructed in a way that prevents trapping other than by loop formation. This crucial property allows the identification of kinetic growth walks (KGWs) on the honeycomb lattice [28] with the hulls of percolation clusters at threshold. The length of the walk is associated with the number of sites in the perimeter of the cluster. The percolation probability of the cluster controls the relative probability of turning left rather than right in the KGWs. These smart KGWs were found to also map to the static problem of interacting self-avoiding walks on that lattice with a particular subset of next-nearest neighbour interactions [24] (the θ'-point). This connection between some static walk problem and the percolation transition inspired Duplantier and Saleur to write down their model [17] where, as mentioned above, the percolation probability was now associated with the walk model temperature. Ziff has examined the critical properties of percolation hulls [29] and confirmed a set of exponents for this problem. Saleur and Duplantier [30] obtained the exact fractal dimension ($\frac{7}{4}$) of the hulls of percolation clusters by using Coulomb gas methods. Hence, the mapping between the KGWs, percolation, and θ'-walks allow the identification of the size exponent, $\nu_t = \frac{4}{7}$. Studies of kinetic growth walks have previously focussed on this exponent and the partition function exponent γ_t. In this paper we shall extract the thermal crossover exponent for the static collapse problem of interacting walks on the honeycomb lattice derived from kinetic growth walks in the manner of Coniglio et al. [24].

This supplements a study [31] on the oriented Manhattan lattice where complementary and further results have been found, including an exact solution, concerning a model isomorphic to a KGW. In addition, we shall provide precise estimates of γ_t and ν_t to illustrate the accuracy of this method.

As stated above, the collapse transition in the θ'-problem is brought about by preferentially weighting a set of nearest neighbour and next-nearest neighbour contacts. We have stochastically enumerated dressed KGWs on the honeycomb lattice. These kinetic growth walks are *dressed* by "remembering" the left (L) and right (R) lattice faces that have been touched by the walk and using the rule that the walk may not proceed between two faces of the same labelling. This ensures that a walk can never enter a dead end unless it contains the walk's origin (see fig. 1) and hence in this way the "smartness" property is achieved. We have generated configurations up to a length of 2×10^5 keeping track of the loop formation probability, the end-to-end distance, the average number of such contacts, and their respective fluctuations. The simulations were completed on an Intel Paragon supercomputer with 50 processors. It took approximately 60 hours of cpu time (per processor) to obtain 5×10^5 samples of length 2×10^5. The code involved was nearly 100% parallelised.

The loop formation probability p_n and the mean-square end-to-end distance $\langle R^2 \rangle_n$ data allow the computation of the exponents $\alpha_t = \gamma_t$ and ν_t via graphical extrapolation of the finite-size approximations

$$\gamma_{t,n} - 1 = \log_2 \frac{p_n}{p_{n/2}} \qquad (1)$$

and

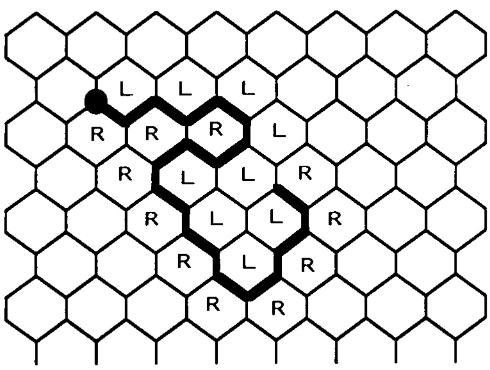

Fig. 1. A portion of the honeycomb lattice with a smart kinetic growth walk of length 19 illustrating the "dressing" necessary to avoid trapping. The beginning of the walk is marked with a bullet.

Table I
Best estimates and exact conjectures for the bulk exponents for the θ'-problem of interacting walks on the honeycomb lattice derived from the smart KGW on that lattice. These are to be compared to the values for the Duplantier and Saleur model.

Exponent	ν_t	γ_t	α_t	ϕ
Estimates	0.571(2)	0.857(2)	0.857(2)	0.44(2)
Exact θ'	$\frac{4}{7}$	$\frac{6}{7}$	$\frac{6}{7}$	$\frac{3}{7}$
DS walks	$\frac{4}{7}$	$\frac{8}{7}$	$\frac{6}{7}$	$\frac{3}{7}$

$$2\nu_{t,n} = \log_2 \frac{\langle R^2 \rangle_n}{\langle R^2 \rangle_{n/2}} \tag{2}$$

over a range of lengths with errors computed from the fluctuations. The results are listed in table I.

