Manifolds in random media: A variational approach to the spatial probability distribution

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Abstract

We develop a new variational scheme to approximate the position dependent spatial probability distribution of a zero dimensional manifold in a random medium. This celebrated 'toy-model' is associated via a mapping with directed polymers in 1+1 dimension, and also describes features of the commensurate-incommensurate phase transition. It consists of a pointlike 'interface' in one dimension subject to a combination of a harmonic potential plus a random potential with long range spatial correlations. The variational approach we develop gives far better results for the tail of the spatial distribution than the hamiltonian version, developed by Mezard and Parisi, as compared with numerical simulations for a range of temperatures. This is because the variational parameters are determined as functions of position. The replica method is utilized, and solutions for the variational parameters are presented. In this paper we limit ourselves to the replica symmetric solution.

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I. INTRODUCTION

Recently a lot of attention has been devoted to the behavior of manifolds in random media. This is partially due to their connection with vortex line pinning in high \(T_c\) superconductors, but also because of the intrinsic interest in the behavior of interfaces between two coexisting phases of a disordered system, like magnets subject to random fields or random impurities. In addition mappings are known to exist between one dimensional manifolds like directed polymers in disordered media and growth problems in the presence of random noise described by the KPZ equation.

The variational method appears to be an important tool in approximating many properties of the system like the calculation of the roughness exponent of a wandering manifold in a disordered medium. Recently we have conducted a numerical study of the spatial probability distribution of directed polymers in 1+1 dimensions in the presence of quenched disorder. Directed polymers refer to an interface in two dimensions with no overhangs. In addition to the width of the interface, it is important to know what is the probability that the interface would wander a certain distance in the transverse direction. We have then exploited a mapping of this system into that of a pointlike interface in one dimension subjected to a combination of a harmonic restoring force and a random potential with long ranged correlations.

Using that mapping combined with a use of the variational approximation, we were able to derive many properties of the spatial probability distribution (PD) of the directed polymers. In particular the function \(f(\alpha)\) associated with the decay of the probability for different realizations of the disorder has been derived using the replica method. Replica symmetry breaking solutions have been used (at low temperatures). The mapping from directed polymers to the so called toy-model is discussed in detail in ref. based on
previous work by Parisi [5] and Bouchaud and Orland [7]. In particular the spatial probability distribution of directed polymers at large times relates to the spatial probability distribution of the toy-model at low temperature. Villain et al. [1] emphasize directly the relation between the toy-model and the commensurate-incommensurate transition in systems with quenched impurities. [1]

Using the replica method the toy-model can be mapped into an n-body problem where the interaction between different particles (replicas) is given by the correlation of the original random potential. The variational method utilizes an effective quadratic Hamiltonian whose parameters are chosen by the stationarity method to give a good approximation for the free energy of the n-body system in the limit n → 0. [8] The results it provides for the tail of the spatial distribution are not very accurate as will be shown below (Section 4.). In this paper we describe a way to directly apply the variational approach to the probability distribution rather than to the Hamiltonian or the free energy. As we shall see it gives a much better approximation for the behavior of the tail of the distribution. For high temperatures the results appear almost exact without the need to break replica symmetry.

II. THE VARIATIONAL METHOD APPLIED TO THE PROBABILITY DISTRIBUTION.

The toy model [1,4,13,14] involves a classical particle in a one-dimensional potential consisting of a harmonic part and a spatially correlated random part. It is the simple prototype of an interface-a point in one dimension- which is localized by a harmonic restoring force, and pinned by quenched impurities the distribution of which may be correlated over large separations. Its Hamiltonian is given by:

\[ H(\omega) = \frac{\mu}{2} \omega^2 + V(\omega), \]  

(2.1)
where $\omega$ denotes the position of the particle and $V(\omega)$ is a random potential with a gaussian distribution characterized by:

$$
\langle V(\omega) \rangle = 0, \quad \langle V(\omega)V(\omega') \rangle = -\frac{g}{2(1-\gamma)} |\omega - \omega'|^{2-2\gamma} + \text{Const.} \equiv -f((\omega - \omega')^2),
$$

(2.2)

where the brackets indicate averaging over the random potential. In the sequel without loss of generality we will take the constant on the r.h.s. of eq.(2.2) to be zero. We will make use of the replica method to replicate the partition function

$$
Z = \int d\omega \exp(-\beta H)
$$

(2.3)

and average it over the random potential to express it in terms of an effective $n$-body hamiltonian:

$$
\langle Z^n \rangle = \int d\omega_1 \cdots d\omega_n \exp(-\beta \mathcal{H}),
$$

$$
\mathcal{H} = \frac{1}{2} \mu \sum_{a=1}^{n} \omega_a^2 + \frac{1}{2} \beta \sum_{ab} f((\omega_a - \omega_b)^2).
$$

(2.4)

For later use let us also define an $n$-body quadratic hamiltonian:

$$
h = \frac{1}{2} \mu \sum_{a=1}^{n} \omega_a^2 - \frac{1}{2} \beta \sum_{ab} \sigma_{ab} \omega_a \omega_b
$$

(2.5)

where the matrix elements of $\sigma_{ab}$ are free parameters at this point.

