LETTER TO THE EDITOR

Universal distance ratios for two-dimensional polymers

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Abstract. By using a quantitative version of the c-theorem in conformal theories, we determine some universal gometrical features of two-dimensional critical systems, with emphasis on the ratios of mean square distances for polymers.

The application of the principle of conformal invariance has provided a variety of new results for two-dimensional critical phenomena. Among these are the calculation of exact values of critical exponents, which can be observed in real or computer experiments. Due to their geometrical nature, polymer systems have often been used as the simplest examples for illustrating predictions of the theory.

Less progress has been made in the understanding of the vicinity of the critical point, where one would like to determine explicity the different universal scaling functions. So far, one of the main results obtained in a quantitative version of the c-theorem [1] of Zamolodchikov, which allows the calculation [2] of the universal product $\lim_{T \to T_c} f_s \xi^2$ in terms of the central charge of the associated critical theory. In this letter, as a further application of the c-theorem, we determine some universal geometrical features of 2D critical systems, with emphasis on the ratios of mean square distances for polymers.

We first consider an $O(n)$ model near the critical point, with both thermal and magnetic perturbations, and continuum limit Hamiltonian

$$\mathcal{H} = \mathcal{H}^* + t \int \varepsilon(r) \mathrm{d}^2 r + h \int s^1(r) \mathrm{d}^2 r. \tag{1}$$

Here $\mathcal{H}^*$ is the fixed-point Hamiltonian, ε and s are the energy and spin operators. Due to the added terms in (1), the stress–energy tensor has a non-vanishing trace given by

$$\Theta(r) = 2\pi[y_t t \varepsilon(r) + y_h h s^1(r)] \tag{2}$$

where $y = 2 - x$, x the scaling dimension. The sum rule established in [2], $\Delta c = (3/4\pi) \int r^2 \langle \Theta(r)\Theta(0)\rangle \mathrm{d}^2 r$ relates the difference of the central charges of the UV and IR stable fixed points to the second moment of the two-point function of Θ. In the case under consideration, the IR stable fixed point is always the trivial one with $c = 0$. Thus the integral

$$\int r^2 [y_t^2 t^2 \langle \varepsilon(r)\varepsilon(0)\rangle + y_h^2 h^2 \langle s^1(r)s^1(0)\rangle + 2y_t y_h t h \langle s^1(r)\varepsilon(0)\rangle] \, \mathrm{d}^2 r \tag{3}$$

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is independent of both t and h in the scaling region. In this expression, correlators are calculated with the Hamiltonian (1), and we can expand them in powers of h. In the high-temperature phase where $s \leftrightarrow -s$ symmetry is not broken, the first-order term vanishes, while the second-order one gives

$$
y_t^2 t^2 \int (r_1 - r_2)^2 \langle \varepsilon(r_1)\varepsilon(r_2)s^1(r)s^1(0)\rangle \, \mathrm{d}^2r\mathrm{d}^2r_1\mathrm{d}^2r_2 + 2y_h^2 \int r^2 \langle s^1(r)s^1(0)\rangle \, \mathrm{d}^2r
$$

$$
- 4y_t y_h t \int r_1^2 \langle \varepsilon(r_1)s_1(r)s^1(0)\rangle \, \mathrm{d}^2r\mathrm{d}^2r_1 = 0 \tag{4}
$$

where correlation functions are now to be evaluated for a Hamiltonian with only a thermal perturbation. In (4) and subsequent equations the connected part of all correlation functions is implied.

The discrete Hamiltonian for the $O(n)$ model is $\mathcal{H} = -\beta \sum_{\langle ij \rangle} s_i \cdot s_j$ where $\langle ij \rangle$ denotes nearest neighbours of a regular lattice, β is the inverse temperature and s are n-component spins with $|s|^2 = n$. We can evaluate the equivalent of integrals in (4) by the usual graphical expansion [3]. In the $n \to 0$ limit, the loops disappear, as well as the subtracted terms in the connected correlators. The mean value $\langle \varepsilon(r_1)\varepsilon(r_2)s^1(r)s^1(0)\rangle$ for instance is interpreted as a sum over self-avoiding walks with extremities in 0 and r, and a bond in r_1, r_2. Note that each insertion of $\varepsilon(r)$ can be connected to the polymer in two ways, giving rise to factors of 2. Thus (4) gives

$$
8y_t^2 t^2 \sum_l \beta^{l-2}\omega_l \langle R_G^2\rangle_l l^2 + 2y_h^2 \sum_l \beta^l \omega_l \langle R^2\rangle_l - 8y_t y_h t \sum_l \beta^{l-1}\omega_l \langle R^2\rangle_l l = 0. \tag{5}
$$

