Analytical model for a crossover between uncorrelated and fractal behaviour of a self-repulsive chain

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Abstract

The thermodynamics of a long self-repulsive chain is studied. In $D < 4$ dimensions it shows two distinctly different regimes, corresponding to weak and strong correlations in the system. A simple microscopic analytical model is presented which successfully describes both the regimes. The self-consistent scheme is used, in which the center of mass of a chain is fixed explicitly. This allows to take correlations into account in an indirect manner.

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Problem of a crossover between the strong-correlation regime and weak correlations is of a general interest for the solid-state physics. A textbook example is here the theory of phase transitions \[1\]. Not too close to the transition point Landau theory is valid, yielding the dimension-independent Landau set of critical indices. On the other hand, correlations in a critical region in a very vicinity of the transition result in different (dimension-dependent) values of critical indices, as it can be described by the renormalisation-group analysis \[2,3\]. While the two regimes are well understood in itself, no general microscopic analytical formula describes them simultaneously.

In this paper we draw a formula of this kind, which describes the behaviour of a simpler system, namely the self-repulsive chain. The peculiarity of this system is that it does not show a phase transition, but the two regimes mentioned above are still present. We believe that an absence of a spontaneous symmetry break makes things simpler, while the physics of a crossover remains somehow similar to more complicated problems like the description of the phase transition; for instance the problem of a self-interacting chain is closely related to the theory of percolation \[3\].

Let us first define the formal (mathematical) problem. We consider paths of a random walker on a cubic lattice in \(D\) dimensions, which returns to the starting point after \(L\) steps (see Figure 1 for the illustration); we suppose that \(L \gg 1\). These paths are closed polygons (maybe, self-crossing); positions of their vertexes \(x_i\) fulfill the condition

\[
||x_i - x_{i+1}|| = 1; \quad x_0 = x_L. \tag{1}
\]

We define the number of self-crosses for a given path \(X = \{x_0, x_1, ..., x_{L-1}\}\) by the formula

\[
N(X) = \frac{1}{2} \sum_{i \neq j} \delta(x_i; x_j), \tag{2}
\]

where \(\delta\) is a Kronecker symbol, and introduce a statistical average as follows:

\[
<f> = Z^{-1} \sum_X f(X) e^{-\beta N(X)}; \quad Z = \sum_X e^{-\beta N(X)}. \tag{3}
\]
Here sums are taken over all paths $X$, $f$ is a function of $X$, and $\beta$ is a small positive parameter. In particular, we shall monitor the dispersion $<(x-u)^2>$, where $u = L^{-1} \sum_i x_i$ is the position of the center of mass of a chain.

Physically, the above equations describe the statistics of a loop-chain with a potential energy equal to the number of its self-crosses $N$, at the inverse temperature $\beta$.

Since $\beta \ll 1$, for a sufficiently small $L$ the statistical weight $e^{-\beta N}$ is always close to 1, i.e. correlations in the system are negligible. Therefore we deal with a standard random-walk problem; for this case $<(x-u)^2> \propto L$. We shall refer to this case as an uncorrelated regime.

Let us establish a parameter which determines the magnitude of fluctuations. Since the typical volume occupied by the chain is proportional to $L^{D/2}$ in the uncorrelated regime, the average number of its self-crosses can be estimated as $N \propto L^{2-D/2}$. Therefore the dimensionless length $\lambda = \beta^{2/(4-D)} L$ can be introduced; the uncorrelated regime occurs at $\beta N \ll 1$, that corresponds to $\lambda \ll 1$.

In the opposite case of a large $\lambda$, correlations in the chain affect its statistics strongly. The problem is similar to the well-studied case of the statistics of a self-avoiding polymer molecule \cite{4,5}. The scaling laws are dimension-dependent and can be calculated by the renormalisation-group technique. For this "fractal" limit $<(x-u)^2> \propto L^\phi$ with $\phi = 2$ in 1D and takes non-integer values in 2D and 3D, which are respectively close to 4/3 and 6/5. In $D \geq 4$ the fractal regime is virtually absent, as $\phi$ takes the "uncorrelated" value 1 (there are logarithmic corrections in $D = 4$).

As it was declared above, the present paper is aimed to establish a formula that describes (at least qualitatively) both the uncorrelated regime and the fractal regime. The outline is as follows. First, the continuous analog (7) of the chain under study is introduced. Then, we switch to a kind of the self-consistent potential approximation (11). It yields simple formulae (15-19), that show the desired asymptotes for $<(x-u)^2>$. The result is then compared with numerical calculations.

Let us construct a continuous analog. One can neglect the short-range correlations,
as the critical behaviour in \( D < 4 \) is due to the long-range ones \[2\]. Let \( \tau \gg 1 \) be a "physically infinitesimal" length, on which correlations can be neglected; accordingly to the above estimations it should be \( \tau \ll \beta^{-2/(4-D)} \). Since \( \beta \) is small, in \( D < 4 \) these two inequalities can be fulfilled simultaneously. Consider the paths passing through some \( x_i \).

