Localization and freezing of a Gaussian chain in a quenched random potential

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The Gaussian chain in a quenched random potential (which is characterized by the disorder strength $\Delta$) is investigated in the $d$-dimensional space by the replicated variational method. The general expression for the free energy within so called one - step - replica symmetry breaking (1-RSB) scenario has been systematically derived. We have shown that the replica symmetrical (RS) limit of this expression can describe the chain center of mass localization and collapse. The critical disorder when the chain becomes localized scales as $\Delta_c \approx b^d N^{-2+d/2}$ (where $b$ is the length of the Kuhn segment length and $N$ is the chain length) whereas the chain gyration radius $R_g \approx b (\Delta^2/\Delta) ^{1/(4-d)}$. The freezing of the internal degrees of freedom follows to the 1-RSB - scenario characterized by the beads localization length $D^2$. It was demonstrated that the solution for $D^2$ appears as a metastable state at $\Delta = \Delta_c$ and behaves similarly to the corresponding frozen states in heteropolymers or in $p$-spin random spherical model.

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I. INTRODUCTION

The behavior of polymer chains (with or without excluded volume) in a quenched random potential is a simple but nontrivial problem of statistical mechanics with disorder. Despite the vast investigations of both statistical [2, 3, 4, 5, 6, 7, 8, 9, 10, 11] and dynamical [12, 13, 14] properties many aspects remain to be elucidated. First of all we emphasize that one should discriminate between the annealed and quenched problems. In the case that the effective diffusion coefficient is large enough, so that the chain experiences different disorder realizations, the problem is equivalent to the annealed one (even though the random potential is quenched). In this case the presence of the effective diffusion coefficient is large enough, so that the chain experiences different disorder realizations, the problem is equivalent to the annealed one (even though the random potential is quenched).

Indeed, as the disorder strength $\Delta$ and the chain length $N$ increase, the diffusion coefficient $D$ falls down dramatically and the chain cannot sample the whole random medium over the course of internal degrees of freedom equilibration. It was shown [4, 5] that in the $d$-dimensional space the center of mass diffusion coefficient $D \approx D_R \exp[-(\Delta/b^d)N^\alpha]$, where $D_R$ is the Rouse diffusion coefficient, $b$ is the Kuhn segment length, $\alpha = 2 - \nu d$ and $\nu$ is the Flory exponent. As a result the time needed to obtain an “averaged” (annealed) statistics grows exponentially with $\Delta$ and $N$. In a recent publication [13] we have treated this problem dynamically by functional tools based on a Langevin dynamics approach. This approach avoids replicas naturally but by averaging over the quenched disorder inevitably couples different dynamic trajectories. This leads ultimately to the non - Markovian diffusional slowing down as well as to the corresponding freezing and non - ergodic regimes for the chain Rouse modes. We have derived the equation of motion for the Rouse mode time - dependent correlation function within a Hartree approximation and found that this equation has a memory kernel which is generic for the mode - coupling theory of the glass transition [16]. The self - consistent treatment of the mode - coupling equations leads to the conclusion that the chain center of mass diffusion coefficient decreases according to the law: $D \approx D_R[1 - \operatorname{const}(\Delta/b^d)N^\alpha]$. The individual Rouse modes of the chain also freeze at a common disorder strength, but their dynamic pathway is strongly selective to the mode number. We have recently launched the intensive Monte - Carlo (MC) simulation [17] to support these analytical calculations. Indeed we have found that the diffusion coefficient as a function of $(\Delta/b^d)N^\alpha$ drops much more dramatic than the exponential law, which is mainly based on the simple Markovian diffusion approximations. Preliminary MC - results [17] can be fitted much better by the form $D \sim [1 - \operatorname{const}(\Delta/b^d)N^\alpha]$. Thus suggests that a critical disorder, $\Delta_c \approx b^d N^{-\alpha}$,exists and that for strong disorder $\Delta > \Delta_c$ the chain center of mass is localized under the conditions of the simulation.

Such a dramatic reduction of the diffusion coefficient shows that because the dynamics of the chain becomes indeed extremely slow the equivalence of the quenched and annealed problems in the infinite volume limit [3, 5, 10, 11] has
to be questioned for strong disorder, i.e., $\Delta > \Delta_c$. As soon as $\Delta > \Delta_c$ the chain center of mass is practically localized and the chain may only sample intermediate disorder environment. We should implement in this case the quenched averaging, i.e. the chain free energy (or any observable physical quantity) must be calculated first for a particular configuration of disorder, only after this the average over the disorder can be taken. In any case, as proposed by the ref. [3, 6], the system volume indicated by the factor \ln \Omega represents then the actually explored volume. For completeness we mention that the MC - simulations [17] also reveal the Rouse modes freezing by showing a plateau in the time - dependent correlation function and has been predicted first in the ref. [12]. Motivated by our dynamic studies we come here back to the static replica approach and reformulate the theory in such a way, that we are able to treat the freezing of the chain on internal scales, which correspond to (Rouse) modes.

The idea is then to use the indication of the center of mass freezing and propose on these grounds a static theory for pinned chains in random medium. Clearly then, the theory has to be formulated in terms of the replica theory in such a way that the behavior internal degrees of freedom can be treated within the same framework. Obviously more than a formulation which is only sensitive to the overall size of the polymer must then be employed. A more refined theory needs then more variables than the overall size of the chain, since the behavior of individual segments of the chain needs to be studied in view of their freezing behavior. Nevertheless we can expect that within the static approach the freezing and nonergodic regimes show up through the replica symmetry breaking (RSB) scheme [18, 19].

We reformulate in this paper the replica freezing theory and discuss the different regimes for a Gaussian chain by making use the replica approach embedded in the variational formalism [10, 21, 22, 23]. Indeed we are going to show that the corresponding free energy can be explicitly calculated in the framework of so - called one-step replica symmetry breaking (1-RSB) scenario [18, 19]. Moreover it will be formulated more generally, that annealed and the replica symmetric theory can be treated as special cases in a more general framework. Within this scenario all replicas are grouped into clusters so that the resulting pattern has only two levels: the intra-cluster overlap has a finite value whereas the inter-cluster overlap is equal to zero. The first special case, when the cluster contains only one self-overlapping replica, corresponds to the replica symmetrical (RS) scenario and in principle leads back to results obtained in ref. [2].

We will show that for such situations a critical value for the disorder exists $\Delta_c \sim N^{-2+2/d}$, which corresponds to the Harris criterion (see [16] and references therein). For stronger disorder the chain is captured by the disorder potential and the chain gyration radius (resulting from the interplay between the entropical and energetical terms) is scaled as $R_g \sim (1/\Delta)^{1/(4-d)}$. This is basically a background for the dynamic localization of the center of mass of the chain and the chain collapse to its localization radius $R_g$.

In the general case of 1-RSB scenario the free energy is a functional of the mean - square beads (inter-replica) deviation within a frozen state $\overline{D^2}$. This corresponds to an order parameter which characterizes the freezing of the internal degrees of freedom inside the chain. We will show that the solution for $\overline{D^2}$ arises through the 1-st order phase transition (first as a metastable state) at some critical disorder $\Delta_A$ which is similar to critical temperature $T_A$ discussed in ref. [21, 22, 23]. It is of interest that for reasonably long chains $\Delta_c < \Delta_A$, so that the center of mass is localized first and then with increasing $\Delta$ internal degrees of freedom become frozen.