In this expression, ω_l is the number of configurations of a SAW of length l attached to the origin. $\langle R_G^2\rangle$ and $\langle R^2\rangle$ are the usual radius of gyration and mean square end-to-end distance, while $\langle R'^2\rangle$ is the mean square distance of a monomer to the origin. Note the relation $\langle R'^2\rangle = \langle R_G^2\rangle + \langle R_1^2\rangle$ where R_1 is the distance of the centre of mass to the origin. Evaluating the asymptotic behaviour of sums in (5), with $\omega_l \sim l^{\gamma-1}\beta_c^{-l}$ and $t = \beta_c - \beta > 0$ gives the result

$$
\lim_{l \to \infty} \left(2 + \frac{y_t}{y_h}\right) \frac{\langle R_G^2\rangle_l}{\langle R^2\rangle_l} + \frac{1}{8} - \frac{\langle R'^2\rangle_l}{\langle R^2\rangle_l} = 0. \tag{6}
$$

The exponents $y_t = \frac{4}{3}$ and $y_h = \frac{91}{48}$ being known from Coulomb gas or conformal invariance techniques [4], (6) provides a precise relation between two universal ratios of geometrical quantities. Unfortunately the c-theorem does not seem to give access to the value of each of these ratios separately. $\langle R_G^2\rangle/\langle R^2\rangle$ has been obtained [5] to second order in ε-expansion as $\frac{1}{6} \times 0.8567$. A second-order calculation [6] gives similarly for $\langle R'^2\rangle/\langle R^2\rangle$ the value $\frac{1}{2} \times 0.8733$. Using these numbers we find for the combination in (6) a value of order 5%.

Identity (3) can also be used in the broken symmetry phase where correlators involving an odd number of spin operators do not vanish. At first order in h one finds then

$$
-ty_t \int (r_1 - r)^2 \langle \varepsilon(r_1)\varepsilon(r)s^1(0)\rangle \, \mathrm{d}^2r_1\mathrm{d}^2r + 2y_h \int r^2 \langle \varepsilon(r)s^1(0)\rangle \, \mathrm{d}^2r = 0 \tag{7}
$$

where averaged quantities are calculated with the Hamiltonian perturbed by the thermal operator, $t < 0$. Using scaling arguments, the last correlator can be replaced, up to a

factor $1+(y_h/y_t)$, by its t-derivative, giving

$$y_t \int (r_1-r)^2 \langle \varepsilon(r_1)\varepsilon(r)s^1(0)\rangle \mathrm{d}^2r\mathrm{d}^2r_1 - \frac{2y_h}{1+(y_h/y_t)} \int r_1^2 \langle \varepsilon(r_1)\varepsilon(r)s^1(0)\rangle \, \mathrm{d}^2r\mathrm{d}^2r_1 = 0. \quad (8)$$

This provides a relation between different moments of the same correlator $\langle \varepsilon\varepsilon s\rangle$.

One can use (8) to predict some geometrical properties of the dense phase of polymers [7]. The subtracted terms in connected correlators disappear due to the $n \to 0$ limit, and $\langle \varepsilon(r_1)\varepsilon(r)s^1(0)\rangle$ is a sum over configurations of a polymer passing through r and r_1, with one extremity in 0, and filling some finite fraction $f > 0$ of the accessible volume since $\beta > \beta_c$. The other extremity, due to this filling, is sent to infinity [7]. Hence from (8) we deduce the relation

$$\langle R_G^2\rangle / \langle R'^2\rangle = \frac{y_h}{y_t + y_h} \quad (9)$$

where the radii have the same definition as in (6). Equation (9) applies to a polymer attached at the origin and filling a fraction $f \to 0$ of the accessible volume, the limit $f \to 0$ being taken after the thermodynamic limit. Using the above values of the exponents, one finds for the right-hand side $\frac{91}{155}$. The ratio $\langle R_G^2\rangle / \langle R'^2\rangle$ is thus larger on the low-temperature side, as expected since the polymer is more compact.