Then the distribution function of \( x \) at \( i + \tau \) is given by

\[
p_{i+\tau}(x; x_i) = p_0 \exp \left( -\frac{D(x - x_i)^2}{2\tau} \right),
\]

where \( p_0(\tau) \) is a normalisation factor. The number of paths passing simultaneously through given \( x_i \) and \( x_{i+\tau} \), is obviously proportional to \( p_{i+\tau}(x_{i+\tau}; x_i) \).

Introduce also the "partial" average number of self-crosse \( n_{ij} \), which counts only the crosses between the "sub-chains" of the length \( \tau \) located near \( i \) and \( j \). It is defined as

\[
n_{ij}(x_{i\tau} - x_{j\tau}, x_{i\tau} - x_{(i+1)\tau}, x_{j\tau} - x_{(j+1)\tau}) = \langle \sum_{k,m} \delta(x_k; x_m) \rangle;
\]

where indices \( k \) and \( m \) run only within the intervals \( i\tau \ldots i(\tau+1) - 1 \) and \( j\tau \ldots j(\tau + 1) - 1 \), respectively, whereas the averaging is carried out over the paths passing through \( x_{i\tau}, x_{(i+1)\tau}, x_{j\tau}, \) and \( x_{(j+1)\tau} \).

Full path \( L \) can be divided into \( L/\tau \) parts of the length \( \tau \), so that, for example, partition function \( Z \) takes the form

\[
Z = Z_0(\tau) \sum \exp \left( -\sum_{i=0}^{L/\tau} \frac{D||x_{i\tau} - x_{(i+1)\tau}||^2}{2\tau} - \frac{\beta}{2} \sum_{i,j=0}^{L/\tau} n_{ij} \right).
\]

Here the pre-exponential sum is taken over all possible sets \( \{x_0, x_\tau, \ldots, x_{L-\tau}\} \).

Obviously, \( n(r, \rho_1, \rho_2) \) peaks near \( r = 0 \) and falls fast at \( r \to \infty \). It can be verified \[3\] that \( \sum_r n(r, \rho_1, \rho_2) = \tau^2 \) at any \( \rho_1, \rho_2 \). So the continuous limit of \( (6) \) is as follows:

\[
Z = Z_0 \int [Dx] \exp \left( -\int_0^L \frac{Dx'^2(l)}{2} dl - \frac{\beta}{2} \int_0^L \int_0^L \delta(x(l) - x(l')) dl dl' \right).
\]

Here \( \delta \) is the Dirac \( \delta \)-function.

Self-parallel shifts of the whole chain are irrelevant for the statistical properties under study, so we can take the path-integral only over the closed paths with the center of mass fixed at zero:
\[ u = \int_0^L x dl = 0; \quad x(0) = x(L). \tag{8} \]

Continuous analog of the formula (3) for statistical averages can be written in the same manner. In particular, the distribution function of \( x \) is equal to

\[ p(x_0) = \frac{Z_p(x_0)}{Z}, \tag{9} \]

where \( Z_p(x_0) \) is a contribution to \( Z \) from the trajectories passing though the given point \( x_0 \) at \( l = 0 \), that is \( x(0) = x_0 \). Function \( p(x_0) \) is normalised:

\[ \int p(x_0) dx_0 = 1. \tag{10} \]

The key assumption of the present model is to approximate the second term in the exponent by the interaction with harmonic potential:

\[ -\frac{\beta}{2} \int_0^L \int_0^L \delta(x(l) - x(l'))dl'dl' \approx \int_0^L \left( U_0 + \frac{D\Omega^2 x^2(l)}{2} \right) dl, \tag{11} \]

where \( \Omega \) is defined in a self-consistent way:

\[ D\Omega^2 = -\beta LD^{-1}(\nabla^2 p)|_{x_0=0} \tag{12} \]

(the value of \( U_0 \) may remain undefined, as it drops out of the final formulae).

After the approximation (11) is done, the distribution function can be found straightforwardly. The problem resembles Feynman’s path-integral expressions for the statistics of a quantum particle [7], with however an additional condition for trajectories \( \int x dl = 0 \). Let us introduce a notation

\[ S_{x(l)} = \int_0^L \left( \frac{Dx'^2}{2} - U_0 - \frac{D\Omega^2 x^2}{2} \right) dl \tag{13} \]

and define the ”minimal-action” trajectory \( \bar{x}(l; x_0) \), which satisfy (8) and delivers a minimum of \( S \) at given \( \bar{x}(0) = x_0 \). The conditional minimisation results in the problem of a classical oscillator in the external field

\[ \frac{d^2\bar{x}}{dl^2} + \Omega^2 \bar{x} - f\bar{x} = 0, \tag{14} \]
where the value of $f$ should be chosen to fulfil the condition (8). The following minimal value of $S$ is obtained:

$$S_{\text{min}}(x_0) = -U_0 L + \frac{6D\Lambda(\omega)x_0^2}{L},$$

$$\Lambda(\omega) = \frac{\omega^2}{3} \left( \frac{1}{1 - \omega \text{ctg} \omega} \right),$$

$$\omega = \Omega L/2.$$

Consider now possible deviations from this trajectory: $x(l) = \bar{x}(l) + \tilde{x}(l)$, where $\bar{x}(0) = 0$ and the conditions (8) are satisfied. As the potential is harmonic it appears that $S_x = S_{\text{min}} + S_{\tilde{x}}$, and $Z_p$ can be factorised:

$$Z_p(x_0) = \tilde{Z} \exp(-S_{\text{min}}(x_0)).$$

Here $\tilde{Z}$ does not depend on $x_0$. The last two formulae and expressions (9, 10) allow to find out the distribution function:

$$p(x_0) = \left( \frac{6D\Lambda(\omega)}{2\pi L} \right)^{D/2} \exp \left( -\frac{6D\Lambda(\omega)x_0^2}{L} \right).$$

The dispersion is equal to

$$< x^2 > = \frac{L}{12\Lambda(\omega)}.$$ 

(17) Substitution of $\nabla^2 p$ in formula (12) gives the equation

$$\Lambda(\omega) = \frac{\pi}{3D} \left( \frac{2D\omega^2}{\pi \beta} \right)^{D/2} L^{-\frac{D+1}{2D+2}}.$$

The left-hand and right-hand sides of this equation are schematically plotted in Figure 2 as functions of $\omega$. There is a single root within the range $(0, \pi)$. Its position is governed by $\lambda = \beta^{2/(1-D)} L$. At $\lambda \ll 1$ we obtain $\omega \approx 0$ and therefore $\Lambda(\omega) \approx 1$, so

$$< x^2 > \mid_{\lambda \ll 1} = \frac{L}{12}.$$ 

(20) The "uncorrelated" dependence $< x^2 > \propto L$ is reproduced; moreover the factor $1/12$ is also correct. At the opposite limit $\omega(\lambda \gg 1) \approx \pi$, and it follows from (18-19) that
\[ <x^2> |_{\lambda \gg 1} = \frac{D}{4\pi} \left( \frac{\beta}{2\pi D} \right)^{\frac{3}{D+2}} L^{\frac{6}{D+2}} \]  

(21)

In particular, \( <x^2> \propto L \) in 4D and \( <x^2> \propto L^2 \) in 1D. The indices in 2D and 3D are also quite reasonable. In \( D > 4 \) the scheme is hardly suitable, as it is impossible to fulfill the inequality \( 1 \ll \tau \ll \beta^{-2/(D-4)} \) and the continuum analog (11) cannot be used.

It is important to discuss the following peculiarity of the approximation made. Usually, the use of mean-field schemes means that correlations like \( <x(l_1)x(l_2)> \) at \( l_1 \neq l_2 \) are totally neglected. In our scheme however some correlations are still present, because the center of mass of the trajectory is fixed (formula (8)). Namely, that circumstance results in a non-trivial dependence of \( S_{min}(L) \) and the dimension-dependent critical index in the last formula.

We have also compared the result obtained with Monte-Carlo calculations in 1D and 2D. Figure 3 shows bi-logarithmic plots for the dispersion \( <x^2> \) versus \( L \) at \( \beta = 10^{-2} \) in 1D and \( \beta = 5 \cdot 10^{-2} \) in 2D. Thin lines are asymptotes (20, 21). An agreement is quite good even quantitatively.

The final remark is that although we have considered only a particular random-walk problem (1) with unitary steps, it is clear that the model can be applied for any random-walk self-repulsing chains. It is only required that (a) the repulsion is short-range and (b) the central limit theorem can be applied, yielding the Gaussian distribution (9). Once these requirements are fulfilled, the continuous analog of the universal form (9) can be established.

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FIGURES

FIG. 1. Examples of the self-crossing closed chains in $D = 2$. In the central chain there is a single self-cross (positions of vertexes 1 and 3 are the same). In the right chain there are 3 whose pairs (3-5, 3-7, and 5-7).

FIG. 2. The sketch of $A(\Omega)$ (thick line) and the right-hand side of the equation (19) (thin lines). Note that in $D < 4$ the later is always a monotonic increasing function of $\omega$, so there is always a single root of (19).

FIG. 3. Monte-Carlo calculations of the dispersion $< x^2 >$ in 1D and 2D (points), compared with estimations from formula (18). Thin lines show the displacive and fractal asymptotes.
\[ \lambda \ll 1 \]
(weak correlations)

\[ \lambda \gg 1 \]
(strong correlations)
\[ \frac{L}{2 D/c^98} = 0.05 \]

\[ \beta = 0.01 \]

\[ \beta = 0.05 \]