II. REPLICAS AND VARIATIONAL APPROACH

A. Model

We consider a Gaussian chain which is characterized by the $d$ - dimensional vector - function $\mathbf{R}(s)$, where $1 \leq s \leq N$ and labels beads of chain. The chain is embedded in a quenched random potential $V\{\mathbf{R}(s)\}$, so that the whole Hamiltonian take the form

$$
H = A \sum_{s=1}^{N} | \nabla_s \mathbf{R}(s) |^2 + \sum_{s=1}^{N} V\{\mathbf{R}(s)\} ,
$$

where $A = d/2b^2$ , $b$ is the Kuhn segment length, $N$ is the length of chain and the finite difference $\nabla_s \mathbf{R}(s) = \mathbf{R}(s+1) - \mathbf{R}(s)$. We will use below the units of measurement where $k_B T = 1$. The quenched random potential $V\{\mathbf{R}(s)\}$ is assumed to be Gaussian distributed with a short-ranged correlator

$$
\langle V(\mathbf{r}) V(\mathbf{r}') \rangle = \frac{\Delta}{(2\pi a^2)^{d/2}} \exp \left[ - \frac{(\mathbf{r} - \mathbf{r}')^2}{2a^2} \right] \rightarrow \Delta \delta^{(d)}(\mathbf{r} - \mathbf{r}') ,
$$

where the dispersion $\Delta$ is the main control parameter of the problem. The correlation length $a$ in eq. (2.2) plays the role of the spatial resolution or a minimal scale length. The second line in eq. (2.2) corresponds to the limit $a \rightarrow 0$. 
B. Replicated variational method

As pointed out in earlier for the quenched disorder problem the free energy must be averaged over the random field $V\{R(s)\}$, i.e. $[F]_{av} = -\ln[Z]_{av}$, where $[\cdots]_{av}$ stands for the average over the quenched field and $Z$ is the partition function.

In order to average $\ln Z$ over $V$ we use the replica trick. After introducing $n$ copies of the chain and averaging over $V$ with the correlator we obtain

$$[F]_{av} = -\lim_{n \to 0} \frac{\ln[Z^n]_{av}}{n} = \lim_{n \to 0} \frac{F_{eff}}{n},$$

(2.3)

where the replicated partition function reads

$$[Z^n]_{av} = \int \prod_{a=1}^{n} D R(s) \exp \left\{-A \sum_{a=1}^{n} \sum_{s=1}^{N} [\nabla_s R_a(s)]^2 + \frac{\Delta}{2} \sum_{a=1}^{n} \sum_{b=1}^{n} \sum_{s=1}^{N} \sum_{s'=1}^{N} \delta (R_a(s) - R_b(s')) \right\},$$

(2.4)

and $R_a(s)$ with $a = 1,2,\ldots n$ is the replicated vector function. The effective free energy

$$F_{eff} = -\ln[Z^n]_{av} = -\ln \int \prod_{a=1}^{n} D R_a(s) \exp \{-H_{eff}\}$$

(2.5)

with the effective Hamiltonian having the form

$$H_{eff} = A \sum_{a=1}^{n} \sum_{s=1}^{N} [\nabla_s R_a(s)]^2 - \frac{\Delta}{2} \sum_{a,b=1}^{n} \sum_{s,s'=1}^{N} \delta (R_a(s) - R_b(s')).$$

(2.6)

Because eq. (2.6) is not amenable for the exact calculation we use the replicated variational method. This method is based on the inequality

$$F_{var} = F_{tr} + \langle H_{eff} - H_{tr}\rangle \geq F_{eff}.$$

(2.7)

We take the trial Hamiltonian $H_{tr}$ in the following bilinear form

$$H_{tr} = A \sum_{a=1}^{n} \sum_{s=1}^{N} [\nabla_s R_a(s)]^2 + B \sum_{a=1}^{n} \sum_{s=1}^{N} R_a^2(s) + C \sum_{s=1}^{N} \sum_{a \neq b} q_{ab} [R_a(s) - R_b(s)]^2$$

(2.8)

with the trial free energy

$$F_{tr} = -\ln \int \prod_{a=1}^{n} D R_a(s) \exp \{-H_{tr}\}$$

(2.9)

It is worthwhile to note that because of the presence of the second term in eq. the “trial” Hamiltonian does not preserve the translational symmetry, $R_a(s) \to R_a(s) + C$, which is respected by the effective Hamiltonian. Nevertheless it does not damage our results because the chain ultimately is captured by the disorder potential at $\Delta > \Delta_c$ in some part of the space (see Sec. III A). Since this part of the space is not specified one should average over the chain locations or (which is equivalent) over the random field realizations (see e.g. Sec. 2.1 in ref. [20]). We might expect that the optimization of $F_{var}$ with respect to $B$ and $C$ leads to a good approximation for $F_{eff}$, i.e. the optimized $F_{var} \approx F_{eff}$. After that with the use of eq. we can estimate the free energy $[F]_{av} = \lim_{n \to 0} F_{var}/n$. In eq. $B$ is a variational parameter conjugated to the chain mean-square gyration radius $R_g^2$ which is responsible for the collapse transition. The second variational parameter, $C$, is conjugated to the mean - square inter-replica deviations $\Delta^2$ which characterizes the freezing transition. The form of the $q_{ab}$ - matrix is related with the pattern of 1-RSB scenario which we have assumed here. This pattern looks as follows: all $n$ replicas are divided into $n/m$ clusters each of which has the size $m$, so that $q_{ab}$ is 1 if $a$ and $b$ ($a \neq b$) belong to the same cluster and 0 otherwise. The averaging $<\cdots>$ in eq. means the expectation value with the trial Hamiltonian $H_{tr}$. 
C. Free energy calculation

The variational free energy $F_{\text{var}}$ can be represented in the form

$$F_{\text{var}} = F_0 + F_1,$$  \hspace{1cm} (2.10)

where the entropy term $F_0$ is

$$F_0 = F_{\text{tr}} - \langle H_{\text{tr}} \rangle + A \left\langle \sum_{a=1}^{n} \sum_{s=1}^{N} [\nabla_s R_a(s)]^2 \right\rangle$$  \hspace{1cm} (2.11)

and the interaction part $F_1$ reads

$$F_1 = -\frac{\Delta}{2} \sum_{a,b=1}^{n} \sum_{s,s'=1}^{N} \left\langle \delta (R_a(s) - R_b(s')) \right\rangle.$$  \hspace{1cm} (2.12)

Let us calculate first $F_{\text{tr}}$. For this purpose we must first diagonalize the quadratic form (2.8) with respect to the replica index. The coefficient matrix of the last part of the quadratic form (2.8) has the $m \times m$ - blocks over diagonal. It can be seen easily that this matrix has $(n/m)$ - modes with the eigenvalue 0 and $(n - n/m)$ modes with the eigenvalue $2m$ \[21\] \[22\] \[23\]. Then the eq. (2.10) take the form of Gaussian integral

$$F_{\text{tr}} = -\ln \int \prod_{a=1}^{n} D R_a(s) \exp \left\{-\frac{\Delta}{2} \sum_{a,b=1}^{n} \sum_{s,s'=1}^{N} \left[ A [\nabla_s R_a(s)]^2 + B R_a^2(s) + C \Lambda_a R_a^2(s) \right] \right\},$$  \hspace{1cm} (2.13)

where $\Lambda_a = 0$ for $1 \leq a \leq (n/m)$ and $\Lambda_a = 2m$ for $(n/m) + 1 \leq a \leq n$. By making use the results of calculation for the harmonic oscillator functional integral \[24\] we have

$$F_{\text{tr}} = -\frac{d}{2} \left( \frac{n}{m} \right) \ln \left[ \frac{\sinh(\lambda_+)}{\sinh(N\lambda_+)} \right] - \frac{d}{2} \left( n - \frac{n}{m} \right) \ln \left[ \frac{\sinh(\lambda_-)}{\sinh(N\lambda_-)} \right] + \frac{(N-1)dn}{2} \ln A,$$  \hspace{1cm} (2.14)

where $\lambda_+$ and $\lambda_-$ can be found from relations

$$\frac{1}{2} \sqrt{\frac{B}{A}} = \sinh \left( \frac{\lambda_+}{2} \right),$$

$$\frac{1}{2} \sqrt{\frac{B + 2mC}{A}} = \sinh \left( \frac{\lambda_-}{2} \right).$$  \hspace{1cm} (2.15)

