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Directed Polymers in Hartree–Fock Approximation

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A replica trick is used to map the problem of directed polymers into a quantum mechanics problem of n-body bound states. This bound-state problem is then treated using a self-consistent method of Hartree–Fock. For $d=2$, the exact result of the DP exponents is reproduced; and for complex DP, the ground-state energy $E_n \sim n^2$ is found, confirming previous numerical results.

KEY WORDS: Directed polymers; replica trick; self-consistent fields.

The problem of directed polymers (DP) in random media has recently drawn considerable attention.(1) The DP problem is related to the Burgers' equation in fluid dynamics,(2) to that of domain walls in the $2d$ random bond Ising model,(3) and to surface growth.(4)

The model can be defined in a Feynman path integral form:

$$W(\mathbf{x}, t) = \int_{(0,0)}^{(\mathbf{x},t)} \mathscr{D}\mathbf{x} \exp - \int_0^t d\tau \left[\frac{1}{2} \left(\frac{d\mathbf{x}}{d\tau} \right)^2 + V(\mathbf{x}(\tau), \tau) \right] \tag{1}$$

where $W(0,0)=1$, and $V(\mathbf{x}, t)$ is a quenched random potential, or disorder, which obeys $\overline{V(\mathbf{x}, t)\, V(\mathbf{x}', t')} = 2\delta(\mathbf{x}-\mathbf{x}')\,\delta(t-t')$, where the overbar denotes the sample average. The above expression is a sum over all possible oriented (in the t direction) paths that connect $(\mathbf{x}, t)$ to $(0, 0)$, with due random weights along each path.

In contrast to the disorder-free, or pure case, the "wave packet" $W(\mathbf{x}, t)$ is not symmetric with respect to the geometric center $\mathbf{x}=0$, for any given single sample. One is thus interested in its transverse deviation, defined as $x_c = \overline{|\langle \mathbf{x} \rangle|}$, where $\langle \cdot \rangle$ denotes the average using the normalized

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probability density $P(\mathbf{x}, t) = W(\mathbf{x}, t) \int d\mathbf{y}\, W(\mathbf{y}, t)$. One expects x_c to be a scaling function of t, $x_c \sim t^{\nu}$.

A generalization of the DP problem is to consider the complex random amplitude $\exp -iV(\mathbf{x}, t)$ in place of $\exp -V(\mathbf{x}, t)$, and the quantity of interest is $|W(\mathbf{x}, t)|^2$ in place of $W(\mathbf{x}, t)$, in Eq. (1). Hence the model is called the complex DP, or CDP problem.(5,6) It has applications in the study of hopping conductivity(7) and electron or light transmission through random media.

For short-range, correlated disorder, the scaling exponents for the DP problem are known analytically only for the $d=2$ case; those for all other cases (including $d=2$ CDP) are only available from direct or indirect numerical simulations. Nevertheless, there is an established exponent relation(8) $\nu = (1+\omega)/2$, where ω is the scaling exponent of the free energy fluctuation: $F(t) = -\ln |W(\mathbf{0}, t)|$ can be called free energy, which varies from sample to sample; its fluctuation is $[\Delta F(t)]^2 = \overline{[F(t) - F_0]^2} \sim t^{2\omega}$, where $F_0 = \overline{F(t)}$.

There is a way to obtain the exponent ω analytically. To this end, we need to consider the moments $\overline{W^n(\mathbf{0}, 0)}$ [here and below $\overline{|W(\mathbf{0}, 0)|^{2n}}$ for CDP], for arbitrary positive integer n. This is essentially a *replica* trick.[2] Our disordered DP and CDP models are thus mapped onto $(d-1)$-dimensional quantum mechanical, n-body bound-state problems.(6,10)

In anticipation of the bound-state energy result, we may express $\overline{W^n} = \exp -tE_0(n)$, where the ground-state energy is $E_0(n) \sim -n^{\beta}$, for asymptotically large t and n. From the knowledge of these moments, we can reconstruct the probability distribution function(5) of the free energy $F(t)$,

$$P(F) \sim \exp\left(-a\,\frac{|F-F_0|^{\eta}}{t^{\eta/\beta}}\right) \tag{2}$$

where $\eta = \beta/(\beta - 1)$, $\beta > 1$, a is a constant. From it we deduce that $\Delta F \sim t^{1/\beta}$, or the desired exponent $\omega = 1/\beta$. The aim of this note is to show a new way of estimating the bound-state energy exponent β [hence $\omega = 1/\beta$ and $\nu = (1 + 1/\beta)/2$]. Note that in general $E_0(n)$ contains subleading terms in n, which depend normally on the schemes or approximations employed. However, it is clear from the above discussion that only the leading term in n determines the scaling behavior. This is to be contrasted with the traditional *replica* trick, where the opposite limit $n \to 0$ is assumed.

