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# Long range anti-ferromagnetic spin model for prebiotic evolution

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## Abstract

I propose and discuss a fitness function for one-dimensional binary monomer sequences of macromolecules for prebiotic evolution. The fitness function is defined by the free energy of polymers in the high temperature random coil phase. With repulsive interactions among the same kind of monomers, the free energy in the high temperature limit becomes the energy function of the one-dimensional long range anti-ferromagnetic spin model, which is shown to have a dynamical phase transition and glassy states.

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## 1. Introduction

With the development of spin-glass theory [1], properties of biological macromolecules have been discussed in terms of spin-glass-like models, which are characterized by complex energy landscapes. Among several suggestions, the origin of monomer sequences in a prebiotic environment has been discussed by assuming some fitness functions which are similar to spin-glass models [2, 3]. In these studies, monomer sequences are regarded as dynamical variables and the evolution of macromolecules is achieved by combinations of simple molecules which make the fitness function increase. The fitness functions are often assumed to be the energy functions of typical spin-glass models, which contain quenched random interactions [4, 5]. By introducing spin-glass models, stability and diversity of macromolecules are naturally explained on physical bases. Although this will be in the right direction, the relevance of quenched randomness in this context may remain to be discussed.

Recently, the study of spin glasses has achieved another finding. Some deterministic spin models were shown to have random glassy states at low temperature, which are referred to as self-induced quenched randomness [6–8]. Although the study of glass transition is a long standing problem [9], these studies clarified that some seemingly simple spin models also have

this fascinating property. We expect the study of these and related models will be fruitful in providing some insight into irregular structures in nature. This naturally leads to a question: are the one-dimensional structures of macromolecules described by some deterministic models? In other words, do polymers themselves have an ability to create stability and diversity of biological information by non-random interactions? Quite recently, it was found that one-dimensional anti-ferromagnetic (AF) Ising spin models belong to the spin models which have a glass transition [10, 11]. This allows us to postulate a simple but non-trivial fitness function for polymers in a prebiotic environment.

To find a simple fitness function for polymers, let us review some fundamental properties of them. A polymer is a one-dimensional flexible chain made of many monomers, which may be of several kinds. Generally, polymers are characterized by two kinds of energy scales. One is the strong binding energy between two adjacent monomers on the chain, which is realized by covalent bonds. The other is the weak and moderate range interactions among monomers. Due to the strong binding energy, a polymer resembles a chain which looks like a random coil at high temperature, while at low temperature, they fold into a compact conformation, or conformations, which are controlled by the weak interactions.

In the process of polymer evolution, monomers on the chain are replaced by other kinds of monomers, i.e., mutation, and/or polymers partially exchange monomer sequences, i.e., crossover. These processes require breaking and recombination of strong bonds. Naively, in the prebiotic environment, we expect that breaking of strong bonds happens simply by thermal activation, whose probability will be greater at higher temperature. Thus, in the framework of statistical physics, a natural suggestion will be that the evolution takes place mainly at rather high temperature, where polymers are in the random coil phase. This leads to the idea of using the free energy of a polymer in the high temperature random coil phase as a cost function of monomer sequences. This is in accordance with the recent idea of the ‘deep hot biosphere’ for origin of life [12].

The purpose of this paper is to explore the idea presented above by introducing a simple polymer model. Before getting into the details of the study, we give an overview on the resulting cost function and its implications. At high enough temperature, polymer configurations are approximately given by random walks of a particle. With a quenched monomer sequence, the free energy is given by the expectation value of monomer interaction energy over these configurations. This free energy defines an energy function of one-dimensional spin model if kinds of monomers are expressed as spin variables. In the conventional idea of statistical physics, one-dimensional short range spin models only have a paramagnetic phase down to zero temperature. However in our model, this is not necessarily the case since the resulting one-dimensional models are long range due to the bending of the polymer. It is known that the one-dimensional long range spin models can have a phase transition at finite temperature. The resulting spin model will be long range anti-ferromagnetic when the same kinds of monomers interact repulsively. Although this model has no quenched randomness, it has frustrations [13], which suggest a complex energy landscape.