The internal energy and specific heat of the KGWs give us the ability to find estimates of the specific heat exponent, α, and crossover exponent, ϕ, [23] which are related to each other via the scaling relation

$$2 - \alpha = 1/\phi \, . \tag{3}$$

At the tricritical-like point in the static walk problems [23] the internal energy U_n and specific heat C_n of walks of length n asymptotically behave as

$$U_n \sim U_\infty + U_0 n^{(\alpha-1)\phi} \tag{4}$$

while if $\alpha < 0$

$$C_n \sim C_\infty + C_0 n^{\alpha\phi} \, . \tag{5}$$

By calculating both the internal energy and specific heat we can either obtain two estimates of ϕ using the scaling relation (3) or alternatively use the relation to check the accuracy of our results. We use the finite-size estimations

$$\phi_n - 1 = \log_2 \frac{U_{n/2} - U_n}{U_{n/4} - U_{n/2}} \tag{6}$$

respectively

$$2\phi_n - 1 = \log_2 \frac{C_{n/2} - C_n}{C_{n/4} - C_{n/2}} \, , \tag{7}$$

with errors computed from the respective fluctuations.

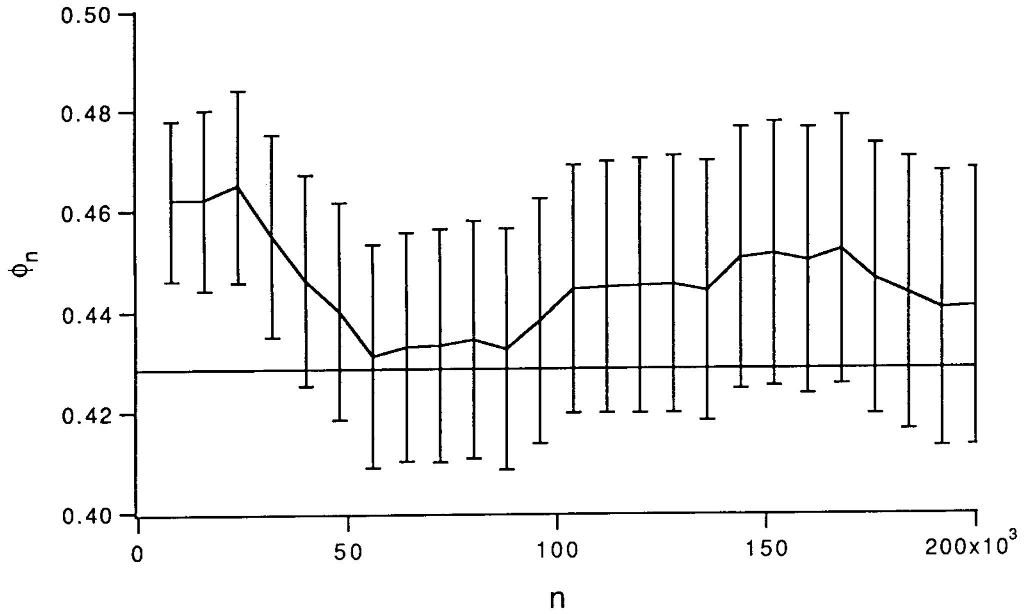

Fig. 2. A plot of local estimates of the crossover exponent ϕ_n against the length n.

The best estimates ϕ_n for the crossover exponent utilise the values of the internal energy. These are plotted in fig. 2 along with 95% confidence intervals on these estimates. The estimates from the specific heat data are consistent with the internal energy data.

We do not use any further extrapolation methods as we have simulated walks of such considerable length and feel that with such statistical errors that are left in the estimates, any extrapolation procedure is open to criticism. However, the estimates of ϕ are fairly constant over the decade plotted while estimates on shorter walks show a downward drift. The results of our estimation for all the exponents are in table I. Each result encompasses the predicted exact value. Assuming $\phi = \frac{3}{7}$, we can further estimate $U_\infty \approx 0.23290(3)$ and $C_\infty \approx 1.02(4)$.

In conclusion, we have stochastically enumerated relatively long (2×10^5) smart or dressed kinetic growth walks on the honeycomb lattice and estimated the thermal crossover exponent for the θ'-model to be $\phi \approx 0.44 \pm 0.02$. This is consistent with the exact crossover exponent $(\frac{3}{7} \approx 0.428)$ for the model proposed by Duplantier and Saleur [17] to be valid at the collapse transition.

Acknowledgements

It is a pleasure to thank R. Brak and A.J. Guttmann for helpful discussions and carefully reading the manuscript. Two of us, A.L.O. and T.P., are grateful to the Australian Research Council and D.B-W. to the Department of Mathematics, Melbourne University for financial support.

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