We consider cases in which the potential has long-range correlations, (i.e. $\gamma < 1$), and in particular we are interested in the case $\gamma = \frac{1}{2}$ because of the above mentioned mapping from directed polymers in $1 + 1$ dimensions. Let us review briefly the variational scheme used by Mezard and Parisi. We start with the well known inequality

$$
\langle e^A \rangle \geq e^{\langle A \rangle}
$$

(2.6)

The Mezard-Parisi variational approximation \[8\] can be obtained from this inequality, by choosing
\[ A(\omega_1, \ldots, \omega_n) = \mathcal{H}(\omega_1, \ldots, \omega_n) - h(\omega_1, \ldots, \omega_n) \]  
\hspace{1cm} (2.7)

And by defining the average as

\[ \langle A \rangle = \frac{TrA \exp(-\beta h)}{Tr \exp(-\beta h)}. \]  
\hspace{1cm} (2.8)

with

\[ Tr = \int_{-\infty}^{+\infty} d\omega_1 \cdots d\omega_n \]  
\hspace{1cm} (2.9)

This yields

\[ nf = -\frac{1}{\beta} \ln Tr \exp(-\beta \mathcal{H}) \leq \langle \mathcal{H} - h \rangle - \frac{1}{\beta} Tr \ln \exp(-\beta h), \]  
\hspace{1cm} (2.10)

where \( f \) is the free energy. The variational free energy is given by the right hand side of eq. (2.10) at the point of stationarity. This procedure provides equations for the variational parameters which are the elements of the matrix \( \sigma_{ab} \). MP \[ 13 \] have solved these equations and found a replica symmetric (RS) solution valid for high temperatures and a solution which breaks replica symmetry (RSB) at low temperatures.

Recall that the limit \( n \to 0 \) has to be taken when making use of the replica method. An important point to bear in mind is that the inequality (2.6) holds only when \( n \) is a positive integer, provided the parametrization of \( \sigma \) is such that \( Tr \exp(-\beta h) < \infty \). This is because only in this case the integration measure

\[ [Tr \exp(-\beta h)]^{-1} \exp(-\beta h) d\omega_1 \cdots d\omega_n. \]  
\hspace{1cm} (2.11)

is a real positive measure on \( R^n \), for which the proof of the inequality (2.6) holds (see e.g. \[ 23 \] p. 61). In the limit \( n \to 0 \) the inequality can change sign and does not hold in general, but one still expects the the stationary point of the r.h.s. of equation (2.10) to give a good approximation to the l.h.s. i.e. to the exact free energy. Support for this contention comes
also from the fact that the variational method becomes exact for a manifold embedded in $d$ spatial dimensions when $d$ becomes infinite, and one can systematically improve it by a $1/d$ expansion. \[\text{[8,13,17,19]}\]

Let us define

$$
\widehat{T}r = \int d\omega_1 \cdots d\omega_n \delta(\omega_1 - \omega).
$$

(2.12)

The function

$$
P_h(\omega) = \widehat{T}r \exp(-\beta h),
$$

(2.13)

(with the parameters $\sigma_{\alpha\beta}$ determined by the stationarity conditions which were discussed above) constitutes an approximation to the exact spatial probability distribution, averaged over the random realizations of the potential, and given by the formula

$$
P_H(\omega) \equiv \left\langle \frac{\exp(-\beta H(\omega))}{\int d\sigma \exp(-\beta H(\sigma))} \right\rangle = \widehat{T}r \exp(-\beta H),
$$

(2.14)

with the limit $n \to 0$ to be understood. Eq. \[\text{[2.13]}\] has been evaluated by us in a previous publication \[\text{[16]}\] and compared with numerical simulations both using the RS and RSB solutions for the variational parameters. The result for $P_h$ is \[\text{[16]}\]:

$$
P_h(\omega) = \left(\frac{\beta}{2\pi G_{11}}\right)^{1/2} \exp\left(-\frac{\beta \omega^2}{2G_{11}}\right),
$$

(2.15)

with

$$
G_{ab} = \left[ \mu I - \hat{\sigma} \right]_{ab}^{-1}.
$$

(2.16)