Equation (8) may also be interpreted for magnetic systems in terms of a droplet picture [8]. Unlike the polymer case, this geometric picture is not exact, but nevertheless gives a useful way of thinking about the low-temperature phase. As an example, consider the Ising model where all the spins at infinity are fixed to be $+1$. At low temperatures, the dominant configurations contributing to a fluctuation in the magnetisation $s(0)$ at the point $r=0$ consist of a single droplet, or domain, surrounding $r=0$, inside of which the spins are all -1. In these configurations, the fluctuations in the energy density $\varepsilon(r)$ occur only on the boundary of the droplet. Thus, the first integral in (8) is proportional to twice the mean squared radius of gyration of the boundary R_1^2. Similarly the second integral is proportional to the mean square distance R_2^2 between a point on the boundary and a point in the interior of the droplet. Equation (8) then predicts that

$$R_2^2/R_1^2 = (y_t+y_h)/y_h. \quad (10)$$

Of course, close to criticality where (8) is supposed to be valid, the oversimplified model described above is not correct due to other fluctuations. However, in the spirit of the droplet model one may assume that these serve only to renormalise the local energy density and magnetisation, without destroying the whole picture. For a disc (indeed for any regular polygon) the above geometrical ratio is $\frac{3}{2}$. For a very filamentary object, where all points of the interior are very close to the boundary, the ratio is 3. For an object shaped like a spermatozoon, where most of the perimeter is well separated from the bulk, the ratio is 4. For the Ising model, the right-hand side of (10) is equal to about 1.53. Thus we conclude that Ising droplets are rather symmetrical, compact objects.

It is interesting to notice that the low-temperature phase of the $O(n)$ model is also critical, with properties that do not depend on β for $n < 2$. Letting $y_t \to 0$ in (9) we find

$$\langle R_G^2\rangle / \langle R'^2\rangle = 1 \quad (11)$$

which should apply to a polymer filling any fraction $f > 0$ of the volume. The result (11) looks reasonable for a dense walk. Indeed one expects the walk to fill the space

in a homogeneous way around its origin which should thus coincide with the centre of mass.

The above method can also be applied to the case of a tricritical point. We discuss here again the example of polymers. If one considers chains for which short distance repulsions and attractions compete, it is well known that a collapse transition can occur at the so-called theta point. The latter is described by a tricritical $O(n)$, $n \to 0$, theory.

In two dimensions, a model has been proposed [9] to study this transition, where the exponents can be calculated exactly. There, a polymer is represented by a self-avoiding walk, and attractions are induced by a gas of annealed forbidden random hexagons. If $n = 0$, the θ point occurs when obstacles percolate.

An advantage of this model is that the two scaling directions are microscopically identified, the associated relevant operators being the two legs (φ_2) and four (φ_4) legs operators with dimensions [9] $x_2 = \frac{1}{4}$, $x_4 = \frac{5}{4}$. φ^2 is coupled to the fugacity β of monomers (φ_2 coincides with the ε operator used above), and φ_4 to the nearest-neighbour attraction energy. Hence we can consider the fixed (θ) point Hamiltonian perturbed by φ_2 and φ_4 as in (1), the c-theorem leading to a formula similar to (3).

At first order one finds then, as in (8)

$$y_2 \int (r_1 - r)^2 \langle \varphi_2(r_1)\varphi_2(r)\varphi_4(0)\rangle \, d^2r d^2r_1$$

$$= \frac{2y_4}{1 + (y_4/y_2)} \int r_1^2 \langle \varphi_2(r_1)\varphi_2(r)\varphi_4(0)\rangle \, d^2r d^2r_1. \quad (12)$$

Taking $n \to 0$ limit keeps a single self-avoiding loop with attractions. In the graphical expansion of integrals in (12), the loops are weighted with the additional factor of their number of nearest-neighbour contacts due to the φ_4 insertions. However, it is known [10] that the probability distribution of this number is sharply peaked when $l \to \infty$, so we can write

$$\lim_{l \to \infty} \frac{\langle R_G^2\rangle_l}{\langle R'^2\rangle_l} = \frac{y_4}{y_2 + y_4} = \frac{3}{10} \quad (13)$$

where $\langle R_G^2 \rangle$ is the usual radius of gyration and $\langle R'^2 \rangle$ is the mean square distance of a monomer to a nearest-neighbour contact. Studying the ratio (13) may be a way of determining numerically the crossover exponent $\phi = y_4/y_2$ at the theta point.

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