Testing a Variational Approach to Random Directed Polymers

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Abstract

The one dimensional direct polymer in random media model is investigated using a variational approach in the replica space. We demonstrate numerically that the stable point is a maximum and the corresponding statistical properties are for the delta correlated potential in good agreements with the known analytic solution. In the case of power-law correlated potential two regimes are recovered: a Flory scaling dependent on the exponent of the correlations, and a short range regime in analogy with the delta-correlated potential case.

1 Introduction

A challenging open problem in statistical mechanics is the behavior of fluctuating random manifolds with quenched disorder (for a review see [1]). New insight has been obtained in the framework of replica formalism [2] and, at least at the level of the tree approximation (Hartree-Fock) which is the exact solution in the limit of infinitely many dimensions, the problem has been hopefully solved [3]. Nevertheless the approximation turned out to be maybe too drastic for take in account the behavior in all dimension and for different structures of correlation of the quenched noise. For instance the prediction

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for the wandering exponent $\zeta$ of one-dimensional direct polymers in random media (DPRM) are wrong even in the case of short range correlations of the random potential.

In the following we will restrict to DPRM, which due to their one-dimensional structure are simpler than random manifolds with generic dimension.

After this short introduction we will present some details on the model and we will define some basic mathematical tools in order to introduce in section 3 the variational approach developed in [5] and reformulating it in a suitable form to implement a numerical simulation. Section 4 is divided in two parts: in the first one we check the agreement of our results with Kardar’s analytic solution [4] for the delta-correlated potential and in the second part we study the power-law correlated potential for different values of its exponent. Two different scaling regimes are recovered: a short-range one analogous to the delta-correlated potential, and a Flory like regime in which the wandering exponent depends from the power-law correlation exponent in agreement with the one loop renormalization group analysis presented in [4]. Finally in section 5 we present comments and perspectives.

2 The Model

Knowledge of end point probability distribution in DPRM is of fundamental importance. In principle it is always possible to determine this probability distribution $P_t[x]$ starting from the explicit structure of the Hamiltonian of the system which depends on the space coordinate set $x$, the time $t$, and the random potential $\eta$:

$$H[x] = \int dl \left\{ \frac{1}{2} \frac{d\mathbf{x}}{dl} + \eta(x, t) \right\}$$

(1)

The related partition function satisfies the imaginary time Schrödinger equation:

$$\frac{\partial Z(x, t)}{\partial t} = 1/2 \nabla^2 Z(x, t) + \eta(x, t) Z(x, t)$$

(2)

The polymer’s end point probability distribution function $\rho(x, t)$ is readily obtained by:

$$\rho(x, t) = \frac{Z(x, t)}{\int d^d\mathbf{y} Z(\mathbf{y}, t)}$$

(3)
We want to implement a variational approach in order to determine a functional of the probability \( P_t[\rho(x,t)] \) which allows direct calculation of the quenched noise average of a generic observable \( O \) by the functional integration:

\[
\overline{O[\rho(x,t)]} = \int d[\rho] P_t[\rho(x,t)] O[\rho(x,t)]
\]  

(4)

Quenched averaging is believed to be a rather difficult problem in spin-glass and DPRM models. Replica technique consists on calculating quenched average of the replicated partition function. We can therefore introduce \( Z(\{x_a\},t) = Z(x_1,t)Z(x_2,t)...Z(x_n,t) \) as the solution of the imaginary time Schrödinger equation:

\[
\frac{\partial Z(\{x_a\},t)}{\partial t} = \left[ \frac{1}{2} \sum_{i=1}^{d} \sum_{a=1}^{n} \frac{\partial^2}{\partial x_{i,a}^2} + \sum_{a<b}^{n} V(x_a - x_b) \right] Z(\{x_a\},t)
\]  