The plan of this paper is as follows. In section 2, introducing a simple polymer model at high temperature, we discuss the high temperature expansion to obtain the free energy as a function of monomer sequence. This is simply the statistical mechanics of a polymer in the random coil phase, resulting in a seemingly simple but interesting spin model. In section 3, taking the free energy as a cost function, we discuss the low energy states. For this purpose, we study another statistical mechanics for spin models by regarding kinds of monomers as dynamical variables. In section 4, we present some numerical results of double dynamics, which consists of fast polymer dynamics and slow monomer dynamics. Section 5 is devoted to some discussions.

## 2. Binary polymer at high temperature

In this section, we introduce a simple polymer model and evaluate the high temperature free energy, which will be regarded as a cost function for monomer sequence evolution. Among various polymer models, we consider a heteropolymer made of binary mixtures of two kinds of monomers. The probability of bond breaking is assumed to be very small and the monomer sequences can be regarded as quenched on the timescale of fluctuations of polymer configurations.

Let us consider binary polymers made of  $L$  monomers, each of which is either kind A or B. Let  $S_i$  ( $i = 1, 2, \dots, L$ ) denote the kind of  $i$ th monomer;  $S_i = 1$  for A and  $S_i = -1$  for B. We assume that the same kind of monomers interact repulsively, while the different kinds are attractive. By this assumption, the condensation of the same kind of monomers is suppressed. The simplest energy function made of  $S_i$  will be given by

$$H_p = \sum_{i < j} S_i S_j f(r_i - r_j) \quad (1)$$

where  $r_i$  are coordinates of monomers in the space on which the polymer is placed and  $f(r)$  is a positive function which characterizes the weak interactions between monomers. This function will be specified later. Since monomers are located on a chain, they should obey the constraints  $|r_i - r_{i+1}| = 1$  for  $i = 1, 2, \dots, L - 1$ . To be specific, we assume that monomers are located on sites of a  $D$ -dimensional simple cubic lattice, that is, each component of  $r_i$  takes integers  $1, 2, \dots, K$  with  $K^D = V$ , where  $V$  is the number of sites of the cubic lattice.

The partition function for the polymer is given by

$$Z_p = \sum_{\{r\}} \exp(-\beta_p H_p) \quad (2)$$

where  $\beta_p = T_p^{-1}$  is the inverse temperature of the polymer and  $\sum_{\{r\}}$  means the summation over possible chain configurations. Usually, the chain configurations are assumed to be self-avoiding due to the hard spheres of monomers. For the sake of simplicity, we avoid this problem by assuming that the lattice has high enough dimension  $D > 4$ , for which self-avoiding walks are approximated by random walks [14]. For  $\beta_p = 0$ , we then have  $Z_p \sim Z_0 \equiv V(2D)^{L-1}$  for large  $D$ . According to the well-known result for random walks [14], the distribution of  $R = |r_L - r_1|$  is given by

$$P(R) = \left(\frac{D}{2\pi L}\right)^{D/2} \exp\left(-\frac{D}{2L}R^2\right) \quad (3)$$

for large  $L$ . The one-dimensional scale of the random coil is given by  $(L/D)^{1/2}$ .

Let us specify the interaction function  $f(r)$ . We assume that the interactions are finite range and decrease rapidly for  $r \rightarrow \infty$ . The relevant parameter is the range of interactions, beyond which  $f(r) \sim 0$ . Note that if it is larger than  $(L/D)^{1/2}$ , the energy function does not depend on the chain configuration. On the other hand, long range interactions will justify the continuous approximation for lattice structure and, more importantly, the mean-field approximation of the resulting spin model. With these points in mind, it is convenient to assume

$$f(r) = \exp\left(-\frac{D}{2l_0}r^2\right) \quad (4)$$

where  $l_0$  is a positive parameter with  $1 \ll l_0 \ll L$ . Other functions will give a similar result as long as they are finite range.