Calculation of $\langle H_{\text{tr}} \rangle$ can be made by using the scaling arguments \[22\]. Because $R_a(s)$ are dummy variables $F_{\text{tr}}$ is not changed if we scale $R_a(s) \rightarrow \sqrt{2} R_a(s)$ and $\langle H_{\text{tr}} \rangle = \langle (\partial/\partial z) F_{\text{tr}} \rangle_{z=1}$. But according to eq. (2.15) $\lambda_+$ and $\lambda_-$ does not depend from the rescaling of coefficients $A, B$ and $C$. The only part of $F_{\text{tr}}(z)$ which depends from $z$ has the form $(N-1)dn \ln(zA)/2$. After that we have

$$\langle H_{\text{tr}} \rangle = n \frac{d}{2} (N - 1)$$  \hspace{1cm} (2.16)

For the calculation of

$$A \left\langle \sum_{a=1}^{n} \sum_{s=1}^{N} [\nabla_s R_a(s)]^2 \right\rangle = A \frac{\partial}{\partial A} F_{\text{tr}},$$  \hspace{1cm} (2.17)

we make use eq. (2.14). The results reads

$$A \left\langle \sum_{a=1}^{n} \sum_{s=1}^{N} [\nabla_s R_a(s)]^2 \right\rangle = \frac{n}{2} d (N - 1) - \left( \frac{n}{m} \right) \frac{d}{2} A \frac{\partial \lambda_+}{\partial A} (\coth[\lambda_+] - N \coth[N\lambda_+])$$

$$- \left( n - \frac{n}{m} \right) \frac{d}{2} A \frac{\partial \lambda_-}{\partial A} (\coth[\lambda_-] - N \coth[N\lambda_-]).$$  \hspace{1cm} (2.18)
For the very long chain, \( N \gg 1/\lambda \), \( \sinh(N \lambda_\pm) \approx (1/2) \exp(N \lambda_\pm), \coth(N \lambda_\pm) \approx 1 \) and eqs. \((2.14) - (2.18)\) can be substantially simplified. For example the trial free energy \((2.14)\) takes the form

\[ F_{tr} = \left( \frac{n}{m} \right) \frac{dN}{2} \lambda_+ + \left( n - \frac{n}{m} \right) \frac{dN}{2} \lambda_- . \]  

(2.19)

After straightforward calculation the entropy term \((2.11)\) becomes

\[ F_0 = \left( \frac{n}{m} \right) \frac{dN}{2} \left[ \lambda_+ - \frac{1}{\sqrt{1 + 4A/\delta}} \right] + n \left( 1 - \frac{n}{m} \right) \frac{dN}{2} \left[ \lambda_- - \frac{1}{\sqrt{1 + 4A/\delta^2}} \right] . \]  

(2.20)

The calculation of the interaction term \( F_1 \) (see eq. \((2.12)\)) is more complicated because it involves the replicated Green function of the bilinear form \((2.8)\). Employing the exponential representation of the \( \delta \)-function in \((2.12)\), we have

\[ F_1 = -\frac{\Delta}{2} \sum_{a,b=1}^{n} \sum_{s,s'=1}^{N} \int \frac{d^4k}{(2\pi)^d} \; Q_{ab}(s,s';k) . \]  

(2.21)

where the replicated correlator

\[ Q_{ab}(s,s';k) = \left\langle \exp \{ i k [ R_a(s) - R_b(s') ] \} \right\rangle \]

\[ = \exp \left\{ -\frac{k^2}{4A} \left[ G_{aa}(s,s) + G_{bb}(s',s') - 2G_{ab}(s,s') \right] \right\} . \]  

(2.22)

In eq. \((2.22)\) the Green function

\[ G_{ab}(s,s') = [H^{-1}]_{ab}(s,s') \]  

(2.23)

is the result of inversion of the coefficient matrix in the quadratic form

\[ H_{tr} = \sum_{c,d=1}^{n} \sum_{s,s'=1}^{N} R_c(s) H_{cd}(s,s') R_d(s') . \]  

(2.24)

The explicit calculation of \( Q_{ab} \) and \( F_1 \) is given in the Appendix A. It turns out, that the \( Q_{ab} \) take different forms in the respective elements of the matrix. The diagonal elements \( Q_{aa} \) read

\[ Q_{aa}(s,s';k) = \exp \left\{ -\frac{k^2}{4A} \left[ \overline{g}(s,s) + \overline{g}(s',s') - 2\overline{g}(s,s') \right] \right\} \]

\[ = \exp \left\{ -\frac{k^2}{4Am \sinh(\lambda_+)} \left[ 1 - e^{-\lambda_+ |s-s'|} \right] - \frac{k^2(m-1)}{4Am \sinh(\lambda_-)} \left[ 1 - e^{-\lambda_- |s-s'|} \right] \right\} . \]  

(2.25)

The off - diagonal elements of \( Q_{ab} \) inside the blocks are calculated to be

\[ Q_{ab}^<(s,s';k) = \exp \left\{ -\frac{k^2}{4A} \left[ \overline{g}(s,s) + \overline{g}(s',s') - 2g(s,s') \right] \right\} \]

\[ = \exp \left\{ -\frac{k^2}{4Am \sinh(\lambda_+)} \left[ 1 - e^{-\lambda_+ |s-s'|} \right] - \frac{k^2}{4Am \sinh(\lambda_-)} \left[ m - 1 + e^{-\lambda_- |s-s'|} \right] \right\} . \]  

(2.26)

Finally the off - diagonal elements of \( Q_{ab} \) outside the blocks can be written as

\[ Q_{ab}^>(s,s';k) = \exp \left\{ -\frac{k^2}{4A} \left[ \overline{g}(s,s) + \overline{g}(s',s') \right] \right\} \]

\[ = \exp \left\{ -\frac{k^2}{4A} \left[ \frac{1}{m \sinh(\lambda_+)} + \frac{m-1}{m \sinh(\lambda_-)} \right] \right\} . \]  

(2.27)

In eqs. \((2.25) - (2.27)\) \( \overline{g} \) and \( g \) stand respectively for the diagonal and off - diagonal elements of the Green - function. In addition we have to see how many elements \( Q_{ab} \) of each type exist for the present problem. It is easily seen that
the number of diagonal elements is \(n\). The number of elements \(Q_{ab}^\prec\) is \(n(m-1)\) and similarly the number of elements \(Q_{ab}^\succ\) is \(n(n-m)\).

The final form of \(F_1\) is given by

\[
F_1(n, m) = \frac{\Delta}{2\pi^{d/2}b^d} \sum_{s, s' = 1}^{N} \left\{ n \left[ 1 - e^{-\lambda_+|s-s'|} \right] \frac{m - 1}{m} \frac{1 - e^{-\lambda_-|s-s'|}}{\sinh(\lambda_-)} \right\}^{-d/2} + n(m-1) \left[ \frac{1}{m} \frac{1 - e^{-\lambda_+|s-s'|}}{\sinh(\lambda_+)} + \frac{m - 1 + e^{-\lambda_-|s-s'|}}{\sinh(\lambda_-)} \right]^{-d/2} + n(n-m) \left[ \frac{1}{m} \frac{1 - e^{-\lambda_+|s-s'|}}{\sinh(\lambda_+)} + \frac{m - 1}{m} \frac{1}{\sinh(\lambda_-)} \right]^{-d/2}
\]

and the complete variational free energy is then given by the sum of all the individual contributions.

D. Order parameters

As have been mentioned in the Introduction there are at least two types of phenomena which we face while the disorder strength \(\Delta\) is growing. At some critical \(\Delta_c\) the chain is captured by the disorder potential, so that the chain center of mass becomes localized and the mean squared gyration radius \(R_{g}^2\) is defined only by disorder. In this case \(R_{g}^2\) play the role of the order parameter and can be expressed in terms of variational parameters \(B, C\) as follow

\[
R_{g}^2 = \frac{1}{nN} \left\langle \sum_{c=1}^{n} \sum_{s, s' = 1}^{N} R_{c}^2(s) \right\rangle = \frac{1}{nN} \frac{\partial}{\partial B} F_{\text{tr}}
\]

\[
= \frac{d}{2} \left\{ \frac{1}{m} \frac{1}{B \sqrt{1 + 4A}} + \frac{m - 1}{m} \frac{1}{(B + 2mC) \sqrt{1 + 4A \frac{B}{B + 2mC}}} \right\} ,
\]

where we have used eqs.(2.15) and (2.19). In the Sec.III we will show that this quenched problem can be treated within RS - scenario, i.e. at \(m = 1\).