Substituting the RS and RSB solutions for $G_{11}$ obtained in ref. \[\text{[13]}\], we find \[\text{[16]}\]

$$
P_h(\omega) = \left(\frac{\beta \mu}{2\pi(1 + \gamma^{-1} T^{-1}(1+\gamma))}\right)^{1/2} \exp\left(-\frac{\beta \mu \omega^2}{2(1 + \gamma^{-1} T^{-1}(1+\gamma))}\right), \quad \hat{T} > 1
$$

$$
P_h(\omega) = \left(\frac{\beta \mu \gamma \hat{T}}{2\pi(1 + \gamma)}\right)^{1/2} \exp\left(-\frac{\beta \mu \gamma \hat{T} \omega^2}{2(1 + \gamma) \omega^2}\right), \quad \hat{T} < 1
$$

(2.17)
with the ‘reduced’ temperature $\hat{T}$ defined as

$$\hat{T} = \beta^{-1} \mu^{\frac{1-\gamma}{1+\gamma}} \left( \frac{\gamma^{2-2\gamma} \Gamma(3/2 - \gamma)}{\Gamma(1/2)} \right)^{-\frac{1}{1+\gamma}}. \tag{2.18}$$

In the sequel we refer to the expressions given in eq. (2.17) as “the hamiltonian variational approximation”.

I proceed to derive a new variational scheme which is more appropriate for approximating the position-dependent spatial probability distribution. The idea is to use the inequality (2.6), but substitute $\hat{\text{Tr}}$ from eq. (2.12) for the trace in eq. (2.8). This means, defining

$$\langle\langle A\rangle\rangle(\omega) \equiv \frac{\hat{\text{Tr}} \left[ A(\omega_1, \cdots, \omega_n) \exp (-\beta h) \right]}{\hat{\text{Tr}} \exp (-\beta h)}. \tag{2.19}$$

The notation $\langle\langle \rangle\rangle$ is used to distinguish the $\omega$-dependent average from the averaged defined in eq. (2.8). Using $A = \mathcal{H} - h$ I find

$$P_H(\omega) = \hat{\text{Tr}} \exp (-\beta \mathcal{H}) \geq \exp (-\beta \langle\langle \mathcal{H} - h \rangle\rangle(\omega)) \times \hat{\text{Tr}} \exp (-\beta h) \equiv P_v(\omega) \tag{2.20}$$

Again, for positive integers $n$, and $\hat{\text{Tr}} \exp (-\beta h) < \infty$, the measure

$$[\hat{\text{Tr}} \exp(-\beta h)]^{-1} \exp (-\beta h) \delta(\omega_1 - \omega) \, d\omega_1 \cdots d\omega_n, \quad \tag{2.21}$$

is a positive measure on $R^n$ for any value of $\omega$ and the inequality (2.6) holds. For $n \to 0$ this is no longer true, but the stationary point of the r.h.s. of eq. (2.20), denoted by $P_v(\omega)$, with respect to the parameters $\sigma_{ab}$ is expected to yield a good approximation to the spatial probability distribution by virtue of analytic continuation. This will be checked in Sec. 4 in comparison with numerical simulations. Such a variational determination of $P_v(\omega)$ is obtained for each value of $\omega$ separately and thus it is expected to provide a better approximation than by just using the $\sigma_{ab}$ obtained globally from extremizing the free energy (see eq. (2.10)), and using eq. (2.13). One should note that it does not follow from our
discussion that \( P_v(\omega) \) is properly normalized. Provided it is a good approximation to the exact probability distribution, its normalization will be close to one, and correcting for the exact normalization will have practically no effect on the behavior in the tail region were the probability is very small and where the variational calculation is most important.

Our next task is to evaluate the quantity \( \langle \langle H - h \rangle \rangle(\omega) \) needed in order to calculate \( P_v(\omega) \), see eq. (2.20). If we use the integral representation for the Dirac \( \delta \)-function in eq.(2.12):

\[
\delta(\omega_1 - \omega) = \int \frac{dk}{2\pi} e^{ik\omega - ik\omega_1} .
\]

we can write

\[
\hat{\text{Tr}} \left[ (H - h) e^{-\beta h} \right] = \int \frac{dk}{2\pi} e^{ik\omega} \int d\omega_1 \cdots d\omega_n 
\left( \frac{\beta}{2} \sum_{ab} f((\omega_a - \omega_b)^2) + \frac{1}{2} \sum_{ab} \sigma_{ab}\omega_a\omega_b \right) \times \exp \left( -\frac{\beta}{2} \sum_{ab} (G^{-1})_{ab}\omega_a\omega_b - ik\omega_1 \right) .
\]