Our problems are reduced to finding the ground-state energies of the Schrödinger equations; the number of particles n is assumed to be large

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[2] See ref. 9 for a somewhat different approach, where bound-state problems are also discussed.

and here we consider the $d=2$ cases only. For the DP problem all n particles are subject to mutual attractive interaction; we have

$$\left\{-\sum_{i=1}^{n} \partial_i^2 - \sum_{i>j} \delta(x_i - x_j)\right\} \Psi(x_1,..., x_n) = E_0(n)\, \Psi(x_1,..., x_n) \tag{3}$$

For the $d=2$ case it has been solved(10) using Bethe ansätze, and it was found that $E_0(n) \sim -n^3$. For the CDP case, we have the analogous equation(6)

$$\left\{-\sum_{i=1}^{2n} \partial_i^2 + \sum_{i>j} e_i e_j \delta(x_i - x_j)\right\} \Psi(x_1,..., x_n) = E_0(n)\, \Psi(x_1,..., x_n) \tag{4}$$

where e_i can be considered the charge (via the contact interaction, though) of the ith particle: $e_i = 1$ for $1 \leqslant i \leqslant n$ and $e_i = -1$ for $n \leqslant i \leqslant 2n$. Thus, for the CDP problem the total system is charge-neutral; bound states can be formed through dipolar and multipolar interactions. I have tried to diagonalize this Hamiltonian along the lines of the traditional Bethe ansatz approach, like that for the DP case, without success. Below I want to follow an alternative approach, tackling both problems on equal footing.

Here a Hartree–Fock approximation can be introduced to solve the above equations for $d=2$. For details of its application to the above n-body attraction problem see a recent textbook,(11) where comparison was made between the exact Bethe ansatz solution and that of the HF mean field approximation—they agree to the leading order in n. This is a consequence of a more general conclusion of $1/n$ expansion.(11) I outline the precedure below. For n attracting particles one can define a single-particle wave function $\phi(x)$, which should satisfy the self-consistent equation

$$\{-\partial^2 - (n-1)\, |\phi(x)|^2\}\, \phi(x) = \varepsilon\phi(x) \tag{5}$$

with the normalization condition $\int dx\, |\phi(x)|^2 = 1$, and the boundedness requirement $|\phi(x \to \pm\infty)| \to 0$; ε denotes the (bound) ground-state energy of a single particle, and $E_0(n) = n\varepsilon$. In the following I will only keep the leading order in n, hence in the above equation $n-1$ will be replaced by n. The above equation is integrable and has the normalizable soliton solution

$$\phi(x) \sim \pm n^{1/2}/\cosh(nx) \tag{6}$$

only when(12) $\varepsilon = -n^2$. Thus, we obtain the result $E_0(n) = -n^3$, in agreement with the exact Bethe ansatz solution.(10) The above soliton solution shows that the typical physical size R of the bound state is $R \sim 1/n$. Recall that in the original n-body bound state problem, if n particles are confined in a (small) region R, the total kinetic energy $\sim n(1/R)^2$ opposing the collapse should be of the same order of magnitude as the ground-state energy $\sim -n^3$. The above solution is consistent with this expectation.

For the CDP case, or Eq. (4), it is not as easy to write down the Hartree–Fock self-consistent equation for a single wave function. We need more physical insight. In Eq. (4) we have n positive charges and n negative charges; they can form a boundstate because they cannot screen each other's charges completely. Two particles of opposite charges can be bound into a pair by the direct attraction, two such pairs can be bound together by a dipolar (attractive) interaction, groups of more particles can be bound together by multipolar attractions, and so on. However, the interaction strength (or coupling constant) per particle for a bound state of *larger* number of particles is *weaker*; this is due to the aforementioned charge screening. Since we are only interested in the final bound state of the $2n$ particles, it suffices to ask what is the necessary interaction strength per particle for this case.

Let us split the total $2n$ charges into two separated groups, in an arbitrary way, so that each contains $\sim n$ charges. As a consequence of the central limit theorem, each group contains $\sim \sqrt{n}$ *unpaired* excess charges (the two groups have opposite signs, due to charge conservation). It is these excess charges that are solely responsible for holding the $2n$ charges bound. Nor knowing exactly which particle actually contributes to these excess charges, we assume that they can be thought of arising uniformly from all the particles $\sim n$, each contributing $\sim 1/\sqrt{n}$. This assumption is consistent with the philosophy behind the Hartree–Fock approximation.

This can be also seen from another perspective: Among the $2n$ particles, there are n^2 attractive bonds (pairs) between opposite charges; $n(n-1)$ repulsive bonds between like charges. As a result, there are n *net* attractive bonds, which can be redistributed among the $2n$ particles, each having an effective strength $\sim 1/\sqrt{n}$.