Now we evaluate the partition function to the first order of  $\beta_p$ . The Boltzmann weight is expressed as a product of monomer pair contributions and the exponential is expanded in terms of  $\beta_p$ , giving

$$Z_p = \sum_{\{r\}} \prod_{i < j} \{1 - \beta_p f_{ij}(r_{ij}) + \dots\} \quad (5)$$

where  $r_{ij} = r_i - r_j$  and  $f_{ij}(r) = S_i S_j f(r)$ . To evaluate the first-order terms, we first sum all configurations with fixed  $r_i$  and  $r_j$ . In the following calculations, the continuous approximation for a lattice is introduced, which will be justified for large  $l_0$ . The number of paths from  $r_i$  to  $r_j$  with length  $l = |i - j|$  is approximately given by  $(2D)^l G_l(r_{ij})$ , where the propagator is given by

$$G_l(r) = \left(\frac{D}{2\pi l}\right)^{D/2} \exp\left(-\frac{D}{2l}r^2\right) \quad (6)$$

for large  $l$  and  $r$ . The expression for the number of chain configurations which starts from  $r_1$ , visits  $r_i$  and  $r_j$ , and ends at  $r_L$  is given by the product of suitable propagators. We note that propagators which contain either  $r_1$  or  $r_L$  can be eliminated by using  $\sum_{r_1} G_{i-1}(r_{1i}) = 1$ , etc. Further, the summations over lattice sites are replaced by integrals over continuous coordinates. The first-order term then becomes

$$\begin{aligned} -\frac{\beta_p}{Z_0} \sum_{i < j} \sum_{\{r\}} f_{ij}(r_{ij}) &= -\frac{\beta_p}{V} \sum_{i < j} \sum_{r_i, r_j} G_{j-i}(r_{ij}) f_{ij}(r_{ij}) \\ &= -\beta_p \sum_{i < j} J_{ij} S_i S_j \end{aligned} \quad (7)$$

where

$$J_{ij} = \frac{l_0^{D/2}}{(l_0 + |i - j|)^{D/2}}. \quad (8)$$

In this way, we obtain the free energy  $F_p = -\ln Z_p / \beta_p$ ,

$$F_p = \sum_{i < j} J_{ij} S_i S_j \quad (9)$$

where an irrelevant constant is dropped. Since  $J_{ij}$  are positive, this function defines the long range AF spin model, if  $S_i$  are regarded as dynamical variables. Note that the sign of  $J_{ij}$  is opposite to that conventionally used in spin models.

The cost function tells us that the interaction strengths between two monomers depend on the distance  $l$  on the chain as  $(l_0 + l)^{-D/2}$ . This  $l$ -dependence is simply the consequence of the probability that a particle comes back to the original point by  $l$ -step random walks. If  $l_0$  is much larger than  $L$ , the spin model reduces to the infinite range AF model, which has a paramagnetic phase down to zero temperature. When  $l_0 \ll L$ ,  $J_{ij}$  become spatially decreasing AF interactions.

Expression (9) is the simplest non-trivial cost function among several modifications. Firstly, the second-order terms of  $\beta_p$  give rise to four-spin long range interactions. These terms will change the following arguments quantitatively but will not greatly change the qualitative aspects. We can control the contribution of these terms by choosing  $\beta_p$ . Secondly, the relevance of nearest neighbour (nn) AF interaction remains to be discussed since nn monomers are bound by strong interactions which do not depend on the kinds of monomers. As discussed in section 5, the change of nn AF interactions may change the nature of the low temperature phase and contain another interesting problem, which is beyond the scope of this paper.

### 3. The study of the effective AF spin model

In the previous section, we have studied the free energy with fixed monomer sequences, assuming that the polymer chain is in the random coil phase. The resulting free energy defines the cost function of monomer sequences. This function can be regarded as the energy function of the long range AF Ising spin model if the kinds of monomers are regarded as dynamical spin variables. In this section, we study the statistical mechanics of the effective spin model by introducing a formal temperature for spin variables. Basically we are interested in the behaviour of the cost function for various monomer sequences. We shall discuss the meaning of the spin dynamics in sections 4 and 5.

As discussed in earlier papers, the long range AF spin models have very interesting properties in spite of their simplicity. They have a dynamical phase transition and glassy low temperature phase. The study performed here is parallel to the ones presented in the previous papers [10, 11].