In the Appendix we show how the integrals can be evaluated for general \( n \). The end result is:

\[
\langle \langle H - h \rangle \rangle(\omega) = 
\frac{\beta}{2} \left( \frac{G_{11}}{\pi} \right)^{1/2} \exp \left( \frac{\beta \omega^2}{2G_{11}} \right) \sum_{ab} \left[ (Z_{ab})^{-1/2} \int_{-\infty}^{\infty} dp \exp\left( -p^2 - \frac{(\omega\sqrt{\beta} + p\sqrt{2}Y_{ab})^2}{2Z_{ab}} \right) \right]
\times f\left( \frac{2}{\beta X_{ab}p^2} \right) - \frac{n}{2\beta} + \frac{\mu}{2\beta} \sum_a G_{aa} + \frac{1}{2\beta G_{11}} (G_{11} - \mu \sum_a G_{1a}^2)(1 - \frac{\beta \omega^2}{G_{11}})
\]

with

\[
X_{ab} = G_{aa} + G_{bb} - 2G_{ab}
\]

\[
Y_{ab} = (G_{1a} - G_{1b}) / \langle X_{ab} \rangle^{1/2}
\]

\[
Z_{ab} = G_{11} - Y_{ab}^2 .
\]

For the special case of interest \( \gamma = 1/2 \) (see eq.(2.2) for \( f \)) we find:
\[ \langle \langle \mathcal{H} - h \rangle \rangle (\omega) = \left( \frac{\beta Y_{ab} X_{ab}^{1/2}}{2G_{11}} \right) \frac{\omega}{2} \text{erf} \left( \left( \frac{\beta Y_{ab}^2}{2Z_{ab}G_{11}} \right)^{1/2} \omega \right) + \left( \frac{\beta X_{ab} Z_{ab}}{2\pi G_{11}} \right)^{1/2} \exp \left( - \frac{\beta Y_{ab}^2 \omega^2}{2Z_{ab}G_{11}} \right) \]

\[ - \frac{n}{2\beta} + \frac{\mu_1}{2\beta} \sum_a G_{aa} + \frac{1}{2\beta G_{11}} \left( G_{11} - \mu \sum_a G_{1a}^2 \right) \left( 1 - \beta \omega^2/G_{11} \right), \] (2.26)

where erf is the usual error function. Eqs. (2.24) and (2.26) together with the expression (2.20) for \( P_v(\omega) \) constitute the main results of this section. In the rest of the paper we consider only the important case of \( \gamma = 1/2 \).

### III. The Replica Symmetric Solution

In this section we consider the replica symmetric solution to the variational stationarity equations. In this case we search for a solution for which all the off diagonal elements of the matrix \( \sigma_{ab} \) are equal as well as all the diagonal elements:

\[ \sigma_{ab} = \sigma \quad a \neq b \]

\[ \sigma_{aa} = \sigma_d \quad a = 1 \cdots n \] (3.1)

we also define

\[ \mu_1 = \mu + \sigma_d + (n - 1)\sigma \] (3.2)

In terms of these parameters one finds

\[ G_{aa} = \frac{1}{\mu_1} \left( 1 + \frac{\sigma}{\mu_1} \right); \quad G_{ab} = \frac{\sigma}{\mu_1^2}; \quad a \neq b \] (3.3)

Thus we have two variational parameters \( \sigma \) and \( \mu_1 \) as contrasted with the hamiltonian variational approach were there is only one variable because in that case translational invariance dictates \( \mu_1 = \mu \). In addition, the variational parameters are of course dependent on \( \omega \) in the present case. We define for convenience:
Using the result of the previous section, eq. (2.26), we can express the probability distribution $P_v(\omega)$ (see also eqs. (2.20) and (2.13)) as

$$P_v(\omega) = \left(\frac{\beta}{2\pi G_{11}}\right)^{1/2} \exp \left(-\frac{\beta\omega^2}{2G_{11}}\right) \exp \left(g(\omega)\right)$$

where the limit $n \to 0$ has been taken. The stationary points of eq. (3.5) in the $\sigma - \mu_1$ plane as functions of $\omega$, have been obtained numerically for various values of the parameters of the model $(\beta, \mu, g)$, and the results have been used back in eq. (3.5) to evaluate $P_v(\omega)$. The results will be summarized below. But first let us examine the simpler behavior in the tail of the probability distribution, that can be investigated analytically.