The above reasoning helps us to identify the leading order (in n) contribution; hence the conclusions that follow are valid only for large n.

A single particle is again immersed in the field of the $\sim n$ other particles, but with a smaller coupling constant $\sim 1/\sqrt{n}$ than that $(=1)$ of the DP case. All we need to change in Eqs. (5) and (6) is to replace the factor n by $\sqrt{n}$. The self-consistent equation for this case should be

$$\Delta\phi(x) + n^{1/2}\phi(x)^3 - \varepsilon\phi(x) = 0 \tag{7}$$

The discussion which leads to this equation shows that it is straightforward to conclude that $\varepsilon = n$ or $E_0(n) = -n^2$. The soliton solution $\phi(x) \sim \pm n^{1/4}/\cosh(n^{1/2}x)$ shows that the bound state now has a physical extension of $R \sim 1/\sqrt{n}$. The kinetic energy $n(1/R)^2$ is of the same order as $E_0(n)$. Note that R for CDP is larger than that of the DP case, consistent with the present general argument. The bound-state energy exponent $\beta = 2$ for $d = 2$ CDP implies that the exponent $\nu = 3/4$, which was previously conjectured on the basis of direct numerical simulations.(5,6)

I have not discussed how to generalize the above approach to $d > 2$ cases. There are difficulties in doing so: First, using a spherical approximation to study an effective one-dimensional nonlinear Hartree–Fock equation is far from being justified—there are indications that particles inside the bound states follow some singular distribution; assumptions of homogeneity and isotropy of particle distribution are suspicious. Even assuming spherical symmetry, i.e., $\phi(\mathbf{x}) = \phi(r)$, the resulting Hartree–Fock equation

$$\left\{-\partial_r^2 - \frac{d-2}{r}\partial_r - (n-1)\,|\phi(r)|^2\right\}\phi(r) = \varepsilon\phi(r) \tag{8}$$

is not integrable. The second term in (8) can be regarded as "dissipative," which spoils the solvability. It can be shown the above equation may not have any solution at all, not even numerically. Only for a discrete set of parameters can numerical solutions be found.(12)

For $d > 2$ DP cases here are plenty of numerical results for the related problem of surface growth, which can be readily transcribed here for our bound state problems. The initial numerical simulations lead to the so-called superuniversality hypothesis, i.e., $E_0(n) \sim -n^3$ for all d. Later, there were more careful numerical simulations on the related surface growth equation, most notably those by Wolf and Kertész(13) (WK), and very recently by Kim and Kosterlitz(14) (KK). Based on numerical results, WK conjecture that (in the present notation) $\omega_{\mathrm{DP}} = 1/(2d-1)$, while the new results of KK indicate $\omega_{\mathrm{DP}} = 1/(d+1)$. The subscript denotes that the exponent is for the DP case. One curious feature shared by both conjectures is that the related bound-state exponent β assumes only *integer* values. For the dimensionalities $d = 2, 3, 4,\ldots$, according to WK, $\beta_{\mathrm{DP}} = 3, 5, 7,\ldots$, and according to KK, $\beta_{\mathrm{DP}} = 3, 4, 5,\ldots$. These integer solutions are *aesthetically* very appealing, especially considering that, when the above authors proposed them, they were not biased by our bound-state problems.

Which one of the above numerical conjectures for the $d > 2$ DP problem may well turn out to be exact, future numerical as well as analytical work may decide. What can one say for the corresponding CDP problem? From the previous discussion on the Hartree–Fock approximation, one may expect that the bound-state energies of the CDP and DP problems are related in the following way: the bound-state energy for DP is $-n^{\beta_{\rm DP}}$, which can be rewritten as $-n \cdot n^{\beta_{\rm DP}-1}$, where the factor n is singled out for the particle number. I propose that the bound-state energy for CDP should be $-n \cdot n^{(\beta_{\rm DP}-1)/2}$. In other words, it should be $\sim -n^{\beta_{\rm CDP}}$, $\beta_{\rm CDP} = 1 + (\beta_{\rm DP} - 1)/2$. I have used the fact that the above argument leading to the $d = 2$ CDP result, that the interaction strength is $1/\sqrt{n}$ per particle, does not depend on the dimensionality d. However, while for the $d = 2$ case one can justify this relation by finding a self-consistent solution, for the $d > 2$ cases the relation can be only considered a speculation. From this conjectured $\beta_{\rm CDP}$, one can deduce two other exponents, $\omega_{\rm CDP} = 2/(1 + \beta_{\rm DP})$ and $\nu_{\rm CDP} = (3 + \beta_{\rm DP})/[2(1 + \beta_{\rm DP})]$ for complex polymers, where $\beta_{\rm DP}$ can assume the above values, conjectured from numerical work.

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