(5)

where \( V(x - y) = \eta(x,t)\eta(y,t') \). A couple of explicit solutions to (5) are already available for \( V(x - y) = \delta(x - y) \) [4] and \( V(x - y) = (x - y)^2 \) [3], both of them in the one dimensional case \( d = 1 \). Unfortunately those are the only known analytical solutions of the problem which in general can be only studied by mean of renormalization group approximate technique [4]. A particular solution of (5) can be decomposed over the eigenstate’s set of the Hamiltonian:

\[
Z(\{x_a\},t) = \sum_{i} c_i \Psi_i(\{x_0\}) \Psi_i(\{x_a\}) e^{-E_i t}
\]  

(6)

From the previous expression it is evident that all the excited states decrease sub-exponentially compared with the ground state, and then the thermodynamic behavior of the model will be ruled in the asymptotic regime by the structure of the ground state. In this regime is possible to calculate for instance:

\[
\overline{\rho(x_1)\rho(x_2)} = \int dP[\rho] \rho(x_1)\rho(x_2) \propto \int dx_3 dx_4...dx_n \psi(x_1, x_2, ..., x_n)
\]  

(7)

where \( \psi(x_1, x_2, ..., x_n) \) is the ground state of (5) and \( dP[\rho] = \lim_{t \to \infty} dP_t[\rho] \).

Since we know the exact solution of the one dimensional delta-correlated potential model, a careful analysis of its ground state structure should be illuminating for further development of the variational principle. In fact a
straight application of the Bethe ansatz - which turns out to be the exact solution of the delta-correlated model - shows that the ground eigenstate is:

$$\psi(x_1, x_2, ..., x_n) = \prod_{a<b} e^{-A|x_a - x_b|}$$  \hspace{1cm} (8)

with energy:

$$E^{(n)} = -\frac{n(n^2 - 1)A^2}{3}$$  \hspace{1cm} (9)

where $A$ is a constant depending on the parameters of the Hamiltonian. So, following M´ezard et al. in [5], in the general case a reasonable choice should restrict the space of $n$-particles test functions to the following:

$$\psi(x_1, x_2, ..., x_n) = \prod_{a<b} f(x_a - x_b)$$  \hspace{1cm} (10)

A direct calculation shows that this is tantamount to choosing the following Gaussian probability distribution $P_g[\phi]$ for $\phi(x) \equiv \ln(\rho(x))$:

$$P_g[\phi] \propto \exp \left[ -\frac{1}{2} \int d^dxd^dy \phi(x)g(x - y)\phi(y) \right]$$  \hspace{1cm} (11)

In fact performing a Gaussian integration we obtain:

$$\int d[\phi] \exp \left[ \sum_{n=1}^n \phi(x_a) - \frac{1}{2} \int d^dxd^dy \phi(x)g(x - y)\phi(y) \right] = \prod_{a,b} f(x_a - y_b)$$  \hspace{1cm} (12)

and the following relation holds:

$$\int d^dz \ g(x - z) \ln[f(z - y)] = \delta^d(x - y)$$  \hspace{1cm} (13)

In the previous one dimensional case $g$ must be chosen in such a way that:

$$\int dx dy \ \phi(x)g(x - y)\phi(y) = \int dx \frac{1}{2} |\nabla \phi|^2$$  \hspace{1cm} (14)

It’s now reasonable to guess for our ground state a functional structure of the following type:

$$\psi(x_1, x_2, ..., x_n) \propto \int dR[\mu] \mu(x_1)\mu(x_2)...\mu(x_n)$$  \hspace{1cm} (15)

The distribution functions $P[\rho]$ and $R[\mu]$ are related by:

$$\frac{\rho(x_1)\rho(x_2)}{\rho(x_1)\rho(x_2)} = \int dP[\rho] \rho(x_1)\rho(x_2) = \int dR[\mu] \frac{\mu(x_1)\mu(x_2)}{I[\mu]^2}$$  \hspace{1cm} (16)

where $I[\mu] = \int d^d x \mu(x)$. 

