Random heteropolymer dynamics

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We study the Langevin dynamics of the standard random heteropolymer model by mapping the problem to a supersymmetric field theory using the Martin-Siggia-Rose formalism. The resulting model is solved nonperturbatively employing a Gaussian variational approach. In constructing the solution, we assume that the chain is very long and impose the translational invariance which is expected to be present in the bulk of the globule by averaging over the center of mass coordinate. In this way we derive equations of motion for the correlation and response functions $C(t,t')$ and $R(t,t')$. The order parameters are extracted from the asymptotic behavior of these functions. We find a dynamical phase diagram with frozen (glassy) and melted (ergodic) phases. In the glassy phase the system fails to reach equilibrium and exhibits aging of the type found in p-spin glasses. Within the approximations used in this study, the random heteropolymer model can be mapped to the problem of a manifold in a random potential with power law correlations.

I. INTRODUCTION

Disordered systems can be extremely hard to solve, as the example of spin glasses shows [1]. It took enormous effort to understand the physics of infinite-dimensional spin glasses, while that of finite-dimensional spin glasses is still debated. Certainly, the complexity of the spin glass energy landscape is the major obstacle one has to deal with, and there are other systems sharing this feature: standard examples are proteins [2] and manifolds in random potentials [3].

The study of simplified random heteropolymer models may provide a useful first step toward understanding the physics of proteins. Here, a central question is whether the trapping of the protein in a valley of the rough energy landscape can hinder, or perhaps even prevent, folding into its native state. Something related to this scenario has actually been observed in some real proteins: the protein can be heated and then, upon recooling, misfold and never be able to find its native state [4,5].

Here, we analyze the kind of dynamical trapping that can occur in the standard model of a random heteropolymer [6,7]. So far, in addition to numerical simulations, two analytic approaches have been used to solve such models: equilibrium analysis employing the replica technique (see, e.g., Refs. [7–13]) and dynamical studies using Langevin dynamics [14–21].

In the equilibrium approach, one studies the properties of Gibbs equilibrium. Even the simplest kind of random heteropolymer model can be approached analytically only in approximate ways. In Refs. [7–13] a model was analyzed with replica variational approximations, which predict ergodicity breaking at low temperature, giving one-step replica symmetry breaking (1RSB) for $d>2$ and continuous replica symmetry breaking for $d<2$. Thus, in three dimensions (3D), below the freezing temperature, the ergodic components lie far apart from each other, and have the same interstate overlap q_0. Given the intrinsic one-dimensional nature of the polymer, it has been argued that RSB could be an artifact of the variational approximation [22]. We believe,

however, that even in this eventuality, implying that a single native state dominates the thermodynamics, RSB in the variational approximation is a signal of a complex energy landscape, which can lead to slow dynamics, with off-equilibrium behavior on long time scales.

Models exhibiting 1RSB (such as the simple random heteropolymer mentioned above, the p-spin glass, or a manifold in a random potential) have been found to have different dynamic and static phase diagrams, with a dynamical energy density higher then the one found at equilibrium. This raises the intriguing possibility that, for a suitable range of temperatures and times, a heteropolymer might find itself dynamically trapped in a local state (as in the scenario described above), while the equilibrium statistical mechanics might give no clue that this was happening. Such trapping would thus be an intrinsically nonequilibrium effect, and a dynamical theory is required to describe it.

For models with this feature, the solutions exhibit a breakdown of time-translation invariance (the correlation functions depend on the time since the system was quenched into the glassy state) and a breakdown of the fluctuation-dissipation relation (which is a fundamental characteristic of Gibbs equilibrium). Together, these properties of the dynamical glassy phase go under the name ''aging,'' and it is one of our goals here to examine the possibility of aging in heteropolymers.

In this paper we consider the simple random heteropolymer model with Langevin dynamics (as in Refs. [16,21]). The equations of motion are constructed in such a way that the Gibbs distribution is the stationary solution of the dynamics. This type of dynamical approach was used successfully in spin glass models.

To derive closed equations of motion for correlation and response functions we resort to a Gaussian variational ansatz similar to the one used at equilibrium. The same approach has been used to study the problem of a manifold in a random potential, for both statics [23,24] and dynamics [25,26]. In related dynamical work on a random heteropolymer model [16] and [21], the slightly different approach of mode

coupling theory is used. Our approach gives results fully coherent with the ones obtained there, although the detailed form of the phase diagram differs, due to the different nature of the approximation.

The analysis of the variational equations indicates that, as expected from static treatments, the random heteropolymer model exhibits spontaneous breaking of ergodicity in a glassy phase. All these states are equally distant from each other; they have the same interstate overlap (naturally, the self-overlap is different). We also discuss the nature of the transition from the frozen (glassy) to the melted (ergodic) phase. Furthermore, we find that, within the Gaussian variational approximation that we employ, the random heteropolymer model can be mapped onto the problem of a manifold in a random potential with power law correlations.

The paper is organized as follows. Section II briefly describes the Langevin model. In Sec. III a mapping to a supersymmetric (SUSY) field theory is made. The resulting action can be simplified by assuming a very long chain. This is discussed in Sec. IV. Dynamical equations in SUSY notation, given in Sec. VII, are obtained via the variational *Ansatz* discussed in Secs. V and VI. Also, in Sec. VII, the connection of the random heteropolymer model to the problem of a manifold in a random potential will be commented upon. After disentangling the SUSY notation, one obtains dynamical equations for correlation and response functions (Sec. VIII). An analytical *Ansatz* for solving these equations is introduced in Sec. IX, and the solution is obtained in Sec. X. Section XI discusses the ergodic phase, while in Sec. XII the spin glass phase is analyzed. Technicalities needed to construct the full phase diagram are given in Sec. XIII.

II. THE MODEL

The model is defined as follows. The Langevin dynamics is assumed to be governed by the Hamiltonian $H[x]$,

$$\partial x(s,t)/\partial t = -\partial H[x]/\partial x(s,t) + \eta(s,t), \quad (1)$$

where $x(s,t)$ is the position of chain bead s at time t. Beads are numbered continuously from $s=0$ to $s=N$. $\eta(s,t)$ is Gaussian noise:

$$\langle \eta(s,t)\eta(s',t')\rangle_T = 2\delta(s-s')\delta(t-t')T \quad (2)$$

due to contact with a heat bath at temperature T. The Hamiltonian $H[x]=H_0[x]+H_{rand}[x]$ contains a deterministic part $H_0[x]$ and a random part $H_{rand}[x]$. The $H_0[x]$ is defined as

$$H_0[x] = \frac{T}{2}\int_0^N ds\{[\partial x(s,t)/\partial s]^2 + \mu x(s,t)^2\} \quad (3)$$

and describes the elastic properties of the chain and a confinement potential that fixes the density of the protein. The random part H_{rand} describes heterogeneity of the interactions between the beads,

$$H_{rand}[x] = \frac{1}{2}\int_0^N ds ds' B_{s,s'} V(x(s,t)-x(s',t)). \quad (4)$$

$B_{s,s'}$ is quenched Gaussian noise with variance B^2:

$$\langle B_{s,s'}^2\rangle_B = B^2, \quad s > s'. \quad (5)$$

$V(\Delta x)$ is a short-range potential, and for simplicity we take it to have a Gaussian form, as in Ref. [16]:

$$V(\Delta x) = \left(\frac{1}{2\pi\sigma}\right)^{d/2} e^{-(\Delta x)^2/2\sigma}. \quad (6)$$

d is the dimensionality of the system, and σ parametrizes the range of the potential. Large (small) σ results in a long-(short-)range potential. In particular, for $\sigma \to 0$, $V(\Delta x) \to \delta(\Delta x)$, and we recover the potential used in [21]. Here and in the following Δx denotes the bead-to-bead distance: $\Delta x = x(s,t) - x(s',t)$ for a pair of beads s,s'.