For large values of $\omega$, the error-function in eq. (3.5) can be approximated by $\text{sign}(\omega)$ and the exponential term in the expression for $g(\omega)$ is negligible. If we further define the tail region as the region for which

$$|\omega| >> \frac{\beta g}{\mu} ,$$

we find that the extremum of $P_v(\omega)$ is obtained for

$$\frac{\sigma}{\mu_1} \approx \frac{\beta g}{\mu|\omega| - \beta g}$$

$$\mu_1 \approx \left[\mu\pi + 2\beta^3 g^2 - 2g\beta(\beta^3 g^2 + \beta\mu\pi)^{1/2}\right]/\pi .$$

Plugging these expressions back into the expression for $P_v(\omega)$ one finds that the behavior of the spatial probability distribution in the tail region defined by eq. (3.6) is
\[ P_v(\omega) \approx \exp(-\mu \beta \omega^2/2 + g \beta^2 |\omega| + C) \]

\[ C = -\frac{\beta^3 g^2}{2\mu} - 2\beta g \left( \frac{\beta}{\pi \mu_1} \right)^{1/2} + \frac{\mu}{2\mu_1} - \frac{1}{2} + \frac{1}{2} \ln \left( \frac{\beta \mu_1}{2\pi} \right), \quad (3.8) \]

where \( \mu_1 \) is given by eq. (3.7).

The extremum in the tail turns out to be a minimum in the \( \sigma - \mu_1 \) plane, as opposed to the situation for \( n \geq 1 \) when it is a maximum as can be seen from eq.(2.20). (On the contrary, for very small values of \( \omega \) we have found numerically, that the stationarity point is actually a saddle point.) The fact that the extremum in the tail region is a minimum seems to suggest that the approximate expression eq. (3.8) constitutes an upper bound to the exact behavior. The behavior in the tail given by eq.(3.8) should be compared with the behavior obtained from the conventional variational approximation given by substituting \( \gamma = 1/2 \) in eq. (2.17). Those formulas give a higher value for the tail than that predicted by eq.(3.8). (This is true even when \( \hat{T} < 1 \) with the RSB solution). More on this in the discussion below.

**IV. COMPARISON WITH NUMERICAL SIMULATIONS**

We proceed to a numerical comparison between simulations and the results of the various variational approximations. Again, we limit the discussion to the case \( \gamma = 1/2 \). We have studied numerically a lattice version of the toy model. A suitable interval of the particle’s position \( \omega \) (\( -12.5/\sqrt{\beta} < \omega < 12.5/\sqrt{\beta} \)) is divided into 5,000 lattice sites. For a given realization, the algorithm generates an independently distributed gaussian random number for each site \( r_i \); it then generates \( V_j \), the correlated random potential at site \( j \), by summing the random numbers in the following way:

\[ V_j \propto \sum_i \text{sign}(i - j) r_i. \quad (4.1) \]

The quadratic term of the hamiltonian is added to this random potential, and then the partition function and probability distribution are calculated.
We consider three sets of values for the parameters \((\beta, g, \mu)\) : \((0.2, 2\sqrt{\pi}, 1)\), \((1.0, 2\sqrt{\pi}, 1)\), \((10.0, 2.2, 4.6)\). The corresponding values of the reduced temperature \(\hat{T}\) for these three cases are 5, 1 and 0.23 respectively. The data for \(\hat{T} = 5\) is plotted in Fig.1 (solid curve). It was obtained from numerical simulations with 50000 realizations of the disorder. The dashed line represents the probability \(P_h\) given in eq.\((2.17)\) and derived from the Hamiltonian variational method. The diamonds represent the approximation developed in the last section. We see that it gives a perfect fit to the data for this value of \(\hat{T}\). We have used Mathematica to find the stationary point of eq.\((3.5)\) in the \(\mu_1 - \sigma\) plane and then substituted these values back into eq.\((3.5)\). The asymptotic formula eq.\((3.8)\) predicts

\[
P_v(\omega) \approx \exp\left(-0.1\omega^2 + 0.142\omega - 2.1\right)
\]

where we used \(\mu_1 = 0.7\) from eq. \((3.7)\). This behavior is also indistinguishable from the data in the range \(10 < \omega < 28\).

Let us proceed to the case \(\hat{T} = 1\). The data is plotted in Fig.2. In this case the noise associated with the random potential is apparent. In this case we found it necessary to average over 500000 realizations. The data for 50000 realizations is also shown in lighter dots. In the tail region it is apparent that the curve corresponding to the lower number of realizations has a lower value, since the average is increased by relatively rare events. The dashed curve is the single parameter Hamiltonian variational fit. The new variational method results are represented by the diamonds. The asymptotic formulas predicts \(\mu_1 = 0.06\) and

\[
P_v(\omega) \approx \exp\left(-0.5\omega^2 + 3.545\omega - 17\right).
\]

It is represented by the solid line in the figure. The diamonds do not lie exactly on this line, because \(\omega\) is still not large enough in this range. Again we see that the variational approximation gives an excellent fit to the data.
The final example is for $\hat{T} = 0.23$ using $10^6$ realizations of the disorder. The data is depicted in Fig. 3. The dashed line is the result of the hamiltonian RS variation. The dot-dashed line is the result of the RSB hamiltonian variation which is the appropriate solution for $\hat{T} < 1$. The diamonds again represent our new variational method results. The range of $\omega$ simulated is lower than the onset of the tail region given by eq.(3.6) which in the present case starts above $\omega \sim 5$, so a comparison with the asymptotic formula eq.(3.8) is not shown.