4
3 The Variational Principle

Since now we have recast our problem in a (hopefully) suitable form to implement the variational principle which consists on minimizing the quadratic form $\langle \psi | H | \psi \rangle$, where $H$ is the replicated Hamiltonian operator which appears in the square brackets of (5). In order to obtain normalized eigenstates we have to enforce this condition by the introduction of a Lagrangian multiplier. Following this procedure described in [5] we easily obtain:

$$\langle \psi | H | \psi \rangle = \int dR[\mu]dR[\sigma] \mathcal{H}_n[\mu, \sigma]$$

where

$$\mathcal{H}_n[\mu, \sigma] = \frac{n}{2} \int d^d x \sum_{\nu=1}^{d} \frac{\partial \mu}{\partial x_\nu} \frac{\partial \sigma}{\partial x_\nu} I[\mu\sigma]^{n-1} + n(n-1) \int d^d x d^d y \mu(x)\mu(y)V(x-y)\sigma(x)\sigma(y) I[\mu\sigma]^{n-2}$$

The normalization in terms of our trial functions is:

$$\langle \psi | \psi \rangle = \int dR[\mu]dR[\sigma] I[\mu\sigma]^n$$

In this new representation the Schrödinger equation reads:

$$\int dR[\sigma] \mathcal{H}_n[\mu, \sigma] = E_n \int dR[\sigma] I[\mu\sigma]^n$$

It’s now possible to consider the $n \to 0$ limit of (20). In this limit we can eventually implement the variational principle in terms of the stationary point of the free energy functional $F[R] = \int dR[\mu]dR[\sigma] \mathcal{H}[\mu, \sigma]$, and $\mathcal{H}$ is now defined by:

$$\mathcal{H}[\mu, \sigma] = \frac{1}{2} \int d^d x \sum_{\nu=1}^{d} \frac{\partial \mu}{\partial x_\nu} \frac{\partial \sigma}{\partial x_\nu} I[\mu\sigma]^{-1} + \int d^d x d^d y \mu(x)\mu(y)\sigma(x)\sigma(y)V(x-y) I[\mu\sigma]^{-2}$$

As far as replica symmetric approximation is concerned, the problem is recast just in finding the proper $g$-function - as defined in (11) - which is stationary against variations of the following functional:

$$\int dP_g[\phi_1]dP_g[\phi_2] \mathcal{H}[\exp(\phi_1), \exp(\phi_2)]$$
Performing analytic calculation on this functional is hopeless, so we are forced to try a numerical approach in order to calculate the critical exponents of the model.

4 Numerical Analysis

4.1 The delta-correlated potential

As already mentioned, 1-dimensional DPRM with delta-correlated random potential is explicitly solvable and so it is a good testing ground for our variational approach. For technical reasons it is simpler to consider the case in which a lattice spacing is introduced. The Hamiltonian, taking lattice spacing, \( a = 1 \) is:

\[
\mathcal{H}[\mu, \sigma] = \frac{1}{2} \sum_{i=1}^{N} (\mu_{i+1} - \mu_{i})(\sigma_{i+1} - \sigma_{i})I[\mu\sigma]^{-1} + G \sum_{i,j}^{N} \mu_{i}\mu_{j}\sigma_{i}\sigma_{j}V_{ij}I[\mu\sigma]^{-2}
\]

(23)

where in the delta-correlated case \( V_{ij} = \delta_{ij} \). The continuum limit can be reached sending the lattice spacing to zero or sending the coupling constant measured in lattice units to zero. Indeed the dimensionless coupling constant is \( Ga^3 \). Although the wandering exponent is supposed to be independent from the lattice spacing, the continuum limit may be interesting as a check to our computation.