This model admits a stationary solution characterized by a Gibbs distribution. The equilibrium partition function for this solution is given by

$$\mathcal{Z} = \int Dx \exp -\frac{1}{2}\left(\int_0^N ds\{[\partial x(s)/\partial s]^2 + \mu x(s)^2\}\right.$$
$$\left. -\frac{\beta}{2}\int_0^N ds ds' B_{s,s'} V(x(s)-x(s'))\right). \quad (7)$$

T in Eq. (3) ensures that the chain constraint and quadratic confinement are temperature independent. (That is, the elasticity is purely entropic in origin.) The same convention was used in Ref. [16]. This differs slightly from the work in Ref. [21], where the elastic term had a factor β in front of it. Our choice ensures that for high temperatures the random heteropolymer behaves as a Gaussian random coil. Also, for very low temperatures, the random part of the interaction with β in front dominates ($\beta \to \infty$; the elastic and confinement terms become negligible). Thus, in principle, for $\beta = \infty$, $\mathcal{Z}$ in Eq. (7) is dominated by minima of $\int ds ds' B_{s,s'} V(x(s)-x(s'))$. Furthermore, in this limit there is nothing that would control the spatial spread of those minima, and $\langle x^2(s,t)\rangle_T$ diverges for very low temperatures. [This happens only when μ is held fixed. If it is adjusted appropriately, one can keep $\langle x^2(s,t)\rangle_T$ fixed instead. In this paper, however, we will be concerned with finite-T phase transitions, not the low-T limit, so we will work with fixed μ.]

III. MAPPING TO THE FIELD THEORY

Using the standard Martin-Siggia-Rose formalism [27], the dynamical average of any observable can be calculated as

$$\langle \mathcal{O}[x,\tilde{x}]\rangle_T = \int Dx D\tilde{x} DD\xi D\bar{\xi} \mathcal{O}(x,\tilde{x}) e^{-S[x,\tilde{x},\xi,\bar{\xi}]}, \quad (8)$$

with the following dynamical action:

$$S[x,\tilde{x},\xi,\bar{\xi}]=\int dtds\left[-T\tilde{x}(s,t)^2+\tilde{x}(s,t)\right.$$

$$\times\left(\frac{\partial}{\partial t}x(s,t)+\frac{\partial H[x]}{\partial x(s,t)}\right)\right]$$

$$-\int dtds\,\bar{\xi}(s,t)\frac{\partial}{\partial t}\xi(s,t)$$

$$+\int dtdsds'\,\bar{\xi}(s,t)\frac{\partial^2 H[x]}{\partial x(s,t)\partial x(s',t)}\xi(s',t).$$

(9)

$\tilde{x},\xi,\bar{\xi}$ are auxiliary fields that appear in the formalism. To compactify the notation we introduce the superfield Φ:

$$\Phi(s,t_1,\theta_1,\bar{\theta}_1)=x(s,t_1)+\bar{\xi}(s,t_1)\theta_1+\bar{\theta}_1\xi(s,t_1)$$

$$+\bar{\theta}_1\theta_1\tilde{x}(s,t_1),$$

(10)

where θ and $\bar{\theta}$ are Grassmann (anticommuting) variables. For $X,X'\in\{\theta,\bar{\theta},\theta',\bar{\theta}'\}$, $\{X,X'\}=0$, and $\int dXX=1$, the rest of the integrals being zero. In the following, for practical reasons, the more compact notation $\Phi(s,1)$ $\equiv\Phi(s,t_1,\theta_1,\bar{\theta}_1)$ will be used. Also, the integral symbol $\int d\theta_1 d\bar{\theta}_1 dt_1$ will be denoted by $\int d1$.

In supersymmetric notation Eqs. (8) and (9) translate into

$$\langle\mathcal{O}[\Phi]\rangle_T=\int D\Phi\mathcal{O}[\Phi]e^{-S[\Phi]},$$

(11)

$$S[\Phi]=S_0[\Phi]+S_{rand}[\Phi],$$

(12)

respectively, where

$$S_0[\Phi]=1/2\int dsd1ds'd2\Phi(s,1)K_{12}^{ss'}\Phi(s'2),$$

(13)

$$S_{rand}[\Phi]=1/2\int d1dsds'B_{s,s'}V(\Phi(s,1)-\Phi(s',1)),$$

(14)

and

$$K_{12}^{ss'}\equiv\delta_{12}\delta_{ss'}K_1^s,\quad K_1^s=T[\mu-(\partial/\partial s)^2]-D_1^{(2)},$$

(15)

$$D_1^{(2)}=2T\frac{\partial^2}{\partial\theta_1\partial\bar{\theta}_1}+2\theta_1\frac{\partial^2}{\partial\theta_1\partial t_1}-\frac{\partial}{\partial t_1}.$$

(16)

As noticed by De Dominicis [28] the expression in Eq. (11) is already normalized, so the average over the quenched random interactions $B_{s,s'}$ can be done directly on Eq. (11):

$$\langle\langle A[\Phi]\rangle_T\rangle_B=\int D\Phi A[\Phi]e^{-(S_0[\Phi]+S_1[\Phi])},$$

(17)

where $\exp(-S_1[\Phi])\equiv\langle\exp(-S_{rand}[\Phi])\rangle_B$. The average over $B_{s,s'}$ can be done easily, leading to

$$S_1[\Phi]=-B^2/4\int dsds'\left[\int d1V(\Phi(s,1)-\Phi(s',1))\right]^2.$$

(18)

The dynamical action $S=S_0+S_1$ closely resembles the effective Hamiltonian obtained in the static replica approach of Refs. [7,8]. (This rather general similarity between replica and SUSY treatments has been discussed in Ref. [29].) Instead of summation over replica indices in [7,8] we have $\int d1$. Our expressions are not identical to those in [7,8], since we use a quadratic well potential instead of two- and three-body interaction terms to confine the polymer. Also, we use a Gaussian $V(\Delta x)$ instead of $\delta(\Delta x)$.