For convenience, we choose  $D = 4$  and include the diagonal terms  $J_{ii} = 1$  in the energy function, which is then given by

$$H = \frac{1}{2} \sum_{ij} J_{ij} S_i S_j \quad (10)$$

where

$$J_{ij} = \frac{l_0^2}{(l_0 + |i - j|)^2}. \quad (11)$$

To discuss the low energy states of  $H$ , it is convenient to express the energy function by Fourier representations as

$$H = \frac{1}{2} \sum_k J(k) |S(k)|^2 \quad (12)$$

where  $\sum_k$  means a sum over  $k$  given by  $k = 2\pi\mu/L$  ( $\mu = -L/2 + 1, \dots, L/2$ ),  $S(k) = \sum_j S_j \exp(ikj)/\sqrt{L}$ , and  $J(k)$  are Fourier representation of  $J_{ij}$ , which are given by

$$J(k) = l_0^2 \int_0^\infty \frac{t(e^t - e^{-t})}{e^t + e^{-t} - 2\cos(k)} \exp(-l_0 t) dt. \quad (13)$$

The property of  $J(k)$  is discussed in appendix A.  $J(k)$  is a positive decreasing function of  $k$ , taking  $J(0) \sim 2l_0$  and  $J(\pi) \sim 1/l_0$ . Unlike the AF models studied previously,  $J(k \sim \pi) \sim 1/l_0$  is not negligibly small, although it tends to zero for  $l_0 \rightarrow \infty$ .

Although  $S(k)$  are not independent variables due to Ising constraints  $|S_i| = 1$ , expression (12) is useful to have some insight into the low temperature properties of the model. We first note that macroscopic condensation of  $S(k)$  is suppressed since all  $J(k)$  are positive. One exception will be the one with the smallest  $J(k)$ , that is  $k = \pi$ , which represents the AF order. The energy density for this state is given by  $J(k = \pi)/2 \sim 1/2l_0$ , which is an absolute minimum state.

Expression (12) also suggests an analogy with the anti-Hebbian (AH) model, which is defined by the energy function

$$H_{\text{AH}} = \frac{1}{2} \sum_\mu \left( \sum_j S_j \xi_j^\mu / \sqrt{N} \right)^2 \quad (14)$$

where  $\xi_j^\mu = \pm 1$  ( $j = 1, 2, \dots, N$ ,  $\mu = 1, 2, \dots, P$ ) are quenched random variables and  $N$  is a system size. This energy function is made of  $P = \alpha N$  constraint terms made of random

linear functions with constant weight. The energy functions of the long range AF model are obtained by setting  $\xi_j^\mu \rightarrow \exp(ikj)$  and introducing suitable weights for each constrains. We also note that the interactions among spins are expressed by the sum of anti-Hebbian amplitude  $-\xi_i^\mu \xi_j^\mu / N$ . By replica treatment along the line in [15] and marginally stable condition [7], it was shown that the AH model has a dynamical phase transition and glassy low temperature states for small  $\alpha$  [16]. Although the long range AF models do not have quenched randomness, they have similar properties as studied in the previous papers.

To study the paramagnetic and possible glassy phase, we construct a mean-field replica theory, making use of the Gaussian approximation, which will be justified for large  $l_0$ . This gives a treatment similar to the one for the AH model. A brief review of the mean-field replica theory is given in appendix B, where a definition of the saddle-point variables is also given. Here we only present the main results.

Let us begin with the high temperature expansion. Introducing a monomer inverse temperature  $\beta = T^{-1}$ , the partition function is defined by

$$Z = \sum_{\{S\}} \exp(-\beta H\{S_i\}). \quad (15)$$

With the Gaussian approximation presented in appendix B, we obtain the high temperature free energy  $f = -\ln Z / \beta L$ , energy  $e$ ,

$$f = \frac{1}{2\beta} \int_{-\pi}^{\pi} \ln(1 + \beta J(k)) \frac{dk}{2\pi} - \frac{1}{\beta} \ln 2 \quad e = \frac{1}{2} \int_{-\pi}^{\pi} \frac{J(k)}{1 + \beta J(k)} \frac{dk}{2\pi}$$

and entropy  $s = \beta(e - f)$ . Roughly,  $s$  is estimated to be  $\ln 2 - \ln(1 + \beta J(0)) / cl_0$  with some constant  $c$ . This expression becomes negative below  $T_s \sim 2l_0 \exp(-cl_0 \ln 2)$ , which is not acceptable for Ising spins. This signals the existence of a phase transition above  $T_s$ . Study of the AH model suggests that there will be a glass transition above  $T_s$ , which can be discussed by replica mean-field theory.