We see that the data in this case falls below the result of our variational method, which is nonetheless better than the hamiltonian RSB variational approximation. Two possibilities come to mind to explain this discrepancy.

1. It seems quite possible that because the relative strength of the random part of the potential is much larger when $\hat{T}$ is small, as compared to the harmonic part, one needs more realizations to accumulate enough statistics for the averaged probability distribution. For $\hat{T} = 5$ even 5000 realizations already gave us good results. In Fig.1 we show the results for 50000 realizations, but these are practically indistinguishable from the average of 5000 realizations. For $\hat{T} = 1$, 50000 realizations are not sufficient and we had to average at least 500000 realizations to accumulate enough statistics. This is because we have to collect enough rare events which contribute to the distinction between the average and typical values of the spatial probability distribution. It is quite plausible that to get better results for $\hat{T} = 0.23$ one has to go to a higher number of realizations. Averaging over more realizations (see e.g Fig. 2 for the distinction between 50000 and 500000 realizations) may narrow the gap between the data and the variational approximation.

2. Another strong possibility is that like the hamiltonian variational case it is necessary for small $\hat{T}$ to look for a solution with replica symmetry breaking when using the current variational scheme. Such a solution may display a different asymptotic behavior for small $\hat{T}$ than the one given by eq.(3.8). It may also yield a lower value in the pretail region (which is
the range of values depicted in Fig. 3). In order to find such a solution one has to go back to the full expressions derived in Sec. 2 without making the simplifying assumptions of replica symmetry made in Sec. 3, and one has to extremize the probability distributions under the more general conditions. The task of finding of a RSB solution is left for future research.

V. DISCUSSION

In this paper we have developed a new variational scheme for approximating the spatial probability distribution. The replica symmetric solution gives an excellent approximation to the numerical data for high temperatures $\hat{T} > 1$. For the tail of the spatial probability it predicts a gaussian decay with a linear exponential correction. At lower temperature, the fit in tail region is not that good, either because the numerical data is insufficient and one needs to average over a higher number of realizations, or a solution with replica symmetry breaking is needed (or both). Of course since we are dealing after all with an approximation, we are never guaranteed a perfect fit. For all temperatures tested the present method gives a much better fit to the probability distribution than using the hamiltonian variational method, both with or without RSB.

When the data for $\hat{T} = 0.23$ is displayed in a log-log plot, a crossover is observed from a behavior $P \sim \exp(-\text{const} \, \omega^2)$ to a behavior like $P \sim \exp(-\text{const} \, \omega^3)$. An empirical fit to the data of the form

$$P(\omega) \sim \exp(-3.5\omega^3 + 20)$$

is depicted as open triangles in Fig. 3 for the range $6 < \omega^2 < 16$. Since in this case we are not really observing the tail region (according to the definition given in eq. (3.6)), this behavior may be a transient or intermediate behavior. We should also be cautious about
the data in this region, because as mentioned in the last section it is possible that more realizations are needed.

On the other hand, if we do take the cubic $\omega$ dependence of the log of the probability distribution seriously, this immediately rings a bell because of some work done by Villain et al. [1] on the toy model. What they actually showed was that the probability for rare realizations of the disorder which make $H(\omega) \sim 0$ and thus $\exp(-\beta H) \sim 1$ behaves like $\sim \exp(-\omega^3 \mu^2/2g)$, for values of $\omega^3 >> 2g/\mu^2$ (I have transformed their notation to ours). This could lead to the conclusion that the spatial probability distribution should also behave like a cubic power of $\omega$. This is true only if the probability distribution is completely dominated by the rare realizations of this kind, a fact that was never claimed by Villain et al. It is certainly possible that other realizations which give lower values to $\exp(-\beta H)$ but are nonetheless more abundant dominate the average value. Villain’s argument is valid for any temperature. Our numerical results show that one certainly does not get a cubic behavior of the probability distribution at high temperature for values of $\omega >> (g/\mu^2)^{1/3}$. In that case the rare realizations of the type considered by Villain still exist but they do not dominate the probability distribution.