IV. LONG-CHAIN APPROXIMATION

The S_1 part of the action can be further simplified. It can be rewritten in the form

$$S_1=-\frac{B^2}{4}A^{(V)}*A^{(\delta)}$$

(19)

with the notation

$$A^{(V)}*A^{(\delta)}=\int d1d2dxdyA_{1,2}^{(V)}(x,y)A_{1,2}^{(\delta)}(x,y),$$

(20)

where $A^{(V)}$ and $A^{(\delta)}$ are given by

$$A_{1,2}^{(V)}(x,y)=\int dsV(\Phi(s,1)-x)V(\Phi(s,2)-y),$$

(21)

$$A_{1,2}^{(\delta)}(x,y)=\int ds'\delta(\Phi(s',1)-x)\delta(\Phi(s',2)-y).$$

(22)

It is useful to transform $\exp(-S_1)$ as

$$\exp\left[\frac{B^2}{4}A^{(V)}*A^{(\delta)}\right]=\exp\left[\frac{B^2}{16}[(A^{(V)}+A^{(\delta)})*(A^{(V)}+A^{(\delta)})\right.$$

$$\left.-(A^{(V)}-A^{(\delta)})*(A^{(V)}-A^{(\delta)})]\right]$$

$$=\int DQ_1DQ_2\exp\left[\frac{B^2}{4}[-(Q_1^*Q_1\right.$$

$$+Q_2^*Q_2)+Q_1^*(A^{(V)}+A^{(\delta)})$$

$$\left.+iQ_2^*(A^{(V)}-A^{(\delta)})]\right].$$

(23)

Then, the dynamical generating functional F defined by

$$e^{-F}=\int D\Phi e^{-S[\Phi]+J*\Phi},$$

(24)

with $J*\Phi=\int dsd1J(s,1)\Phi(s,1)$, can be written as

$$e^{-F}=\int DQ_1DQ_2e^{-(B^2/4)(Q_1^*Q_1+Q_2^*Q_2)}\int D\Phi e^{L[Q_1,Q_2,\Phi]},$$

(25)

with L given by

$$L = \frac{B^2}{4}[Q_1^*(A^{(V)}+A^{(\delta)})+iQ_2^*(A^{(V)}-A^{(\delta)})]$$
$$- S_0[\Phi]+J*\Phi. \qquad (26)$$

So far everything was exact. $A^{(V)}$ and $A^{(\delta)}$ are both of order N and for very long chains one can calculate integrals over Q_1 and Q_2 in Eq. (25) using a saddle point approximation. The saddle point equations read

$$Q_1^{s.p.} = \frac{1}{2}\langle A^{(V)}+A^{(\delta)}\rangle_{L'}, \qquad (27)$$

$$Q_2^{s.p.} = \frac{i}{2}\langle A^{(V)}-A^{(\delta)}\rangle_{L'}, \qquad (28)$$

where $\langle\rangle_{L'}$ denotes the average with L taking $Q_1,Q_2 \to Q_1^{s.p.}, Q_2^{s.p.}$. This leads to self-consistent equations for $Q_1^{s.p.}$ and $Q_2^{s.p.}$.

Thus, Eq. (25) can be approximated as

$$e^{-F} \approx \int D\Phi e^{-S'[\Phi]+J*\Phi}, \qquad (29)$$

with $S'[\Phi]=S_1'[\Phi]+S_0[\Phi]$ and

$$S_1'[\Phi] = \frac{B^2}{4}[\langle A^{(V)}\rangle_{S'}*\langle A^{(\delta)}\rangle_{S'} - A^{(V)}*\langle A^{(\delta)}\rangle_{S'}$$
$$- A^{(\delta)}*\langle A^{(V)}\rangle_{S'}]. \qquad (30)$$

$\langle A^{(V)}\rangle_{S'}$ and $\langle A^{(\delta)}\rangle_{S'}$ have to be calculated self-consistently with S':

$$\langle A^{(V,\delta)}\rangle_{S'} = \frac{\displaystyle\int D\Phi A^{(V,\delta)}e^{-S'+J*\Phi}}{\displaystyle\int D\Phi e^{-S'+J*\Phi}}. \qquad (31)$$

In the limit $N\to\infty$ Eqs. (29)–(31) provide an exact description of random heteropolymer dynamics.

V. VARIATIONAL *ANSATZ*

To solve the model we proceed by using a variational *Ansatz*, assuming that the fields Φ are approximately described by a Gaussian action

$$S_{var} = \frac{1}{2}\int d1 ds d2 ds' \Phi(s,1)G(s,1;s',2)^{-1}\Phi(s',2). \qquad (32)$$

This approach has been widely used in statics. Here we apply it to a dynamical calculation. The goal is to calculate F given by Eq. (29). Since the variational parameter $G(s,1;s',2)$ is the only quantity we are interested in, there is no need to keep the source J. It is convenient to write Eq. (29), with $J=0$, formally as

$$e^{-F}=\langle e^{-(S'-S_{var})}\rangle_{var}e^{-F_{var}}, \qquad (33)$$

where

$$e^{-F_{var}}=\int D\Phi e^{-S_{var}}, \quad \langle\rangle_{var}=e^{F_{var}}\int D\Phi(\ )e^{-S_{var}}. \qquad (34)$$

In the usual statics, for problems without disorder, the variational approach is related to a maximum principle. The equivalent of Eq. (33) leads to the inequality

$$e^{-F}\geq e^{-\langle(S'-S_{var})\rangle_{var}}e^{-F_{var}}. \qquad (35)$$

In the present dynamical problem, as well as in the static problem with replicas, unfortunately such a maximum principle is not known, and the variational free energy cannot be claimed to be an upper bound on the true one. Despite that, the variational approach has been argued to give exact results in some limiting cases [23,24], giving a justification for its use in general.

The dynamical variational free energy $F_{dyn}=\langle(S'-S_{var})\rangle_{var}+F_{var}$ is given by

$$F_{dyn}=F_{dyn}^{(1)}+F_{dyn}^{(2)}+F_{dyn}^{(3)}, \qquad (36)$$

with

$$F_{dyn}^{(1)}=\frac{d}{2}\int ds d1 ds' d2 K_{12}^{ss'}G_{12}^{ss'}, \qquad (37)$$

$$F_{dyn}^{(2)}=-\frac{d}{2}\mathrm{Tr}\ln G, \qquad (38)$$

$$F_{dyn}^{(3)}=-\frac{B^2}{4}\langle A^{(V)}\rangle_{var}^*\langle A^{(\delta)}\rangle_{var}. \qquad (39)$$

Note that in calculating $F_{dyn}^{(3)}$ the average $\langle\rangle_{S'}$ in Eq. (30) is performed over the trial distribution [and therefore denoted $\langle\rangle_{var}$].

VI. CALCULATING $\langle A^{(V)}\rangle*\langle A^{(\delta)}\rangle$

The term $\langle A^{(V)}\rangle_{var}^*\langle A^{(\delta)}\rangle_{var}$ is the only nontrivial term in F_{dyn}. Before calculating it we simplify each of the factors in the product further:

$$A_{1,2}^{(V,\delta)}(x,y)\approx A_{1,2}^{(V,\delta)}(u)\equiv 1/v\int d^d R A_{1,2}^{(V,\delta)}(u,R), \qquad (40)$$

where v is the volume of the protein and a new coordinate system has been introduced:

$$R=(x+y)/2, \quad u=(x-y)/2. \qquad (41)$$

R is the center of mass and u a relative distance coordinate. Thus, translational invariance is introduced by hand via Eq. (40). This approximation is not necessary; the model could be solved without it. However, as we shall see later on, this

approximation leads to dynamical equations that are identical to those for the random manifold model studied in [25,26,30].