By introducing  $n$  replicas, the replicated partition function is defined by

$$Z^n = \frac{1}{2^L} \sum_{\{\eta, S\}} \exp\left(-\beta \sum_{\rho=1}^n H\{\eta_i S_i^\rho\}\right) \quad (16)$$

where  $\eta_i = \pm 1$ .

With the approximation for the limit  $l_0^{-1} \rightarrow 0$ , we reach the replica mean-field theory, which is described by order parameter matrix  $q_{\rho\sigma}$  ( $\rho, \sigma = 1, 2, \dots, n, \rho \neq \sigma$ ). Non-trivial replica symmetry (RS) solutions continuously appear at the temperature given by

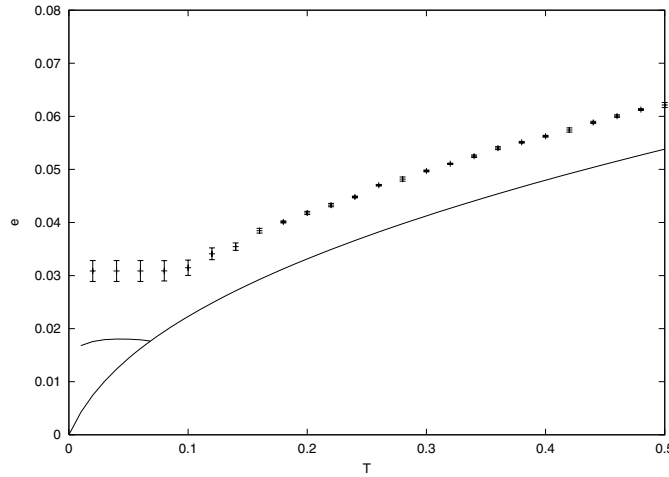
$$1 = -\beta^2 2g''(\beta) \quad (17)$$

where

$$g''(x) = -\frac{1}{2} \int_{-\pi}^{\pi} \frac{J^2(k)}{(1 + xJ(k))^2} \frac{dk}{2\pi}. \quad (18)$$

At this point, it will be convenient to compare this expression with the one of the AH model, which has  $N\alpha$  constraint terms for  $N$  spins in the energy function. In this model, a RS transition appears at  $\beta$  given by  $1 = \alpha\beta^2 / (1 + \beta)^2$ , which does not have a positive solution for  $\alpha < 1$ . Similarly, since  $J(k) > 0$  for all  $k$ , equation (17) does not have a solution down to zero temperature.

Having negative entropy and no RS solution, we study one-step RSB solutions, which are defined by assuming  $q_{\rho\sigma} = q_1$  ( $\rho \neq \sigma$ ) in the diagonal blocks of size  $m \times m$  and zero elsewhere. There are two kinds of RSB solutions; one is the usual one and the other is the



**Figure 1.**  $T$ -dependence of energies for the AF spin model with  $l_0 = 40$ . The full line for all temperatures is the result of high temperature expansion. The full line for  $T < T_g = 0.068$  is the replica result with the marginally stable condition. Dots with error bars represent the result of simulated annealing for five runs with  $L = 200$ .  $10^4$  MC steps have been performed at each temperature.

one with the marginally stable condition [6]. It was suggested that the marginally stable RSB solution describes the glass transition, while the usual RSB solution describes the lowest glassy state. The latter appears at a temperature very close to  $T_s$ , while the former appears at a temperature  $T_g$  much higher than  $T_s$ . The marginal stability condition is given by

$$1 = -\beta^2 \frac{\int \cosh^{-4}(\sqrt{\lambda_1}x) \cosh^m(\sqrt{\lambda_1}x) Dx}{\int \cosh^m(\sqrt{\lambda_1}x) Dx} 2g''(\beta(1 - q_1)) \tag{19}$$

where  $Dx = \exp(-x^2/2) dx/\sqrt{2\pi}$  and  $\lambda_1$  is given by the saddle-point equation. In figure 1, the temperature dependence of energies of marginally stable RSB as well as high temperature energy are presented for  $l_0 = 40$ , for which  $T_g = 0.068$ .