This is actually easy to understand. Let us define two different length scales in the problem. The first, introduced by Villain et al. which we call $\xi_1$ is defined as

$$\xi_1 \simeq \left(\frac{2g}{\mu^2}\right)^{1/3}.$$  

(5.2)

is the length above which the probability for rare events of magnitude 1 goes like

$$A \exp\left(-\frac{\omega^3}{\xi_1^3}\right).$$  

(5.3)

with some undetermined constant $A$. The second length, which I introduced in eq.(3.6),

$$\xi_2 \simeq \frac{\beta g}{\mu},$$  

(5.4)
is the length for which the asymptotic behavior in the tail starts according to our investigation in Sec. 3. For \( \omega \) above this value we have found the behavior

\[
P(\omega) \simeq \exp(-\beta \mu \omega^2/2 + g\beta^2|\omega| + C(\beta)),
\]

(5.5)

where \( C(\beta) \) is given in eq. (3.8). Since

\[
\xi_2 \simeq \xi_1 \times \frac{(2\pi)^{1/3}}{\hat{T}}
\]

(5.6)

We see that for \( \hat{T} > 1.8 \), the cubic behavior is never realized since the contribution of the rare realizations of the Villain type to the averaged probability is smaller than the behavior given by eq.(5.3). This explain the perfect fit of the asymptotic behavior given in eq.(4.3) and the numerical data, starting at a very low value of \( \omega \).

On the other hand for \( \hat{T} \ll 1.8 \) it is conceivable to have two tail regimes, the first with \( \xi_1 < \omega < \xi_2 \) in which the probability has the cubic behavior in \( \omega \) because it is dominated by rare configurations of the Villain type, and a second tail regime for \( \omega > \xi_2 \) for which the asymptotic behavior is changed to a quadratic behavior given by eq.(5.5), if the results of the RS solution are valid (or possibly to a different asymptotic behavior which will emerge from a RSB solution). This is because one can easily check that at the border between these two regimes the two expressions given by eq.(5.3) and eq.(5.5) become comparable in magnitude, and the quadratic behavior wins for \( \omega > \xi_2 \). As the (reduced) temperature is lowered from 1 the first regime (cubic behavior) is expected to grow in size and include all of the tail at \( \hat{T} = 0 \). Simulations of directed polymers at zero temperature, which can be mapped into corresponding results for the toy-model, \[\] showed the beginning of a change in the form of the spatial probability distribution from \( \sim \exp(-c\omega^2) \) to \( \sim \exp(-c\omega^{2.2}) \) at the onset of the tail, but did not go far enough into the tail region to confirm a cubic dependence. See also ref. 14. We have previously observed cubic dependence in the tail of the directed polymers’ spatial probability distribution at finite temperature. 15
There is some difficulty though, to explain the apparent cubic behavior in Fig. 3 purely in terms of Villain’s configurations because we simulated “only” over $10^6$ realizations and thus if the average is dominated by a single realization whose contribution is unity, the value of the average should be of the order of $10^{-6} \simeq \exp(-14)$ which far exceeds the value of the distribution in most of this region (except at the very beginning). One might argue that there are other realizations with somewhat smaller contributions to the average than Villain’s which also gives rise to a similar cubic behavior but this needs to be verified.

We hope that this work will stimulate further investigation of the behavior of the tail of the probability distribution at low temperatures. Three important questions that need a definite answer are

1. Is there a RSB solution to our new variational equations?
2. Is a cubic dependence of the log of the probability indeed realized over a large region when the temperature is very low?
3. Is the asymptotic behavior given by eq. (3.8) which works so well for high temperatures when $\omega > \xi_2$, also valid asymptotically at low temperatures?

We also hope that it will be possible to extend the variational method developed in this paper for the zero-dimensional manifold directly to higher dimensional manifolds in random media.

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In this Appendix we derive eq. (2.24) starting from eq. (2.23). Let us shift the variables \( \omega_a \) in eq. (2.23)

\[
\omega_a \rightarrow \omega_a + \lambda_a
\]

such that the linear term in \( \omega_1 \) in the exponential is eliminated. This is achieved by choosing

\[
\lambda_a = -\frac{i}{\beta} G_{1a} k
\]

We then find:

\[
\hat{T}r \left[ (\mathcal{H} - \hbar) e^{-\beta \hbar} \right] = \int \frac{dk}{2\pi} e^{ik\omega} e^{-\frac{1}{2\beta^2} G_{11} k^2} \int d\omega_1 \cdots d\omega_n \\
\times \left( \frac{\beta}{2} \sum_{ab} f((\omega_a - \omega_b + \lambda_a - \lambda_b)^2) + \frac{1}{2} \sum_{ab} \sigma_{ab}(\omega_a + \lambda_a)(\omega_b + \lambda_b) \right) \\
\times \exp \left( -\frac{\beta}{2} \sum_{ab} (G^{-1})_{ab} \omega_a \omega_b \right) .
\]