On the other hand within 1-RSB scenario the (meta)stable solution for the variational parameter \(C\) appears at some critical \(\Delta_A\). Parameter \(C\) is conjugated to the mean square beads deviation within a frozen state \(\overline{D^2}\) which can be written as

\[
\overline{D^2} = \frac{1}{n(m-1)N} \sum_{a,b=1}^{N} \left\langle (R_a(s) - R_b(s))^2 \right\rangle = \frac{1}{n(m-1)N} \frac{\partial}{\partial C} F_{\text{tr}}
\]

\[
= \frac{d}{(B + 2mC) \sqrt{1 + 4A \frac{B}{B + 2mC}}} .
\]

The order parameter \(\overline{D^2}\) is an inter-replica value which characterizes the mean squared beads localization length and freezing. On the other hand, \(\overline{D^2}\) can be also interpreted as the long - time limit correlation, i.e. \(\overline{D^2} = \lim_{t \to \infty} N^{-1} \sum_{s=1}^{N} \left\langle (R(s, t) - R(s, 0))^2 \right\rangle\). We will consider this in Sec. IV.

III. CENTER OF MASS LOCALIZATION AND COLLAPSE

A. RS - scenario

We will now investigate the quenched problem when the chain is captured by the disorder potential and collapse, so that the chain size is determined only by the disorder strength \(\Delta\). The schematic pictorial representation of this situation is given in Fig.1.
FIG. 1: a) At the critical disorder $\Delta_c$ chain is captured by the random potential in some part of the space, i.e. becomes localized. b) The characteristic scales of the problem: $a$ is the correlation length of the random potential (or the spatial resolution), $b$ is the Kuhn segment length, $R_g$ is the chain gyration radius. Scales satisfy the following relations: $a \ll b \ll R_g$

For the purpose of calculations let us take the RS - limit (i.e. $n \to 0$ and $m = 1$) in the interaction (2.28) and entropy (2.20) terms. Using eq. (2.28) and switching from the summation to the integration over the contour variable $s$ leads us (after using eq. (2.3)) to the following RS - interaction free energy part

$$F^{(1)}_{RS} = -\frac{\Delta}{2\pi d/2} N \int_0^\infty ds \left\{ \frac{1}{R^2(s)^{d/2}} - \frac{1}{R^2(\infty)^{d/2}} \right\},$$  \hspace{1cm} (3.1)

where the mean - square distance

$$\overline{R^2(s)} = \frac{b^2}{\sinh(\lambda_+)} (1 - e^{-\lambda_+ s}) \hspace{1cm} (3.2)$$

Note that this form of the polymer radius corresponds to a simple solution of a Gaussian chain in a harmonic potential. The chain statistics is still Gaussian on the interval $0 < s < 1/\lambda_+$ while the collapsed configurations can be revealed on the larger contour length $1/\lambda_+ < s < N$. As a result (and because of $N\lambda_+ \gg 1$) the chain size is completely independent of its total contour length $N$. Note that the eigenvalue $\lambda_+$ in the limit $B \ll A$ (see below) is small and reads

$$\lambda_+ \approx \sqrt{\frac{B}{A}} \ll 1 \hspace{1cm} (3.3)$$

The free energy (3.1) is typical for the variational method and corresponds to the one - loop approximation. For the problem under discussion it was obtained first in [2]. Unfortunately the integral in eq. (3.1) has the divergence at small $s$ and must be regularized. The reason for this divergence lies in the contradiction between the Gaussian statistics on the interval $0 < s < 1/\lambda_+$ and the effective segment - segment attraction which shows up on all scales within the variational method (see eq. (3.1)). The integral regularization can be obtained by the reasonable coarse - graining. Namely, we should apply our variational method to the string of statistically independent segments of length $l \approx 1/\lambda_+$ (see Appendix B for more details). On this coarse - grained level of description the variational method with only one parameter $B$ (as opposed to the case when $B(s)$ is a trial $s$ - dependent function [25]) is getting self - consistent and the integral in eq. (3.1) can be regularized. It should be mentioned another approach [10] regarding similar point.
RS - entropy contribution, $F^{(0)}_{RS}$, resulting from eq. (2.20) in the limit $m = 1, n \to 0$ and taking into account eqs. (2.15) and (3.3). The final expression for the full RS - free energy $F_{RS}$ can be put in a following form

$$F_{RS} = F^{(0)}_{RS} + F^{(1)}_{RS},$$

where we have used also eqs. (B3) - (B4) for $F^{(1)}_{RS}$ and $I_d$ respectively. For the mean - square gyration radius from (2.29) we get

$$R_g^2 \approx \frac{1}{\sqrt{AB}}.$$  

Minimization of the free energy (3.4) with respect to $B$ leads to the solution

$$B^* \simeq A \left( \frac{\Delta}{b^d} \right)^{\frac{1}{4-d}}.$$  

The resulting $R_g^2$ becomes

$$R_g^2 \approx b^2 \left( \frac{b^d}{\Delta} \right)^{\frac{2}{4-d}}$$  

at $d < 4$. This result has been obtained first in ref. [2]. We can meet the condition $B \ll A$ (see eq. (3.3)) if $\Delta \ll b^d$, i.e. $R_g^2 \gg b^2$ (see Fig. 1b). The free energy at the minimum $B = B^*$ reads

$$F_{RS}\{B^*\} \sim -N \left( \frac{\Delta}{b^d} \right)^{\frac{2}{4-d}} < 0,$$

which corresponds indeed to the form the the free energy confinement $F_{conf} \propto N b^2 / R_g^2$ for localized chains. As a result we conclude that that the chain is captured by the disorder potential at some critical disorder provided that $N \left( \Delta_c / b^d \right)^{2/(4-d)} \approx 1$, i.e.

$$\Delta_c \simeq b^d N^{-2+\frac{d}{4}}.$$  

This criterion has been recently obtained by us within the dynamical consideration in ref. [15] in various representations. It corresponds to the usual Harris criterion for chains in disorder. The quenched RS - free energy (3.4) and the chain confinement is shown in Fig. 2.

The RS - scenario reveals two facets of the problem: the chain center of mass localization (or confinement) which is described by the criterion (3.9) and the collapse with the characteristic chain size given by eq. (3.7). Here it should be recorded that as distinct from the results of ref. [3, 6, 10] the expression for the chain size does not contain the factor $\ln \Omega$ (where $\Omega$ is the volume of the whole random medium) since the chain is effectively pinned for $\Delta > \Delta_c$.

B. Annealed problem

In this case, as we have discussed in the Introduction, the chain is fairly mobile and can span the whole system during the time of an experiment. The chain experiences all possible quenched field realizations and the replica trick is actually not necessary. The corresponding interaction part of free energy results from eq. (2.28) at $n = m = 1$. The entropy term follows from eq. (2.20) at $n = m = 1$ as well. The resulting annealed free energy reads

$$F_{ann} = \frac{dN}{2} \sqrt{\frac{B}{A}} - \frac{\Delta}{2\pi^{d/2}b^d} \sinh(\lambda_+) \left[ \sum_{s,s'} \frac{1}{[1 - e^{-\lambda_+|s-s'|}]} \right]^{d/2}. $$

By making use eqs. (3.2) and (3.3) we can substitute the result of double summation by $N^2 / R_N^d$ whereas the entropy term leads to the form $b^2 N / R_N^2$. As a result we have

$$F_{ann} \simeq \frac{b^2 N}{R_N^2} - \frac{\Delta N^2}{R_N^2}. $$
FIG. 2: RS - free energy as a function of the variational parameter $B$ and different disorder strength $\Delta/b^3$. The confinement is guaranteed by the condition that the minimum depth is large enough, i.e. $N(\Delta/b^3)^{2/(4-d)} > 1$. The upper curve demonstrates the entropy term.