Changing integration variables from $d^d x \, d^d y$ to $d^d R \, d^d u$ (the Jacobian is 2^d) gives

$$\int d1d2d^dx d^dy \langle A_{1,2}^{(V)}(x,y)\rangle_{var} \langle A_{1,2}^{(\delta)}(x,y)\rangle_{var}$$

$$\approx \frac{2^d}{v} \int d1d2d^du \int d^dR' A_{1,2}^{(V)}(u,R') \int d^dR'' A_{1,2}^{(\delta)}(u,R''). \tag{42}$$

The integrals over R' and R'' can easily be performed and one gets

$$\frac{2^d}{v} \int d1d2d^du ds ds' d^d\alpha d^d\beta V(\alpha)V(\beta)$$

$$\times \langle \delta[2u-\alpha+\beta-\Phi(s,1)+\Phi(s,2)]\rangle_{var}$$

$$\times \langle \delta[2u-\Phi(s,1)+\Phi(s,2)]\rangle_{var}, \tag{43}$$

which can be further written as

$$\frac{2^d}{v} \int d1d2d^du ds ds' d^d\alpha d^d\beta V(\alpha)V(\beta)$$

$$\times \int \frac{d^dp}{(2\pi)^d} \frac{d^dq}{(2\pi)^d} e^{i(p+q)2u} e^{ip(\beta-\alpha)} e^{-p^2 B_{12}^s/2} e^{-q^2 B_{12}^{s'}/2}, \tag{44}$$

where averages over S_{var} have been evaluated as

$$\langle e^{ip[\Phi(s,1)-\Phi(s,2)]}\rangle_{var} = e^{-p^2 B_{12}^s/2}, \tag{45}$$

with $B_{1,2}^s$ given by

$$B_{1,2}^s = \langle [\Phi(s,1)-\Phi(s,2)]^2\rangle_{var}$$

$$= G(s,1;s,1)+G(s,2;s,2)-2G(s,1;s,2). \tag{46}$$

Integrating Eq. (44) first over u and then over q and p finally gives

$$\frac{1}{v}(2\pi)^{-d/2} \int d1d2ds ds' d^d\alpha d^d\beta V(\alpha)V(\beta)(B_{12}^s+B_{12}^{s'})^{-d/2}$$

$$\times \exp -\frac{(\alpha-\beta)^2}{2(B_{12}^s+B_{12}^{s'})}. \tag{47}$$

Equation (47) holds for any $V(\Delta x)$. However, technically, it is of little use unless the integrals over α and β can be performed explicitly. For the Gaussian form for $V(\Delta x)$ [see Eq. (6)] it is possible to perform the integrals, and one gets

$$\langle A^{(V)}\rangle_{var}^* \langle A^{(\delta)}\rangle_{var} \approx \frac{1}{v}(4\pi)^{-d/2} \int d1d2ds ds'$$

$$\times [(B_{12}^s+B_{12}^{s'})/2+\sigma]^{-d/2} \tag{48}$$

and finally

$$F_{dyn}^{(3)} \approx \frac{d}{2N} \int d1d2ds ds' \mathcal{V}[(B_{12}^s+B_{12}^{s'})/2] \tag{49}$$

with

$$\mathcal{V}(z) = -\frac{\tilde{B}^2}{d}(z+\sigma)^{-d/2}, \quad \tilde{B}^2 = \frac{B^2}{2}\frac{N}{v}(4\pi)^{-d/2}. \tag{50}$$

Equations (36)–(39) and (49) fully determine F_{dyn}.

VII. EQUATIONS OF MOTION IN SUSY NOTATION

Given F_{dyn}, one can derive the equations of motion from the stationarity condition

$$\frac{\delta}{\delta G_{12}^{ss'}} F_{dyn} = 0. \tag{51}$$

The most complicated term is $(\delta/\delta G_{12}^{ss'})F_{dyn}^{(3)}$. From Eq. (49), it is

$$\frac{d}{2N} \int d3d4dudv \mathcal{V}'[(B_{34}^u+B_{34}^v)/2]$$

$$\times \delta_{ss'} \frac{\delta_{us}+\delta_{vs}}{2}(\delta_{13}\delta_{23}+\delta_{14}\delta_{24}-\delta_{13}\delta_{24}-\delta_{14}\delta_{23}). \tag{52}$$

Due to translational invariance in s, B_{12}^s is independent of s. After dropping the index s Eq. (52) simplifies to

$$\frac{\delta}{\delta G_{12}^{ss'}} F_{dyn}^{(3)} = d\delta_{ss'}\left[\delta_{12}\int d3 \mathcal{V}'(B_{13})-\mathcal{V}'(B_{12})\right]. \tag{53}$$

The variations of $F_{dyn}^{(1)}$ and $F_{dyn}^{(2)}$ are trivial. Using Eqs. (51) and (36) leads to

$$K_{12}^{ss'}-(G_{12}^{ss'})^{-1}+2\delta_{ss'}\left[\delta_{12}\int d3\mathcal{V}(B_{13})-\mathcal{V}(B_{12})\right]=0, \tag{54}$$

which can be written as

$$K_1^s G_{12}^{ss'} = \delta_{12}\delta_{ss'}+2\int d3\mathcal{V}'(B_{13})(G_{32}^{ss'}-G_{12}^{ss'}). \tag{55}$$

Due to translational invariance in the variable s it is useful to define the following Fourier transforms:

$$G_{12}^{ss'} \equiv \int_{-\infty}^{\infty} \frac{dk}{2\pi} e^{ik(s-s')} G_{12}^k. \tag{56}$$

Then Eq. (55) translates into

$$[T(\mu+k^2)-D_1^{(2)}]G_{12}^k = \delta_{12}+2\int d3\mathcal{V}'(B_{13})(G_{32}^k-G_{12}^k). \tag{57}$$

Equation (57) is identical to the one obtained in Ref. [26] for a D-dimensional manifold $\varphi(\omega)$ ($\omega \in R^D$, $\varphi \in R^d$) in a random potential $V(\varphi(\omega), \omega)$, where the correlations of the potential are described by

$$\langle V(\varphi, \omega) V(\varphi', \omega') \rangle = -d\,\delta^D(\omega - \omega')\hat{\mathcal{V}}[(\varphi - \varphi')/d]. \tag{58}$$

These equations of motion were derived using the Gaussian variational approximation (GVA), which is exact for the random manifold problem in $d = \infty$. We expect the same behavior for the random heteropolymer. However, in this study we work at finite d, so the equations of motion are approximate.

There have been several studies of random manifolds where $\hat{\mathcal{V}}$ describes power law correlations as in Eq. (59), employing static [23,24,31] and dynamical [30,32,33] approaches:

$$\hat{\mathcal{V}}(z) = (z + \sigma)^{1-\gamma}/2(1-\gamma). \tag{59}$$

By comparing Eqs. (50) and (59) one notices that $\mathcal{V}(z)$ is identical to $\hat{\mathcal{V}}(z)$ (up to a proportionality factor $\tilde{B}^2$) if one identifies $\gamma = 1 + d/2$. Accordingly, we conclude that, within the Gaussian variational approximation used in this study, random heteropolymer dynamics is identical to the dynamics of the manifold in a random potential with power law correlations. (We cannot say anything rigorous outside the framework of the Gaussian variational approximation scheme, of course.)

Furthermore, correlations of the random manifold potential are classified as short range for $\gamma > 2/(2-D)$ and long range for $\gamma < 2/(2-D)$ [23,24]. This classification of random manifolds helps to classify random heteropolymer models in the same way. Using $\gamma = 1 + d/2$, the random heteropolymer has $D = 1$, and short-range correlations for $d > 2$ and long-range correlations for $d < 2$. (Again, this all makes sense only within the Gaussian variational approximation.)