(A3)

We now expand the function \( f \) in a power series about 0, (this is used only as a tool derive our result. It may not be necessary for \( f \) to be analytic about 0)

\[
f(x) = \sum_{l=0}^{\infty} f_l x^l
\]

(A4)

We use the following formula to integrate over \( \omega_1 \cdots \omega_n \):

\[
\int d\omega_1 \cdots d\omega_n (\omega_a - \omega_b)^{2s} \exp \left( -\frac{\beta}{2} \sum_{ab} (G^{-1})_{ab} \omega_a \omega_b \right) =
\]

\[
(2\pi/\beta)^{n/2} (\text{Det } G)^{1/2} \frac{2^s \Gamma(1/2 + s)}{\beta^s \Gamma(1/2)} (G_{aa} + G_{bb} - 2G_{ab})^s ,
\]

providing \( s \) is a non-negative integer. For \( s \) being half-integer the integral is 0. We obtain

\[
\hat{T}r \left[ (\mathcal{H} - \hbar) e^{-\beta \hbar} \right] = \left( \frac{G_{11}}{2\pi \beta} \right)^{1/2} \exp \left( \frac{\beta \omega^2}{2G_{11}} \right) \int dk \left\{ \exp \left( ik\omega - \frac{1}{2\beta} G_{11} k^2 \right) \times \\
\frac{\beta}{2} \sum_{ab} f \left( -(G_{1a} - G_{1b})^2 k^2 / \beta^2 , \ (G_{aa} + G_{bb} - 2G_{ab}) / \beta \right) \exp \left( -\frac{\beta}{2} \sum_{cd} (G^{-1})_{cd} \omega_c \omega_d \right) \right\} \\
- \frac{n}{2\beta} + \frac{\mu}{2\beta} \sum_a G_{aa} + \frac{1}{2\beta G_{11}} \left( G_{11} - \mu \sum_a G_{1a}^2 \right) \left( 1 - \frac{\beta \omega^2}{G_{11}} \right) ,
\]

(A6)
where

\[
\hat{f}(x, y) = \frac{1}{\sqrt{\pi}} \sum_{l=0}^{\infty} f_l \left( 2y \right)^l \sum_{s=0}^{l} g(l, s) \Gamma(s + 1/2) \left( \frac{x}{2y} \right)^{l-s}
\]

\[
g(l, s) = \sum_{j=0}^{l} \sum_{m=0}^{j} \delta_{(j+m)/2, s} \left( \begin{array}{c} l \\ j \end{array} \right) \left( \begin{array}{c} j \\ m \end{array} \right) 2^{j-m}.
\] (A7)

Since

\[
\int_{-\infty}^{\infty} dp \, e^{-p^2} (p + q)^{2l} = \sum_{s=0}^{l} g(l, s) \Gamma(s + 1/2) q^{2(l-s)},
\] (A8)

we see that \( \hat{f}(x, y) \) can be expressed in the form

\[
\hat{f}(x, y) = \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dp \, e^{-p^2} \left( 2y \left( p + \sqrt{\frac{x}{2y}} \right) \right)^2
\]

\[
= e^{-\frac{x}{4y}} \frac{1}{\sqrt{\pi}} \int_{-\infty}^{\infty} dp \, f(2yp) \, e^{-p^2 + 2\sqrt{x/(2y)} \, p}.
\] (A9)

Using this representation for \( \hat{f}(x, y) \) the integral over \( k \) in eq.(A6) can be performed, and we obtain the desired result given in eq.\((2.24)\).
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Figure Captions

Figure 1: Plot of the log of spatial probability distribution vs. $\omega^2$ for $\hat{T} = 5$ (solid line). The dashed line is the result of the hamiltonian variational approximation and the diamonds the results of our new variational scheme.

Figure 2: Plot of the log of the spatial probability distribution vs. $\omega^2$ for $\hat{T} = 1$. The wiggly solid curve represent the result of averaging over 500000 realizations. The light wiggly curve is for 50000 realizations. The dashed curve and the diamonds are explained in the caption of Fig. 1. The solid smooth curve result from the asymptotic formula, eq.(3.8).

Figure 3: Plot of the log of the spatial probability distribution vs. $\omega^2$ for $\hat{T} = 0.23$. The wiggly solid curve represent the result of averaging over $10^6$ realizations. The dashed and dashed-dotted lines represent the hamiltonian RS and RSB approximations respectively. The diamonds are the results of the new variational scheme. The open triangles represent the empirical cubic approximation.