This expression was obtained first in ref. [2, 3]. The minimization of eq. (3.11) leads to the following result. At $d \geq 2$ $F_{\text{ann}} \to -\infty$ and $R_N \to 0$, or by cutting - off we can state that the chain is collapsed to a size of the order of the Kuhn length $b$. At $d < 2$ the free energy has a minimum at $R_N \simeq b (\Delta N/b^d)^{1/(d-2)} \to b$ in the long chain limit if the cut - off is imposed again. The chain crushing down is of course a result of a Gaussian model. It is well known [15] that the more realistic chain with the second $v > 0$ and the third $w$ virial coefficients chain is collapsed at $\Delta > v$ to the globule state with a finite density.

IV. FREEZING OF INTERNAL DEGREES OF FREEDOM

As shown in Sec.III the Gaussian chain is getting immobile or localized at some critical value of disorder $\Delta_c$. This can be treated by making use the RS - scenario. As a relevant question, we can ask what happened with internal motions of the chain beads as the disorder $\Delta$ increases further? It is clear that the chain still experiences the free energy landscape and can stay in the different minima or the conformational states. The measure of the distance between these states is given by the order parameter $D^2$ which discussed in Sec. II D. The parameter $D^2$ is used extensively for the heteropolymers, where the landscape dominated statistics can be clearly seen [26]. There is a natural mapping in the replica approach [18, 19] between sets of states and replicas. The 1- RSB - assumption about the clustering in the replica space reflects our view of the states subdivision. The general pattern looks as follows. We put together in the same cluster all states that are within a certain distance $D^2$ from each other. The distance between different clusters is infinitely large. From the expression for the entropy (2.20) it can be seen that the fraction of states with a distance $D^2$ between them is equal to $1 - 1/m$. Fig.3 illustrates schematically a cluster which is made up of three states: $a$, $b$ and $c$. In this section we will show that within 1 - RSB - scenario upon disorder growing the parameter $D^2$ can take fairly small value. This means that beads are localized in the globule interior, i.e. the system is freezeed. Indeed, deep in the frozen regime the change of the chain conformation can only take place on the smallest length scales, i.e. $D^2 \approx a^2$. 


FIG. 3: States subdivision in the space of conformations. States of the chain within 1-RSB - scenario (marked as a, b, c) form a cluster, so that the distance between them is equal $\overline{D^2}$. To find the distance one traces back the points a, b, c along the branches until they merge. The chain can move between these states.

A. RSB - free energy

The frozen phase is characterized by small fluctuations around individual minima. In this case we assume that Debye - Waller factor, $2mC$, is large, i.e.

$$2mC \gg A \gg B$$

(4.1)

and the order parameter given by eq. (2.30) takes a simple form

$$\overline{D^2} \simeq \frac{d}{2mC}.$$  

(4.2)

In the opposite limit of small $2mC$, i.e. at

$$2mC \ll B \ll A$$

(4.3)

$\lambda_- \simeq \lambda_+$ and it can be seen that the free energy functional $F_1(n, m)$ in eq. (2.28) and the entropy (2.20) goes back to RS - free energy as it should be.

In the limit (4.3) the order parameter $\overline{D^2}$ reads

$$\overline{D^2} \simeq \frac{d}{B \sqrt{1 + \frac{4A}{B}}} \simeq \overline{R_g^2}.$$  

(4.4)

This is a natural result because in the case when the center of mass is localized but the internal degree of freedom are still not frozen (because of small $C$) the beads localization length is of the order of the gyration radius.

Let us calculate the RSB - free energy $F_{RSB}$. For the sake of simplicity we should find first of all the expressions for the entropy $F_{RSB}^{(0)}$ (see eq. (2.24)) and interaction $F_{RSB}^{(1)}$ (see eq. (2.25)) terms in the both limits, (4.1) and (4.3). After that we can find a reasonable interpolating expression, which is suitable for the theoretical investigation. These calculations are represented in Appendix C. The overall RSB - free energy which consists of the entropy (4.4) and the
interaction (RS) terms is given by

\[ F_{\text{RSB}}/N = \frac{(F_{\text{RSB}}^{(0)} + F_{\text{RSB}}^{(1)})}{N} = \frac{m-1}{m} \frac{d}{2} \ln (y+1) - \frac{d}{2\pi^{3/2}b^d} \frac{\lambda_+^{d-1}(m^{d+1}-1) \lambda_+^{d+1}}{y + \frac{m(m^{d+1}-1)2\lambda_+^d}{m-1} \lambda_+^{d+1}}, \]  

(4.5)

where the dimensionless Debye - Waller factor \( y \equiv 2mCb^2 \).

### B. Freezing transition

Now we discuss the transition related with the freezing of the internal degree of freedom and based on the RSB - free energy expression eq.(4.5). Minimization of eq.(4.5) with respect of \( y \) yields the solution

\[ y^* \simeq \left( \frac{\Delta}{b^d} \right)^{\frac{6}{m^2(m^{d+1}-1)^2}} \left( \frac{m-1}{2} \right)^{\frac{1}{m-1}^2} \]  

(4.6)

where we have used for \( \lambda_+ \) the results of RS - solution (3.10), i.e. \( \lambda_+ \sim (B^*/A)^{1/2} \sim (\Delta/b^d)^{2/(4-d)} \). When minimizing eq. (4.5) we also took into account that \( y^* \) is close to \( y_{\text{max}} \), i.e. \( y^* \approx y_{\text{max}} \), where \( y_{\text{max}} \) is given by

\[ y_{\text{max}} = 2mC_{\text{max}}b^2 \simeq \frac{b^2}{a^2} > 1. \]  

(4.7)

The stationary condition with respect to \( m \), i.e. \( \partial F_{\text{RSB}}/\partial m \) for \( y = y_{\text{max}} \) = 0, leads to the optimal result for \( m = m^* \) defined by

\[ m^* \simeq \frac{[\ln y_{\text{max}} + \frac{2\pi}{\Delta}]^{\frac{1}{2}}}{\left( \frac{\Delta}{b^d} \right)^{\frac{1}{2}}} \geq 1. \]  

(4.8)

Solution \( y = y^* \) appears first as a metastable one at some \( \Delta = \Delta_A \), which is similar to the critical temperature \( T_A \) in heteropolymers discussed in ref. 22 23. This transition in a metastable state is also of the same nature as in the \( p \) - spin glass model studied in ref. 27.

In Fig.3 we have plotted the RSB - free energy expression eq.(4.5) as a function of Debye - Waller factor \( y \) at the different disorder strength; in doing so we have used for \( m \) the optimal value given by eq.(4.8). The metastable solution shows up at \( \Delta_A = 0.753 \), so that \( y^* \) grows with the disorder until it hits the \( y_{\text{max}} \), i.e. \( y^* \approx y_{\text{max}} = b^2/a^2 \). In our case it is happened at \( \Delta_G/b^d \approx 0.796 \) with \( y_{\text{max}} = 66.3 \). At this point all beads are totally localized or frozen.

It is interesting to make a link with the heteropolymer theory 22 23. At \( m^* \rightarrow 1 \) the RSB - free energy \( F_{\text{RSB}} = 0 \) and eq.(4.8) immediately leads to the corresponding expression for \( \Delta = \Delta_K \) which meets this condition, i.e.

\[ \frac{\Delta_K}{b^d} \approx \left[ \ln y_{\text{max}} + \frac{2\pi}{\Delta} \right]^{\frac{1}{2}}. \]  

(4.9)

This expression quantitatively corresponds to the Kauzmann temperature \( T_K \) in heteropolymers 22. In ref. 22 it was found that \( \sigma/k_B T_K \) (where \( \sigma \) is the variance of the random interaction) is proportional to the square root of the entropy loss, which is similar to eq.(4.9). The dependence of \( y^* \) from \( \Delta \) at the different \( y_{\text{max}} = b^2/a^2 \) is shown in Fig.4. The angular points, where \( y^* \) hits \( y_{\text{max}} \), correspond to \( \Delta = \Delta_G \) where the chain becomes fully frozen.