In order to implement a numerical integration of (22) we need as a first step to generate the fields \( \phi \) which follow the distribution \( P_g[\phi] \). The Fourier representation of this probability distribution is:

\[
P_g[\phi]d[\phi] \propto \prod_{k<\Lambda} d[\phi_k] \exp(g_k|\phi_k|^2)
\]

(24)

where \( k \in \{(\pi n)/L\}_{n=1,2,...,N} \), \( N \) are equally spaced intervals in which we consider discretized the field \( \phi(x) \) \( x \in \{0, L\} \) and \( \phi_k \) are Fourier coefficients of \( \phi \). The integration in Fourier space “decouples”, in the sense that now the probability distribution is the product of the individual \( k \)-wave vector probability distributions.
Assuming that the wave function on the lattice is the same as in the continuum (the difference among the two going to zero in the continuum limit), a little algebra reveals that:

\[
\prod_{a<b} e^{-A|x_a - x_b|} = \int d[\phi] \prod_{a=1}^{n} \exp \left\{ \phi(x_a) - \int dx \frac{|
abla \phi(x)|^2}{4A} \right\}
\]

(25)

which means that for delta-correlated noise we straightforwardly obtain:

\[
dP[\phi] \propto \exp \left\{ \int dx \frac{|
abla \phi(x)|^2}{2A} \right\} d[\phi] \propto \prod_{k<\Lambda} \exp \left\{ \frac{k^2|\phi_k|^2}{2A} \right\} d[\phi_k]
\]

(26)

From the structure of (26) we can reasonable guess the following structure for the probability distribution:

\[
dP[\phi] \propto \prod_{k<\Lambda} \exp \left\{ -\frac{\lambda k^2 \alpha |\phi_k|^2}{2} \right\} d[\phi_k]
\]

(27)

in which both \(\alpha\) and \(\lambda\) are to be considered as variational parameters related with the fluctuations of \(\phi\), since:

\[
\langle (\phi(x) - \phi(y))^2 \rangle = \int dP[\phi]|(\phi(x) - \phi(y))^2| = \lambda |x - y|^{\alpha}
\]

(28)

Comparing (24) with (27) it’s easy to deduce that the delta-correlated case is obtained setting \(\alpha = 1\), so we used this result to a first tuning of the variational parameters. We have generated statistically uncorrelated random numbers distributed as (27) with \(\alpha = 1\). Back Fourier transforming via FFT algorithms \[\text{[6]}\] the coefficients \(\phi_k\), we are able to obtain statistically uncorrelated realizations of \(\phi(x)\). Let \(\Gamma\) be the set of \(M\) realizations of \(\phi(x)\), we have found a suitable interval of values for \(\lambda\) in which:

\[
\frac{1}{M} \sum_{a \in \Gamma} (\phi((x_a) - \phi(y_a)))^2 = C |x - y| \quad C = O(1)
\]

(29)

The \(\phi(x)\) fields built following this prescription are the configurations used for calculating the value of the free energy functional \(\mathcal{H}\) defined in (21). It is obvious that such a value should depend on the realization of the fields and so we have to average over a significative number of this realizations, or more formally, \(|\phi_a\) and \(|\psi_a\) being the \(a\)-th of \(M\) realizations, we can compute:

\[
\langle F \rangle = \frac{1}{M^2} \sum_{a,b=1}^{M} \langle \psi_a | \mathcal{H} | \phi_b \rangle
\]

(30)
where in this case we use the delta-correlated potential $V(x-y) = \delta(x-y)$.

It’s easier to use intensive variational parameters, so we redefine (27) as:

$$dP_g[\phi] = \prod_{k<\Lambda} d[\phi_k] \exp \left( -N^{3/2} \alpha k^{2\alpha} \lambda \right)$$

(31)

where $\alpha$ and $\lambda$ are new variational parameters.