VIII. DISENTANGLING SUSY

$G_{12}^{ss'}$ encodes 16 correlation functions, out of which only two, the correlation and response functions, are independent and nonzero:

$$\langle\langle x(s,t_1) x(s',t_2) \rangle\rangle \equiv C(s,t_1;s',t_2)$$

$$= \int \frac{dk}{2\pi} e^{ik(s-s')} C_k(t_1,t_2), \tag{60}$$

$$\langle\langle x(s,t_1) \tilde{x}(s',t_2) \rangle\rangle \equiv R(s,t_1;s',t_2)$$

$$= \int \frac{dk}{2\pi} e^{ik(s-s')} R_k(t_1,t_2). \tag{61}$$

Also, by adding an external field term to the original Hamiltonian $H[x] \to H[x] + \int ds\,dt\,x(s,t)h(s,t)$ one gets

$$\langle\langle x(s,t_1)\tilde{x}(s',t_2) \rangle\rangle = \frac{\delta}{\delta h(s',t_2)}\langle\langle x(s,t_1) \rangle\rangle, \tag{62}$$

i.e., $R(s,t_1;s',t_2)$ describes the response to an infinitesimal field applied at time t_2 and bead s'. Thus, G_{12}^k reduces to

$$G_{12}^k = C_k(t_1,t_2) + (\bar{\theta}_1 - \bar{\theta}_2)[\theta_1 R_k(t_2,t_1) - \theta_2 R_k(t_1,t_2)], \tag{63}$$

and, accordingly, with $G_{11}^{ss} = C(s,t_1;s,t_1)$, $G_{22}^{ss} = C(s,t_2;s,t_2)$, and Eqs. (60),(61), one gets

$$B_{12} = B(t_1,t_2) - 2(\bar{\theta}_1 - \bar{\theta}_2)[\theta_1 r(t_2,t_1) - \theta_2 r(t_1,t_2)] \tag{64}$$

with

$$B(t_1,t_2) = \int \frac{dk}{2\pi}[C_k(t_1,t_1) + C_k(t_2,t_2) - 2C_k(t_1,t_2)] \tag{65}$$

and

$$r(t_1,t_2) = \int \frac{dk}{2\pi} R_k(t_1,t_2). \tag{66}$$

After disentangling the equations of motion in SUSY notation [see Eq. (57)] using Eqs. (63)–(66) gives

$$[T(\mu + k^2) + \partial/\partial t]C_k(t,t')$$

$$= 2TR_k(t',t) + 2\int_0^t ds\,\mathcal{V}'[B(t,s)]R_k(t',s)$$

$$+ 4\int_0^t ds\,\mathcal{V}''[B(t,s)]r(t,s)[C_k(t,t') - C_k(s,t')], \tag{67}$$

$$[T(\mu + k^2) + \partial/\partial t]R_k(t,t')$$

$$= \delta(t-t') + 4\int_0^t ds\,\mathcal{V}''[B(t,s)]r(t,s)$$

$$\times [R_k(t,t') - R_k(s,t')]. \tag{68}$$

The equations of motion (67) and (68) are almost identical to the ones found in Ref. [25] (here $D = 1$, while in [25] $D = 0$).

IX. *ANSATZ* FOR $C_k(t,t')$ AND $R_k(t,t')$

These equations of motion are coupled integro-differential equations which in principle can be solved; the initial conditions are given by $C_k(0,0)$ and we use Ito's convention $R(t+\epsilon,t) \to 1$ as $\epsilon \to 0$. It is well known that asymptotic solutions of such equations can be characterized by few parameters and it is possible to solve those equations analytically [25,26,30,34–36].

For $t,t' \to \infty$, $\tau/t' \ll 1$, and $\tau = t - t'$, time-translational invariance (TTI) holds:

$$\lim_{t\to\infty} C_k(t,t)=\tilde{q}_k, \tag{69}$$

$$\lim_{t\to\infty} C_k(t+\tau,t)=C_k(\tau), \tag{70}$$

$$\lim_{\tau\to\infty} C_k(\tau)=q_k, \tag{71}$$

and

$$\lim_{t\to\infty} R_k(t+\tau,t)=R_k(\tau). \tag{72}$$

In addition to the TTI regime, there is another long-time nontrivial regime, characterized by $t,t'\to\infty$, fixing $\lambda=h(t')/h(t)$ and $0<\lambda<1$, where the function $h(t)$ is an increasing function of t, which the asymptotic analysis performed here is not able to determine. In this aging regime one has

$$\lim_{t\to\infty} C_k(t,h^{-1}[\lambda h(t)])=q_k\hat{C}_k(\lambda), \tag{73}$$

$$\lim_{\lambda\to 0} q_k\hat{C}_k(\lambda)=q_{0,k}, \tag{74}$$

$$\lim_{\lambda\to 1} \hat{C}_k(\lambda)=1, \tag{75}$$

and

$$\lim_{t\to\infty} R_k(t,\lambda t)=\frac{1}{t}\hat{R}_k(\lambda). \tag{76}$$

Also, for future convenience, it is useful to introduce the following order parameters:

$$\tilde{q}\equiv\lim_{t\to\infty}\langle\langle x(s,t)x(s,t)\rangle\rangle=\int\frac{dk}{2\pi}\tilde{q}_k, \tag{77}$$

$$q\equiv\lim_{\tau\to\infty}\lim_{t\to\infty}\langle\langle x(s,t+\tau)x(s,t)\rangle\rangle=\int\frac{dk}{2\pi}q_k, \tag{78}$$

$$q_0\equiv\lim_{\lambda\to 0}\lim_{t\to\infty}\langle\langle x(s,t)x(s,\lambda t)\rangle\rangle=\int\frac{dk}{2\pi}q_{0,k}, \tag{79}$$

together with

$$b=2(\tilde{q}-q),\quad b_0=2(\tilde{q}-q_0). \tag{80}$$

X. EQUATIONS RELATING ASYMPTOTIC VALUES OF CORRELATION AND RESPONSE FUNCTIONS

Using the *Ansatz* discussed in Sec. IX one can derive the following equations for $C_k(t,t')$ in the TTI regime:

$$[T(\mu+k^2)+\partial/\partial\tau]C_k(\tau)$$

$$=2TR_k(-\tau)+\frac{2}{T}\mathcal{V}'(b)[C_k(\tau)-q_k]$$

$$-\frac{2}{T}\int_0^\tau d\tau'\mathcal{V}'(B(\tau-\tau'))\frac{\partial C_k(\tau')}{\partial\tau'}$$

$$+2\int_0^1 d\rho\mathcal{V}'(\hat{B}(\rho))\hat{R}_k(\rho)+4\int_0^1 d\rho\mathcal{V}''(\hat{B}(\rho))\hat{r}(\rho)$$

$$\times[C_k(\tau)-q_k\hat{C}_k(\rho)]. \tag{81}$$

It is also possible to derive similar equations for $R_k(\tau)$ which, due to the fluctuation-dissipation theorem (FDT)

$$R_k(\tau)=-\frac{1}{T}\frac{dC_k(\tau)}{d\tau}, \tag{82}$$

are completely equivalent to Eq. (81).