In the disorder interval \( \Delta_A < \Delta < \Delta_G \) the chain is in a metastable state and the beads localization length lies in the range \( a^2 \leq \Delta^2 \leq \Delta^2 \). The beads become localized when the effective barrier height between the minimum \( F^* \) and maximum \( F^{**} \) in Fig.3 is large enough to assure the beads confinement. Fig. 5 shows the result of the numerical estimation of the effective barrier height \( F^*/N \equiv (F^{**} - F^*)/N \). The result of the fitting can be written as

\[ F^*/N = 2.03 (\Delta - \Delta_A)^{1.49}. \]  

(4.10)

The beads confinement condition, \( F^* > 1 \), leads to the following finite chain scaling for the transition disorder

\[ \Delta_A(N) = \Delta_A + \frac{5b^2}{N^{0.66}} \]  

(4.11)

The eq. (4.11) means that for the reasonably long chain the internal freezing does not depend from the chain length. The comparison with the scaling low eq.(4.9) for the center of mass localization critical disorder \( \Delta_c \) leads us to the conclusion that \( \Delta_c < \Delta_A \). By this is meant that as the disorder increases the chain center of mass is localized first at \( \Delta = \Delta_c \) and then at \( \Delta = \Delta_A \) the internal degree of freedom start to freeze. Furthermore at \( \Delta = \Delta_G > \Delta_A \) the whole system is freezed out with the beads localization length \( \Delta^2 \approx a^2 \).
FIG. 4: RSB - free energy at the different disorder $\Delta/b^3$ and fixed $y_{\text{max}} = 66.3$. The arrow shows the minimum position $y^*$ when it hits $y_{\text{max}}$, i.e. $y^* = y_{\text{max}}$.

The corresponding disorder strength $\Delta = \Delta_G = 0.796 b^3$

V. CONCLUSION

We have studied the behavior of the Gaussian chain in a quenched random short correlated field which is specified by the field dispersion $\Delta$. The consideration is based on the variational method in replica space which was previously used for the heteropolymer problem [21, 22, 23] within the simplest 1-RSB - scenario. This assumption allows to calculate the general free energy functional in an explicit form and consider its RS and RSB cases.

We have shown that the RS - limit ($n \to 0$ and $m = 1$) allows to treat the center of mass localization at some critical $\Delta_c$ (see eq.(3.9)) as well as the chain collapse (see eq.(3.7)). In line with eq.(3.9) it was found by the methods based on the analytical Langevin dynamics calculations [15] that the localization threshold for the center of mass of the self - avoiding chain is scaled as $\Delta_c \simeq b^d N^{-\nu_d}$, where $\nu$ is the Flory exponent. More precisely, for the problem in question there are two characteristic time scales. One of them is the time of the chain capture $t_{\text{cap}}$ by the disorder potential. Within our dynamical calculation based on the Hartree approximation [15] (which in turn is reminiscent of the mode - coupling approximation [16]) $t_{\text{cap}} \to \infty$. The other time scale is the equilibration time of the internal degrees of freedom $t_{\text{eq}}$. It should be realized that our results are valid for $t_{\text{cap}} \gg t_{\text{eq}}$.

The main conclusions of ref.[15] have been recently corroborated by the direct MC - simulations [17] which among other things shows a pronounced decrease of the center of mass diffusion coefficient in the vicinity of $\Delta_c$. The resulting eq.(3.7) corresponds to the size of this trapped chain. Nevertheless the size itself is not sufficient to describe the physical situation. Here we added the discussion of the internal degrees of freedom by dividing the replicated system into $n/m$ blocks.

Then the 1-RSB - limit (i.e. at $n \to 0$ and $m = m^*$, where $m^*$ is an optimized value of the breaking point parameter $m$) of the free energy expression reveals the nontrivial solution for the inter-replica value $D^2$, the beads localization length. This solution appears discontinuously at the critical disorder $\Delta = \Delta_A$ which corresponds to the freezing of the chain internal degree of freedom. Beads localization length $D^2$ falls to $D^2 \simeq a^2$ with the disorder increasing in the interval $\Delta_A < \Delta < \Delta_G$. These results are in a qualitative agreement with the freezing scenario in heteropolymers [22, 23]. On the other hand, according the findings based on the dynamical approach [17] the nonergodicity function shows up (at least for the long Rouse modes) continuously. Moreover the critical threshold for internal Rouse modes freezing is scaled as $\Delta_c \simeq b^d N^{-0.25}$ which at first sight can not be reconciled with eq.(4.11). At the moment it is not clear what is the reason for this discrepancy. Presumably by going beyond the scope of 1 - RSB - scenario to the full scale RSB - hierarchy we could fill the gap between dynamical and replica methods.
FIG. 5: Dependence of the minimum position $y^*$ from the $\Delta/b^3$ at the different $y_{\text{max}}$. The angular point corresponds to the disorder, $\Delta_G$, when the localization length $D^2 \approx a^2$, i.e. the chain becomes fully frozen.

FIG. 6: The barrier height $F^1$ as a function of the disorder. The scaling form fitting corresponds to the eq. (4.10).

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APPENDIX A: REPLICAED GREEN FUNCTION FOR THE GAUSSIAN TRIAL CHAIN

Diagonalization of the quadratic form \(2.8\) in the replica space leads to eq.\((2.13)\). The corresponding Green function has two components, \(G^\pm(s, s')\), which associated with two types of eigenvalues. The Green function satisfies the equation of motion

\[
\left[ -\nabla_s \nabla_s + (\omega^\pm)^2 \right] G^\pm(s, s') = \delta_{ss'} ,
\]  

subjected to free ends boundary conditions

\[
\nabla_s G^\pm(s, s') \big|_{s=0} = \nabla_{s'} G^\pm(s, s') \big|_{s=N} = 0 .
\]

In eqs. \((A1) - (A2)\) the finite differences are defined as follows: \(\nabla_s G^\pm(s, s') \equiv G^\pm(s + 1, s') - G^\pm(s, s')\); the “characteristic frequencies” \(\omega^+ = \sqrt{B/A}\) and \(\omega^- = \sqrt{(B + 2C)/A}\). The exact solution of eq. \((A1)\) becomes the form \(21, 22\)

\[
G^\pm(s, s') = \begin{cases} 
\cosh[\lambda_+ (s - s')] \cosh[\lambda_+ (N - s' + \frac{1}{2})] \sinh[\lambda_1 \lambda_2] \sinh[\lambda_1 N], & \text{if } s \leq s' \\
\cosh[\lambda_+ (s - s')] \cosh[\lambda_+ (N - s' + \frac{1}{2})] \sinh[\lambda_1 \lambda_2] \sinh[\lambda_1 N], & \text{if } s \geq s'
\end{cases}
\]

(A3) where \(\lambda_+\) and \(\lambda_-\) are defined by eq.\((2.15)\).

For the large chain, \(N \gg 1/\lambda_\pm\), eq.\((A3)\) can be written in a much simpler form

\[
G^\pm(s, s') \approx \frac{1}{2 \sinh(\lambda_\pm)} \exp \left\{ -\lambda_\pm |s - s'| \right\} .
\]

(A4)

In order to calculate the Green function matrix elements \(G_{ab}(s, s')\) we recall that the \(n \times n\) - matrix has the block - diagonal structure with each block of size \(m\). Let us denote all diagonal elements \(G_{aa} = \overline{g}\), off - diagonal elements which belong to blocks \(G_{ab} = g\) and all elements outside of blocks are equal to zero. For the purpose of diagonalizing the matrix \(G_{ab}\) we diagonalize first each \(m \times m\) - block. The corresponding characteristic equation for the eigenvalues \(\chi\) is

\[
\begin{vmatrix}
\overline{g} - \chi & g & \cdots & g \\
g & \overline{g} - \chi & \cdots & g \\
\vdots & \vdots & \ddots & \vdots \\
g & g & \cdots & \overline{g} - \chi
\end{vmatrix} = 0
\]

(A5)

It is easy to find that the eq.\((A5)\) has one solution

\[
\chi_+ = \overline{g} - (1 - m)g
\]

(A6) and \((m - 1)\) - solutions

\[
\chi_- = \overline{g} - g
\]

(A7)