A crucial question now is whether the free energy functional should be maximized or minimized, since from a strictly formal point of view we are considering the $n \rightarrow 0$ limit, a regime in which thermodynamic behavior is not evident at all. In the general theory proposed in [7] it is proved that Hartree Fock approximation consists in a saddle point on the number of components of the field going to infinity, and the solution is a maximum of the functional. A possible argument which explains this rather unusual feature of replica theory is that the Hamiltonian (5) is translational invariant, so if we choose the center of mass reference frame we are left with $n-1$ degree of freedom (a number which is negative as soon as $n < 1$!). This is the regime in which the stationary point becomes a maximum of the functional.

The numerical simulations have clearly pointed out that the stationary point of the functional is really a maximum confirming the reasonment. Let us first present what happens for the coupling constant $G = 1$. Setting $\lambda = 1$ the free energy functional develops a maximum for $\alpha = 1.1$. The maximum value is obtained by varying also the $\lambda$ parameter. Iterating this procedure in the interval $\lambda \in \{0.8 : 1.3\}$ we find that as the value of $\lambda$ grows
Figure 2: Plot of free energy $F$ vs. $\alpha$. The maximum value of $F$ is obtained for $(\alpha = 1.0, \lambda = 1.4)$.

inside the interval, the free energy maximum shifts from $(\alpha = 1.15, \lambda = 1.0)$ to $(\alpha = 1.0, \lambda = 1.4)$ increasing monotonically its value. Over the point $(\alpha = 1.0, \lambda = 1.4)$ we observe a decrease of functional. The range of the free energy functional in this window of parameters belongs to the interval $\{0.24 : 0.26\}$.

The value given in (9), is $F = 1/3$ which is of the same magnitude of our simulation but significatively outside the error bar. This difference from the analytic value must be addressed to the fact that we are replacing a continous model with a unitary step discretization so that only wave functions which vary on a length scale bigger than our discretization make sense. It is therefore reasonable to introduce a modulation on the coupling between replicas in (21) tuning the coupling constant $G$. The corresponding ground state energy is now $G^2/3$. As far as values of $G < 1$ are concerned, the binding between replicas is lowered, and bound states with variations on a wider length scale are favored. We can’t consider anyway too small values of $G$ since in this case it’s impossible to build a bound state and the stationary wave function turns out trivially to be constant.

Following the previous considerations for each value of the coupling constant $G$ in the interval $\{0.5 : 1.2\}$ we have generated $10^5$ realizations of $\phi$ with $(\lambda = 1.4, \alpha = 1.0)$. As showed in figure (3), we were able extrapolate from the linear fit of $E(G)/G^2$ vs. $G^2$ the value of the abscissa $F = 0.331 \pm 0.005$ which fits surprisingly well the analytic value of $1/3$.

The variance around mean value overestimates the statistical error related
Figure 3: Plot of $E(G)/G^2$ vs. the square of the coupling constant $G^2$. Here $N = 64$ and $(\lambda = 1.4, \alpha = 1.0)$. From the linear fit extrapolate $\lim_{G^2 \to 0} E(G)/G^2 = 0.331 \pm 0.005$.

with our numerical estimates of free energy, since as we can see from the normalized histogram of energy distribution in figure, relevant power-law tails are present. In order to give a reasonable estimate of statistical errors, we have generated for each experimental point $10^6$ realizations of free energy, which we have randomly divided into 10 subsets of $10^5$ elements. If - say $K$ - is the number of subsets, the statistical estimate of variance made using the whole number of data we have, is $K - 1$ times bigger than the estimate given from averaging every variance in the subsets built under the previous prescription.

It’s worth noting that the variational parameter $\alpha$ is strictly related with critical exponents of the model like for instance the wandering exponent $\zeta$ defined by the relation $\langle |x| \rangle \sim t^\zeta$. As pointed out in [8] $\phi(x) \sim x^2/t$, and since from (28) we know that $\phi(x)^2 \sim x^\alpha$, is possible to argue that $\zeta = 2/(4 - \alpha)$. In one dimension delta-correlated potential we found the stationary point for $\alpha = 1$, which means $\zeta = 2/3$, in complete agreement with Kardar’s analytical solution [4].