In the aging regime one gets the following equation for $q_k\hat{C}(\lambda)$:

$$\left[T(\mu+k^2)-4\int_0^1 d\rho\mathcal{V}''(\hat{B}(\rho))\hat{r}(\rho)\right]q_k\hat{C}_k(\lambda)$$

$$=2\int_0^1 d\rho\mathcal{V}'(\hat{B}(\rho))\hat{R}_k(\rho)+\frac{2}{T}\mathcal{V}'(\hat{B}(\lambda))(\tilde{q}_k-q_k)$$

$$-4\int_0^\lambda d\rho\mathcal{V}''(\hat{B}(\rho))\hat{r}(\rho)q_k\hat{C}_k(\rho/\lambda)$$

$$-4\int_\lambda^1 d\rho\mathcal{V}''(\hat{B}(\rho))\hat{r}(\rho)q_k\hat{C}_k(\lambda/\rho). \tag{83}$$

For $\hat{R}_k(\lambda)$ we obtain

$$\left[T(\mu+k^2)-4\int_0^1 d\rho\mathcal{V}''(\hat{B}(\rho))\hat{r}(\rho)\right]\hat{R}_k(\lambda)$$

$$=-\frac{4}{T}\mathcal{V}''(\hat{B}(\lambda))\hat{r}(\lambda)(\tilde{q}_k-q_k)$$

$$-4\int_\lambda^1\frac{d\rho}{\rho}\mathcal{V}''(\hat{B}(\rho))\hat{r}(\rho)\hat{R}_k(\lambda/\rho). \tag{84}$$

Again, one can see that both Eq. (83) and Eq. (84) can be solved by the *Ansatz*

$$\hat{R}_k(\lambda)=\frac{x}{T}q_k\frac{d\hat{C}_k(\lambda)}{d\lambda}. \tag{85}$$

Equation (85) is commonly referred to as a generalized FDT (GFDT). In principle, Eq. (85) could have been written as

$$\hat{R}_k(\lambda)=\frac{x_k[q_k\hat{C}_k(\lambda)]}{T}q_k\frac{d\hat{C}_k(\lambda)}{d\lambda}, \tag{86}$$

which could be applied to a many-step RSB scheme. However, as previously discussed, the present random heteropolymer model can be identified with the random manifold problem with short-range potential correlations. As such, it has one-step RSB, and it is sufficient to use the simpler ansatz given in Eq. (85).

For $t=t'$ and $t \to \infty$ Eq. (67) gives

$$T(\mu+k^2)\tilde{q}_k = T + \frac{2}{T}\mathcal{V}'(b)(\tilde{q}_k-q_k)$$

$$+ 2\int_0^1 d\rho \mathcal{V}'(\hat{B}(\rho))\hat{R}_k(\rho)$$

$$+ 4\int_0^1 d\rho \mathcal{V}''(\hat{B}(\rho))\hat{r}(\rho)[\tilde{q}_k-q_k C_k(\rho)]. \tag{87}$$

Equation (81) for $t \to \infty$ and then $\tau \to \infty$ results in

$$T(\mu+k^2)q_k = \frac{2}{T}\mathcal{V}'(b)(\tilde{q}_k-q_k) + 2\int_0^1 d\rho \mathcal{V}'(\hat{B}(\rho))\hat{R}_k(\rho)$$

$$+ 4\int_0^1 d\rho \mathcal{V}''(\hat{B}(\rho))\hat{r}(\rho)q_k[1-C_k(\rho)]. \tag{88}$$

Also, Eq. (83) for $\lambda \to 0$ gives

$$T(\mu+k^2)q_{0,k} = 2\mathcal{V}'(b_0)\int_0^1 d\rho \hat{R}_k(\rho) + \frac{2}{T}\mathcal{V}'(b_0)(\tilde{q}_k-q_k). \tag{89}$$

Equations (87), (88), and (89) [and, equivalently, Eqs. (81), (83), and (84) contain TTI and aging parts. Thus, in principle, there are two *Ansätze* for solving them, leading to two phases: an ergodic one (without aging) and a glassy one (with aging).

XI. ERGODIC PHASE

Technically, assuming that aging is absent amounts to setting $\hat{R}_k(\lambda)=0$ and $\hat{C}_k(\lambda)=1$ in Eqs. (87), (88), and (89). [Equivalently, one could start from Eqs. (67) and (68) and exclude the aging part from the beginning, leading to the same equations.] Thus, in the ergodic phase, Eqs. (87), (88), and (89) reduce to

$$T(\mu+k^2)\tilde{q}_k = T + \frac{2}{T}\mathcal{V}'(b)(\tilde{q}_k-q_k), \tag{90}$$

$$T(\mu+k^2)q_k = \frac{2}{T}\mathcal{V}'(b)(\tilde{q}_k-q_k), \tag{91}$$

$$T(\mu+k^2)q_{0,k} = \frac{2}{T}\mathcal{V}'(b_0)(\tilde{q}_k-q_k). \tag{92}$$

Note that Eqs. (91) and (92) enforce $q_k=q_{0,k}$ which is just equivalent to $\hat{C}_k(\lambda)=1$, so one gets only two equations. Solving them for $\tilde{q}_k$ and q_k gives

$$\tilde{q}_k - q_k = \frac{1}{\mu+k^2}, \tag{93}$$

$$\tilde{q}_k = \frac{1}{\mu+k^2} + \frac{2}{T^2}\mathcal{V}'(b)\frac{1}{(\mu+k^2)^2}. \tag{94}$$

After integrating over k and using

$$\int \frac{dk}{2\pi}\frac{1}{\mu+k^2} = \frac{1}{2\sqrt{\mu}}, \quad \int \frac{dk}{2\pi}\frac{1}{(\mu+k^2)^2} = \frac{1}{4\mu^{3/2}}, \tag{95}$$

we obtain

$$q = \frac{1}{2\mu^{3/2}T^2}\mathcal{V}'(1/\sqrt{\mu}), \tag{96}$$

$$\tilde{q} = \frac{1}{2\sqrt{\mu}} + \frac{1}{2\mu^{3/2}T^2}\mathcal{V}'(1/\sqrt{\mu}). \tag{97}$$

For T very small, q and $\tilde{q}$ blow up since the confinement term $\mu x(s,t)^2$ becomes ineffective [see Eq. (7)]. For very large temperature q approaches zero but is never exactly equal to zero.

XII. SPIN GLASS PHASE

Keeping the aging parts and using the GFDT, Eqs. (87), (88), and (89) can be transformed into

$$T(\mu+k^2)\tilde{q}_k = T + \frac{2}{T}\mathcal{V}'(b)(1-x)(\tilde{q}_k-q_k)$$

$$+ \frac{2}{T}\mathcal{V}'(b_0)x(\tilde{q}_k-q_{0,k}), \tag{98}$$

$$T(\mu+k^2)q_k = \frac{2}{T}[\mathcal{V}'(b)-x\mathcal{V}'(b_0)](\tilde{q}_k-q_k)$$

$$+ \frac{2}{T}\mathcal{V}'(b_0)x(\tilde{q}_k-q_{0,k}), \tag{99}$$

$$T(\mu+k^2)q_{0,k} = \frac{2}{T}\mathcal{V}'(b_0)(1-x)(\tilde{q}_k-q_k)$$

$$+ \frac{2}{T}\mathcal{V}'(b_0)x(\tilde{q}_k-q_{0,k}). \tag{100}$$

Solving Eqs. (98), (99), and (100) for $\tilde{q}_k$, q_k, and $q_{0,k}$ gives

$$\tilde{q}_k - q_k = \frac{1}{\mu+k^2+\Sigma}, \tag{101}$$

$$\tilde{q}_k - q_{0,k} = \frac{1}{x}\frac{1}{\mu+k^2} - \frac{1-x}{x}\frac{1}{\mu+k^2+\Sigma}, \quad (102)$$

$$\tilde{q}_k = (\tilde{q}_k - q_{0,k}) + \frac{2}{T^2}\mathcal{V}'(b_0)\frac{1}{(\mu+k^2)^2}, \quad (103)$$