The determinant of \(G_{ab}\) is an invariant of orthogonal transformations and can be represented in the form

\[
\det \{ G_{ab} \} = (\chi_+) (\frac{1}{m}) (\chi_-) (n-\overline{g})
\]

\[
= (G^+) (\frac{1}{m}) (G^-) (n-\overline{g}) ,
\]

(A8)

which leads to the identity \(\chi_+ = G^+\) and \(\chi_- = G^-\) and allows to wright down

\[
G^+ = \overline{g} - (1 - m)g
\]

\[
G^- = \overline{g} - g
\]

(A9)

As a result the expressions for non - zero matrix - elements read

\[
g = \frac{1}{m} [G^+ - G^-]
\]

\[
\overline{g} = \frac{1}{m} G^+ + \left(1 - \frac{1}{m}\right) G^- .
\]

(A10)
Now we are in a position to calculate correlators $Q_{ab}(s, s'; k)$ in eq. (2.22). The diagonal element $Q_{aa}$ is
\[
Q_{aa}(s, s'; k) = \exp \left\{ -\frac{k^2}{4A} \left[ \overline{g}(s, s) + \overline{g}(s', s') - 2\overline{g}(s, s') \right] \right\}
\]
\[
= \exp \left\{ -\frac{k^2}{4Am \sinh(\lambda_+)} \left[ 1 - e^{-\lambda_+|s-s'|} \right] - \frac{k^2(m-1)}{4Am \sinh(\lambda_-)} \left[ 1 - e^{-\lambda_-|s-s'|} \right] \right\}, \tag{A11}
\]
where we have used eqs. (A10) and (A4). The off-diagonal elements of $Q_{ab}$ inside the blocks are
\[
Q_{ab}^<(s, s'; k) = \exp \left\{ -\frac{k^2}{4A} \left[ \overline{g}(s, s) + \overline{g}(s', s') - 2\overline{g}(s, s') \right] \right\}
\]
\[
= \exp \left\{ -\frac{k^2}{4Am \sinh(\lambda_+)} \left[ 1 - e^{-\lambda_+|s-s'|} \right] - \frac{k^2}{4Am \sinh(\lambda_-)} \left[ m - 1 + e^{-\lambda_-|s-s'|} \right] \right\}. \tag{A12}
\]
Finally the off-diagonal elements of $Q_{ab}$ outside the blocks can be written as
\[
Q_{ab}^>(s, s'; k) = \exp \left\{ -\frac{k^2}{4A} \left[ \overline{g}(s, s) + \overline{g}(s', s') \right] \right\}
\]
\[
= \exp \left\{ -\frac{k^2}{4A} \left[ \frac{1}{m \sinh(\lambda_+)} + \frac{m-1}{m \sinh(\lambda_-)} \right] \right\}. \tag{A13}
\]
How many elements $Q_{ab}$ of each type exist? It is easily seen that the number of diagonal elements is $n$, the number of elements $Q_{ab}^<$ is $n(m-1)$ and finally the number of elements $Q_{ab}^>$ is $n(n-m)$. After that the interaction part of free energy (see eq. (2.21)) can be represented in the general form
\[
F_1(n, m) = -\frac{\Delta}{2} \sum_{s, s'=1}^{N} \int \frac{d^d k}{(2\pi)^d} \left\{ n \exp \left\{ -\frac{k^2}{4Am \sinh(\lambda_+)} \left[ 1 - e^{-\lambda_+|s-s'|} \right] - \frac{k^2(m-1)}{4Am \sinh(\lambda_-)} \left[ 1 - e^{-\lambda_-|s-s'|} \right] \right\}ight.
\]
\[+ n(m-1) \exp \left\{ -\frac{k^2}{4Am \sinh(\lambda_+)} \left[ 1 - e^{-\lambda_+|s-s'|} \right] - \frac{k^2}{4Am \sinh(\lambda_-)} \left[ m - 1 + e^{-\lambda_-|s-s'|} \right] \right\}
\[+ n(n-m) \exp \left\{ -\frac{k^2}{4A} \left[ \frac{1}{m \sinh(\lambda_+)} + \frac{m-1}{m \sinh(\lambda_-)} \right] \right\} \right\}
\]
\[= \frac{\Delta}{2\pi^{d/2}} \sum_{s, s'=1}^{N} \left\{ n \left[ \frac{1 - e^{-\lambda_+|s-s'|}}{m \sinh(\lambda_+)} + \frac{m-1}{m} \frac{1 - e^{-\lambda_-|s-s'|}}{\sinh(\lambda_-)} \right]^{-d/2} \right.
\[+ n(m-1) \left[ \frac{1 - e^{-\lambda_+|s-s'|}}{m \sinh(\lambda_+)} + \frac{m-1}{m} \frac{1 - e^{-\lambda_-|s-s'|}}{\sinh(\lambda_-)} \right]^{-d/2}
\[+ n(n-m) \left[ \frac{1}{m \sinh(\lambda_+)} + \frac{m-1}{m} \frac{1}{\sinh(\lambda_-)} \right]^{-d/2} \left\} \tag{A14}
\]
\[= \frac{\Delta}{2\pi^{d/2}} \sum_{s, s'=1}^{N} \left\{ n \left[ \frac{1 - e^{-\lambda_+|s-s'|}}{m \sinh(\lambda_+)} + \frac{m-1}{m} \frac{1 - e^{-\lambda_-|s-s'|}}{\sinh(\lambda_-)} \right]^{-d/2} \right.
\[+ n(m-1) \left[ \frac{1 - e^{-\lambda_+|s-s'|}}{m \sinh(\lambda_+)} + \frac{m-1}{m} \frac{1 - e^{-\lambda_-|s-s'|}}{\sinh(\lambda_-)} \right]^{-d/2}
\[+ n(n-m) \left[ \frac{1}{m \sinh(\lambda_+)} + \frac{m-1}{m} \frac{1}{\sinh(\lambda_-)} \right]^{-d/2} \right\} \tag{A15}
\]
\[
\text{APPENDIX B: REGULARIZATION BY THE COARSE-GRANING}
\]
First of all it is pertinent to note that the chain statistics is Gaussian on the interval $0 < s < 1/\lambda_+$ (see eq. (3.2)) whereas the collapse shows up on the larger contour variable, $1/\lambda_+ < s < N$. The whole collapsed chain can be seen as made up of the statistically independent segments of length $l \approx 1/\lambda_+$. The number of such segments $n_l = N/l = N\lambda_+ \gg 1$. The statistical independence and the equipartition of energy imply that the free energy is proportional to $k_BT n_l$, i.e.
\[
F \approx k_BT n_l = k_BT N \sqrt{\frac{B}{A}} = k_BT N \left( \frac{\Delta}{B^2} \right)^{1/2}. \tag{B1}
\]
and we go back to eq. (3.8). Now we can consider the chain as a string of totally collapsed statistically independent segments of length $l \approx 1/\lambda_+$. This coarse-grained picture provides a basis for the regularization of the integral in eq. (3.1).

The reason for the divergency of this integral at small $s$ is the following. There is a mismatch between the Gaussian chain in the external field $B$ and the variational method where the value of $B$ is expected to find from the variational free energy minimization. The divergency on the interval, $0 < s < 1/\lambda_+$ shows that the effective segment-segment interaction within the variational method comes in a contradiction with the Gaussian statistics on this interval. One way to resolve this contradiction is to take the trial free energy in a more general form, $\sum_{s=1}^{N} R(s)B(s-s')R(s')$, i.e. now $B(s)$ is a trial function but not a constant field. That actually what we have considered in the recent papers [25].

Nevertheless, at the moment it is enough to stay with only one variational parameter $B$ which correctly describes the behavior of the string of statistically independent segments. In other words, the variational method should be applied to the coarse-grained model which we have discussed above.