4.2 The power-law correlated potential

The verification test implemented for delta-correlated potential of the variational principle is in good agreement with theoretical predictions. Unfortunately no solution is available for more general correlation of the random
potential like power-law. It would be interesting for instance to know how the wandering exponent depends on power-law correlation’s exponent. An approximate answer to this question arise from the one loop renormalization group analysis presented in [4], which lead to the following scenario (defining $\langle V(x)V(y)\rangle \propto |x - y|^{-(2\rho - 1)} \equiv |x - y|^{-\nu}$):

- $\nu > 1/2$  
  Renormalization group flux with one stable point which scales to the delta-correlated potential behavior. This regime is characterized by a fundamental length scale bigger then the length scale over which the effects of the correlation of the potential are sensible. Here $\zeta = 2/3$ ($\alpha = 1$) independently from $\nu$.

- $\nu < 1/2$  
  In this regime correlations extends on the same length scale of correlations and wandering exponent depends on $\rho$. It is known sometimes as the Flory’s regime and the relation found is $\zeta(\nu) = 3/(4 + \nu)$ which following our notation also reads $\alpha(\nu) = (4 - 2\nu)/3$.

In order to verify the approximated predictions above, we have inserted in the functional (21) a potential of the following type:

$$V(x - y) = \frac{|x - y|^{-\nu} - 1}{\nu} \quad \nu = 1 - 2\rho$$

(32)

It has to be notice that functional structure of the correlations has been chosen in order to obtain a logarithmic behavior in the limit $\nu \to 0$, so that
Figure 5: On the left is presented the behavior of parameter $\alpha$ which maximizes the functional vs. $\nu$ ($N = 64$). A transition to the Flory long-range scaling regime is clearly observable for $\nu > 1/2$. On the left a zoom on the transition point is presented for $N = 128, 256, 512$. We can observe a more sharp transition from short to long range behavior as the volume increases.

formation of bound states is still allowed in this limit.

The interval $\nu \in \{-2 : 10\}$ has been subjected to investigation. Since negative values of the exponent $\nu$ obviously correspond to correlations which grow with the distance, the finite size effects become more and more relevant. That’s why was impossible to analyze the behavior of the system for values of $\nu < -2$.

For each value of $\nu$ we have calculated the corresponding pair $(\alpha, \lambda)$ which maximize (32), calculating free energy and errors with the probabilistic prescription stated above. The results are presented in figure (for details see caption). From figure (5) we find a rather smooth behavior around the transition point $\nu = 1/2$. Iterating our analysis for polymers of different lengths ($N = 128, 256, 512$) we can observe a more sharp transition since finite size effects are less important. Figure (5) shows that for larger volume the different curves develop a real discontinuity in the first derivative in $\nu = 1/2$ in agreement with the approximate results of [4].
5 Conclusions

The variational method developed seems to correctly describe unidimensional polymers in random environment. For delta-correlated potential, stationary point is effectively a maximum of our replicated free energy functional in the $n \to 0$ limit according with replica theory. The value of the maximum free energy is in very good agreement with Kardar’s solution [2].

The power-law correlated potential has been subjected to investigations and the results are in agreement with the perturbative result in [4]: for $\nu > 1/2$ the wandering exponent equals the delta-correlated one ($\zeta = 2/3$), and for $\nu < 1/2$ the standard Flory regime is recovered ($\zeta(\nu) = 3/(4 + \nu)$).

A number of recently published papers pointed out that one dimensional DPRM are characterized by replica symmetry breaking. Our formulation can be in principle enriched introducing the replica symmetry breaking as pointed out in [5].

Another development of the theory should be the analysis of $d + 1$-dimensional DPRM with $d > 1$. Some preliminary tests performed in $d = 2$ pointed out that for the delta-correlated potential one must chose a probability distribution which is not a simple power-law in $k$. Further inquiry are required maybe in the direction of a more complex functional structure of equilibrium probability distribution function.

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