where

$$\Sigma = x\frac{2}{T^2}[\mathcal{V}'(b) - \mathcal{V}'(b_0)]. \quad (104)$$

Integration over k and using Eq. (95) gives

$$b = \frac{1}{\sqrt{\mu+\Sigma}}, \quad (105)$$

$$b_0 = \frac{1}{x}\frac{1}{\sqrt{\mu}} - \frac{1-x}{x}\frac{1}{\sqrt{\mu+\Sigma}}, \quad (106)$$

$$\tilde{q} = b_0 + \frac{1}{2\mu^{3/2}T^2}\mathcal{V}'(b_0). \quad (107)$$

Furthermore, Eq. (84) with $\lambda = 1$ gives

$$\hat{R}_k(1)(\mu+k^2+\Sigma) = -(\tilde{q}_k - q_k)\frac{4\mathcal{V}''(b)}{T^2}\hat{r}(1), \quad (108)$$

and, after using Eq. (101), integrating over k, and using $\mu + \Sigma = b^{-2}$ [see Eq. (105)], one gets

$$0 = \hat{r}(1)[T^2 + b^3\mathcal{V}''(b)]. \quad (109)$$

Equation (109) with $\hat{r}(1) \neq 0$ implies the marginal stability condition

$$-T^2 = b^3\mathcal{V}''(b). \quad (110)$$

Also, Eqs. (105) and (106) can be rewritten as

$$\frac{\mathcal{V}'(b) - \mathcal{V}'(b_0)}{b_0 - b} = \frac{T^2}{2}\frac{\sqrt{\mu}}{b}\left(\frac{1}{b} + \sqrt{\mu}\right), \quad (111)$$

$$b_0 - b = \frac{1}{x}\left(\frac{1}{\sqrt{\mu}} - b\right). \quad (112)$$

Equations (110), (111), and (112) fully solve the model: (110) gives b as function of T, (111) determines b_0 as function of T and μ, (112) determines $x(T,\mu)$, and Eq. (107) gives $\tilde{q}(T,\mu)$. Knowing $b(T)$, $b_0(T,\mu)$, and $\tilde{q}(T,\mu)$ determines $q(T,\mu)$ and $q_0(T,\mu)$. Were we to impose the spherical constraint $\tilde{q} = $ const, Eq. (107) could be used to relate μ and T, and all order parameters could be expressed as functions of T only ($\tilde{q}$ being fixed). However, in this study we work with fixed T and μ, allowing $\tilde{q}$ to change.
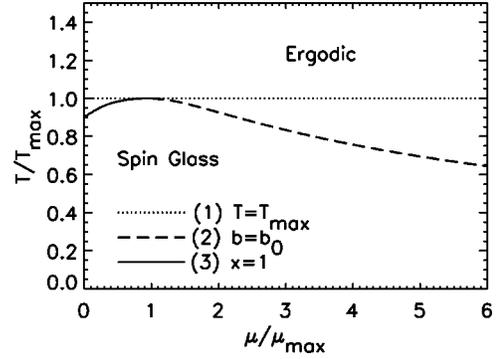
FIG. 1. Phase diagram of dynamic random heteropolymer model in μ, T plane. Critical lines are denoted by (1) $T = T_{max}$; (2) $b = b_0 = \mu^{-1/2}$ (x ranges from 1 to 0); (3) $x = 1$, $b_0 = \mu^{-1/2} > b$. Below lines 2 and 3 lies the glassy phase and above the ergodic phase.

XIII. SOLVING THE EQUATIONS (PHASE DIAGRAM)

The procedure of solving equations similar to the ones given in Eqs. (110), (111), and (112) has been discussed in Ref. [25]. We apply a similar analysis to the random heteropolymer problem. In principle, there are three critical lines in the T, μ plane separating different phases (as shown in Fig. 1).

Critical line 1. $T = T_{max}$ is the uppermost critical line [denoted in Fig. 1 by (1)]; above this line Eq. (110) has no solution. The value of T_{max} can be determined from the graphical solution of Eq. (110) depicted in Fig. 2. Once T has been chosen (horizontal line labeled T/T_{max}) b is found from the intercept of the T/T_{max} line with the $-b^3\mathcal{V}''(b)/T_{max}^2$ curve. From Fig. 2 it is clear that at $b = b_{max}$ the right hand side of Eq. (110) reaches a maximum; requiring $(d/db) \times [b^3\mathcal{V}''(b)] = 0$ gives $3\mathcal{V}''(b) + b\mathcal{V}'''(b) = 0$ and $b_{max} = 3\sigma/(\gamma-2)$. Accordingly, $T_{max} = [-b_{max}^3\mathcal{V}''(b_{max})]^{1/2}$.

Also, note that for fixed T Eq. (110) has two solutions for b (denoted by I and II in Fig. 2); a first, physical solution ($b_I \to 0$ for $T \to 0$) in the interval $[0, b_{max}]$ and a second, unphysical solution ($b_{II} \to \infty$ for $T \to 0$) in the interval $[b_{max}, \infty)$. Accordingly, a model with $\sigma = 0$ [i.e., $V(\Delta x) = \delta(\Delta x)$] leads to an unphysical phase diagram, since for $\sigma \to 0$ the physical branch $[0, b_{max}]$ disappears ($b_{max} \to 0$).
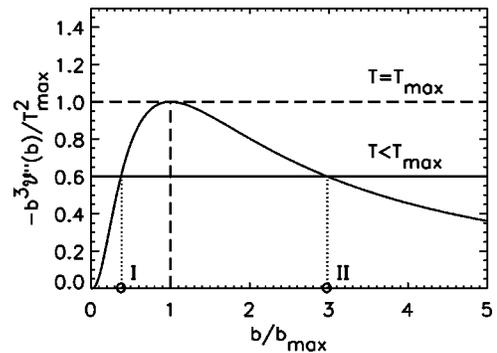
FIG. 2. Graphical solution of Eq. (110). The equation has two solutions for $T < T_{max}$ denoted by I and II. For $T = T_{max}$ there is only one solution $b = b_{bmax}$. Solution I is physical and solution II is unphysical.

Clearly, the form of $\mathcal{V}(b)$ for small b has to be modeled carefully and the choice $V(\Delta x) = \delta(\Delta x)$ simply fails in that respect, giving $\mathcal{V}(0) = \infty$. Thus, when formulating the problem, if there is to be a possibility of freezing at low temperatures ($b \to 0$ as $T \to 0$), the bead-bead interaction $V(\Delta x)$ has to be regular for small Δx. A similar small-distance regularization problem of the bead-bead interaction was encountered in Ref. [21].

Critical line 2. This corresponds to $b = b_0$. From Eq. (112) it follows that $b = b_0 = 1/\sqrt{\mu}$. The equation of the critical line is obtained by inserting $b = 1/\sqrt{\mu}$ into Eq. (110):

$$(T/\tilde{B})^2 = \frac{\gamma}{2} \mu^{-3/2} (\mu^{-1/2} + \sigma)^{-(\gamma+1)}. \tag{113}$$

$\mu \in [\mu_{max}, \infty)$, where μ_{max} solves Eq. (113) with $T = T_{max}$.