Mathematically this simply amounts to the limiting of the contour variable $s$ on the interval $1/\lambda_+ < s < \infty$, i.e. eq. (3.1) reads

$$F^{(1)}_{RS} = -\frac{\Delta}{2\pi^{d/2}bd}N \left[ \sinh(\lambda_-) \right]^{d/2} \int_{1/\lambda_+}^{\infty} ds \left[ \frac{1}{[1-e^{-\lambda_+s}]^{d/2}} - 1 \right]. \quad (B2)$$

After that the RS - free energy becomes

$$F^{(1)}_{RS} = -\frac{\Delta}{2\pi^{d/2}bd}N \left[ \sinh(\lambda_-) \right]^{d/2} \frac{1}{\lambda_+} I_d, \quad (B3)$$

where

$$I_d = \int_{1}^{\infty} dx \left[ \frac{1}{[1-e^{-x}]^{d/2}} - 1 \right], \quad (B4)$$

so that the integral in eq. (3.1) is regularized.

**APPENDIX C: RSB - FREE ENERGY FUNCTIONAL: LIMITS AND INTERPOLATION**

Let us calculate first the entropy term (2.20) in the limits (4.1) and (4.3). For the eigenvalue $\lambda_-$ (see eq. 2.15) one can write

$$\lambda_- = 2 \ln \left[ \frac{1}{2} \sqrt{B + 2mC} + \sqrt{1 + B + 2mC} \right] + 4A,$$

i.e. at $C = 0$ $\lambda_- = \lambda_+$. We expand eqs. (C1) with respect to small $C$ retaining only the main terms. Then the corresponding RSB - entropy term (after subtraction of RS - term, i.e. $F^{(0)}_{RSB} \approx [\lim_{n\to0} F_{0}/n] - F^{(0)}_{RS}$) reads

$$F^{(0)}_{RSB} \approx \frac{m-1}{m} \frac{dN}{2} \frac{mC}{4A} \quad (C2)$$

For the large $C$ using again eq. (C1) in eq. (2.20) yields the result

$$F^{(0)}_{RSB} \approx \frac{m-1}{m} \frac{dN}{2} \ln \left( \frac{2mC}{A} \right) - 1 \quad (C3)$$

The suitable interpolating expression which embraces both, eqs. (C2) and (C3) can be written in the simple form

$$F^{(0)}_{RSB} \approx \frac{m-1}{m} \frac{dN}{2} \ln \left( \frac{2mC}{A} + 1 \right) \quad (C4)$$

In such form the entropy term has been obtained in ref. [22, 23].
Now we can make the same calculations for $F_1(n,m)$ in eq. (A15). Because the dependence from $C$ is contained now only in $\lambda_-$ it is convenient for small $C$ to represent

$$\lambda_- \simeq \lambda_+ \left(1 + \frac{mC}{B}\right).$$  \hspace{1cm} (C5)

Expansion of the first term in eq. (A15) has the form

$$\left[\frac{1 - e^{-\lambda_+|s-s'|}}{m \sinh(\lambda_+)} + \frac{m - 1 - e^{-\lambda_-|s-s'|}}{m \sinh(\lambda_-)}\right]^{-d/2} \approx \left[\frac{1 - e^{-\lambda_+|s-s'|}}{\sinh(\lambda_+)}\right]^{-d/2} + \frac{d}{m} \frac{m - 1 - e^{-\lambda_-|s-s'|}}{m B} \left[\frac{1 - e^{-\lambda_+|s-s'|}}{m \sinh(\lambda_+)}\right]^{-d/2} \times \frac{\lambda_+|s-s'| - e^{-\lambda_+|s-s'|}}{1 - e^{-\lambda_+|s-s'|}} - \lambda_+ \coth(\lambda_+) \right].$$  \hspace{1cm} (C6)

By the same way the 2nd and 3rd terms in eq. (A15) yields correspondingly

$$\left[\frac{1 - e^{-\lambda_+|s-s'|}}{m \sinh(\lambda_+)} + \frac{m - 1 + e^{-\lambda_-|s-s'|}}{m \sinh(\lambda_-)}\right]^{-d/2} \approx \left[\sinh(\lambda_+)^{d/2} + \frac{d}{m} \frac{m - 1 - e^{-\lambda_-|s-s'|}}{m B} \left[\sinh(\lambda_+)^{d/2}\lambda_+ \coth(\lambda_+)\right]\right] \times \frac{\lambda_+|s-s'| - e^{-\lambda_+|s-s'|}}{m} + \frac{\lambda_+ \coth(\lambda_+)}{m} \left[\frac{1 - e^{-\lambda_+|s-s'|}}{m \sinh(\lambda_+)}\right]^{-d/2} \right] \hspace{1cm} (C7)

and

$$\left[\frac{1}{m \sinh(\lambda_+)} + \frac{m - 1}{m} \frac{1}{\sinh(\lambda_-)}\right]^{-d/2} \approx \left[\sinh(\lambda_+)^{d/2} + \frac{d}{m} \frac{m - 1 - mC}{m B} \left[\sinh(\lambda_+)^{d/2}\lambda_+ \coth(\lambda_+)\right]\right] \hspace{1cm} (C8)

The 3rd term in eq. (A15) has the factor $n(n - m)$ which at $n \to 0$ takes the form $n(n - m) \approx -n - n(m - 1)$, so that we can combine the 3rd term with the 1st and 2nd terms correspondingly. After that by switching from the summation to the integration over $s$ and $s'$ we arrive at the following two contributions to the RSB - interaction free energy part

$$F^{(1)}_{\text{RSB}} = \left[\lim_{n \to 0} \frac{F_1(n,m)}{n}\right] - F^{(1)}_{\text{RS}} = J_1 + J_2,$$  \hspace{1cm} (C9)

where

$$J_1 = -\frac{\Delta dN}{2\pi^{d/2}b^d} \frac{m - 1}{m} \frac{mC}{B} \left[\frac{\sinh(\lambda_+)^{d/2}}{\lambda_+} \right] \left[\lambda_+ \coth(\lambda_+) - \frac{2}{d} I_d\right],$$

$$J_2 = -\frac{\Delta dN}{2\pi^{d/2}b^d} \frac{m - 1}{m} \frac{mC}{B} \left[\frac{\sinh(\lambda_+)^{d/2}}{\lambda_+} \right] \left[\lambda_+ \coth(\lambda_+) + 1\right],$$  \hspace{1cm} (C10)

where $I_d$ is given by eq. (B13). At small $\lambda_+$ it can be seen that $\lambda_+ \coth(\lambda_+) \simeq 1 + \lambda_+^2/2$ and both terms, $J_1$ and $J_2$ are negative. Then the resulting expression for $F^{(1)}_{\text{RSB}}$ at small $C$ is given by

$$F^{(1)}_{\text{RSB}} = -\frac{\Delta dN}{2\pi^{d/2}b^d} \frac{m - 1}{m} \frac{mC}{B} \left[\frac{\sinh(\lambda_+)^{d/2}}{\lambda_+} \right] I_d \hspace{1cm} (C11)

In the limit of large $C$ the eigenvalue $\lambda_-$ is large also and all terms which include $1/ \sinh(\lambda_-)$ can be neglected. After that from eq. (A15) for $F^{(1)}_{\text{RSB}} = \left[\lim_{n \to 0} F_1(n,m)/n\right] - F^{(0)}_{\text{RS}}$ we immediately have

$$F^{(1)}_{\text{RSB}} = -\frac{\Delta dN}{2\pi^{d/2}b^d} \left(m^\delta + 1 - 1\right) \left[\frac{\sinh(\lambda_+)^{d/2}}{\lambda_+} \right] I_d \hspace{1cm} (C12)

Let us denote

$$y \equiv \frac{2mC}{A} = 2mC\delta^2.$$

$$\hspace{1cm} (C13)$$
Then the parameter \( m C / B \simeq y / (2\lambda_+^2) \), where we have used \( \lambda_+^2 \simeq B / A \). After that the expression which interpolates between eqs. (C11) and (C12) can be written in the form

\[
F_{\text{RSB}}^{(1)} \simeq -\frac{\Delta dN}{2n^d/2b^d} \frac{[\sinh(\lambda_+)]^{d/2}}{\lambda_+} \frac{(m^2 + 1) y}{y + m (m^2 + 1) / m - 1} \frac{2 \lambda_+^2}{2 \lambda_+^2}
\]

(C14)

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