The value of x_c at the critical line cannot be directly obtained from Eq. (112). Instead, one has to approach the critical line and obtain the limiting value of x: for example, first one assumes that the point (T_c, μ_c) is at the critical line [T_c and μ_c satisfy Eq. (113)] and then $T(\epsilon)$, $\mu(\epsilon)$, $b(\epsilon)$, $b_0(\epsilon)$, and $x(\epsilon)$ approach their values at the critical line for $\epsilon \to 0$. Naturally, the dependence on ϵ has to be chosen consistently with Eqs. (110), (111), and (112). Since one has five variables and three equations that relate them, two variables have to be specified as, e.g., $b_0(\epsilon) = b_c + \epsilon$, with $b_c = 1/\sqrt{\mu_c}$ and $T(\epsilon) = T_c$. The other three variables $b(\epsilon)$, $\mu(\epsilon)$, and $x(\epsilon)$ have to be determined from Eqs. (110), (111), and (112):

$$\frac{\mathcal{V}'(b_c) - \mathcal{V}'(b_c + \epsilon)}{\epsilon} = \frac{T_c^2}{2} \frac{\sqrt{\mu(\epsilon)}}{b_c} \left(\frac{1}{b_c} + \sqrt{\mu(\epsilon)} \right), \tag{114}$$

$$\epsilon = \frac{1}{x(\epsilon)} \left(\frac{1}{\sqrt{\mu(\epsilon)}} - b_c \right). \tag{115}$$

Equation (110) is trivially satisfied and does not enter the analysis. At first order in ϵ Eqs. (115) and (114) give

$$x(0) = -\frac{1}{2\mu_c^{3/2}} \mu'(0), \quad \mu'(0) = -\frac{2}{3} \frac{\mathcal{V}'''(b_c)}{T_c^2 \sqrt{\mu_c}}, \tag{116}$$

which, together with $T_c^2 = -\mu_c^{-3/2} \mathcal{V}''(b_c)$, gives the value for x at the critical line 2,

$$x_c = -\frac{1}{3} \frac{\mathcal{V}'''(b_c)}{\mathcal{V}''(b_c)}. \tag{117}$$

Using the explicit form for $\mathcal{V}$ gives

$$x_c = \frac{\gamma+1}{3} \frac{b_c}{b_c + \sigma} \tag{118}$$

with b_c on the critical line. $b_c = b_{max}$ gives $x_c = 1$ while for $b_c = 0$ one gets $x_c = 0$.

Thus, at the critical line 2, close to T_{max}, x_c is very close to 1 and as $T(\mu)$ decreases (increases) x_c drops to zero.

Also, at the critical line 2, the transition to the ergodic phase is continuous in b and b_0 and discontinuous in x.

Critical line 3. At this line $x = 1$ and Eq. (112) gives $b_0 = 1/\sqrt{\mu} > b$. The equation for this critical line is given by

$$\frac{\mathcal{V}'(b) - \mathcal{V}'(1/\sqrt{\mu})}{1/\sqrt{\mu} - b} = \frac{T^2}{2} \frac{\sqrt{\mu}}{b} \left(\frac{1}{b} + \sqrt{\mu} \right). \tag{119}$$

Once T is chosen, b is determined from Eq. (110) and upon solving Eq. (119) one obtains μ as a function of T. Critical line 3 is depicted in Fig. 1, where it was obtained by solving Eq. (119) numerically. The line starts from (μ_{max}, T_{max}) and then drops to $(0, T^*)$ where T^* is given from Eq. (110) with $b = b^*$ and $b^* = 2\sigma/(\gamma - 2)$. Thus, as $b \to b^*$, $b_0 \to \infty$, as can easily be checked by inserting those assumptions in Eq. (119). Also, $b_0 \to b$ as $\mu \to \mu_{max}$. Thus, unlike line 2, on line 3 the transition to the ergodic phase is discontinuous in b and b_0 but continuous in x.

Also, for arbitrary μ, when T gets close to zero b approaches 0 and b_0 grows to infinity. This simply means that for low temperatures the heteropolymer freezes completely: $x(s, t + \tau) = x(s, t)$ for arbitrary τ and t sufficiently large. On the other hand, for fixed T and vanishing μ, Eq. (111) gives $b_0 \to \infty$, while b stays fixed by Eq. (110).

For small μ Eqs. (96) and (97) give $q/\tilde{q} \propto \mu^{(d-2)/4}$. Thus, for $\mu = 0$ one gets $q/\tilde{q} = 0$. Also, as discussed at the end of the preceding paragraph, in the glass phase for $\mu \to 0$ one has $b_0 \to \infty$ and $b = $ const, which gives $q/\tilde{q} = 1$. Thus in contrast to the ergodic phase, where vanishing μ leads to paramagneticlike behavior, in the glass phase the system gets trapped in one of many states separated by diverging barriers. Interestingly enough, adjusting μ so that the radius of gyration R_g scales according to $R_g^d \sim N$ and using the relation $R_g^2 \sim 1/\sqrt{\mu}$ (which is exact for the Gaussian coil) [16] gives $\mu \propto N^{-4/d}$ and $q/\tilde{q} \propto N^{-(d-2)/d}$. Thus, in the thermodynamic limit $q/\tilde{q} \to 0$.

XIV. DISCUSSION

We have presented a detailed derivation of the equations of motion of a random heteropolymer using SUSY formalism and a Gaussian variational *Ansatz*. In deriving these equations, we have used a long-chain approximation, considerably simplifying the dynamical action. Furthermore, by imposing translational invariance, we have shown that, as happens in statics, within the Gaussian variational *Ansatz* the equations of motion become identical to those for a manifold in a random potential with power law correlations.

Clearly, this result is closely related to the particular variational *Ansatz* employed here, and its generality beyond this framework remains an open question. Nevertheless, the existence of this mapping at the level of the GVA is rather intriguing. It connects the random heteropolymer model with many physical systems, such as a manifold pinned by impurities, interfaces in a random field, the glassy phase of vortices in high-T_c superconductors, directed polymers in a random potential, and surface growth on disordered substrates. It would be interesting to understand to what extent the map-

pings to these problems extends beyond the GVA.

By making the standard 1RSB aging *Ansatz* for response and correlation functions we found the asymptotic solution of the dynamical equation. The validity of this *Ansatz* has been carefully checked elsewhere: in the context of the random manifold problem it was shown that the one-step replica symmetry breaking *Ansatz* can be used to describe a random manifold with short-range correlations, and we have applied this result to the random heteropolymer.

The analytic solutions show that, as expected, the random heteropolymer has characteristic properties of spin glass systems: aging and ergodicity breaking. Furthermore, the dynamical phase diagram is different from that for statics. In dynamics starting from a random condition, the polymer get stuck at energies higher than the ones of the native state.

In a more realistic approach to heteropolymers, we expect that finite-dimensional, and finite-length chain effects will be responsible for ultimate restoration of ergodicity. Our study should be taken as an indication of a time regime where the trapping effect and aging could be observed.

One of the motivations for this paper, mentioned at the beginning of the Introduction, was the hope that it might provide some insight into the dynamics of proteins, including their folding. However, it is fairly well understood by now that protein dynamics are influenced strongly by the existence of an energetically favored native state, a feature absent from the random heteropolymer model we have studied here. In work currently in progress, we are extending the analysis presented here to models in which the two-body interactions $B_{s,s'}$ are systematically biased, with a tunable strength, to favor particular ''native'' states. Such models provide an opportunity to study the competition between the attraction to a native state and the glassiness produced by the randomness and frustration. (References [37–40] treat equilibrium aspects of this competition.)

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