The simulated annealing of the AF model is performed by Monte Carlo (MC) method of Metropolis type, where spin flips are accepted with the probability  $\min[1, \exp -\beta(\Delta H)]$ ,  $\Delta H$  is the change of energy. The simulation results for  $l_0 = 40$  are presented in figure 1, which shows the temperature dependence of energy. The simulation result is systematically higher than the results of the replica method, but it shows a breakpoint close to  $T = T_g$ . We should note that the energy obtained by the Gaussian approximation tends to zero as  $T \rightarrow 0$ , while the energy by simulation should tend to the lowest energy  $J(\pi)/2 \sim 1/2l_0$  if the system has no phase transition. Actually, the discrepancy is very close to  $1/2l_0$ . This was not visible in the case of the AF model studied before, for which  $J(k)$  for  $k \sim \pi$  is exponentially small or zero. We suppose that  $l_0 = 40$  is not large enough to have a long range version of the present model.

Although it is not presented in the figures, we have studied the Edward–Anderson (EA) order parameter and the acceptance rate for the same runs. The EA order parameter is defined by  $q_{EA} = \sum_i \langle S_i \rangle^2 / L$ , where  $\langle S_i \rangle$  is an average of  $S_i$  over the configurations generated by the MC method. These quantities show strong fluctuations for  $T_g \lesssim T \lesssim 0.1$  when the MC step at each temperature is not large enough. The EA order parameter becomes 1 and the



acceptance rate becomes 0 rapidly around  $T_g$ . These aspects are consistent with the results of replica theory.

To see what the low energy states look like, we studied the low energy stable states up to system size  $L = 30$  by enumeration of all configurations. As expected, the lowest state is the AF configuration, which seems isolated from higher energy states. The configurations above AF states are very similar to AF states but have a few kinks such as AA and BB. Although the system size is not large enough to have a translational invariance, the states with very low energy seem to show this property approximately. As the energy increases, the number of kinks increases and the number of states also increases quite rapidly.

In this section, we have studied the long range AF model defined by (10) along a line which was presented in the previous papers. Almost all aspects are similar to those which were found in the previously studied AF models, except for the energy values at low temperature and strong fluctuations just above  $T_g$ . We suppose that finite  $J(k \sim \pi)$  gives rise to these aspects. Concerning the value of energy, the relation  $\sum_k |S(k)|^2 = L$ , which holds for Ising spins, gives positive  $H$  for positive  $J(k)$ , while the Gaussian approximation at high temperature gives energy tending to zero as  $T \rightarrow 0$ . This makes the theoretical results lower than the simulation results. On the strong fluctuation, finite  $J(k \sim \pi)$  seems to make the annealing process near the glass transition more complicated than the case  $J(k \sim \pi) \sim 0$ , since the distribution of  $S(k)$  at low temperature will be strongly controlled by finite and varying  $J(k \sim \pi)$ . However, qualitatively, the result of simulated annealing is consistent with the replica theory and very similar to those of the AF models studied before, supporting the existence of a glass transition.

Are these results relevant to understanding the polymer evolution problem? We first note that the density of cost function  $H/L$  varies from 0.5 to about  $1/2l_0$  depending on the monomer sequences. This means that the  $L$ -dependence of monomer interaction energy  $H - 0.5L$  changes from  $L^{1/2}$  to  $L$  by the arrangements of monomer sequence. Further, the existence of a glass transition implies that there are many monomer configurations which are stable with respect to one-monomer change. This gives an interesting idea on the states of monomer sequences. In spin models, we may say that the spin direction is right if it is in the same direction as the local field, and wrong if not. We can use the same terminology for monomer sequences. That is, a monomer in the sequence is right if the cost function value increases by the replacement by the other kind of monomer and wrong if it decreases. However, in the polymer problem, we need to break two bonds to replace a monomer by the other kind. This process will not take place so easily as in the spin model. In the following section, we discuss the meaning of the spin model and directly study the double dynamics of polymer chain and monomer sequences to see the consistency of the results obtained in this section.

#### 4. Double dynamics simulation of a polymer

The result in the previous section implies that the density of monomer interaction energy  $H_p/L$  in the random coil phase varies from 0 to about  $-0.5 + 1/2l_0$  as the monomer sequence varies. Below the glass transition temperature, the acceptance rate of monomer change becomes practically zero. This section is devoted to presenting some primary results of numerical simulations of the polymer itself. We only give some results which provide a consistency check between the effective spin model and the original polymer problem. The scale of simulations will be too small to give any conclusion on the glass transition.

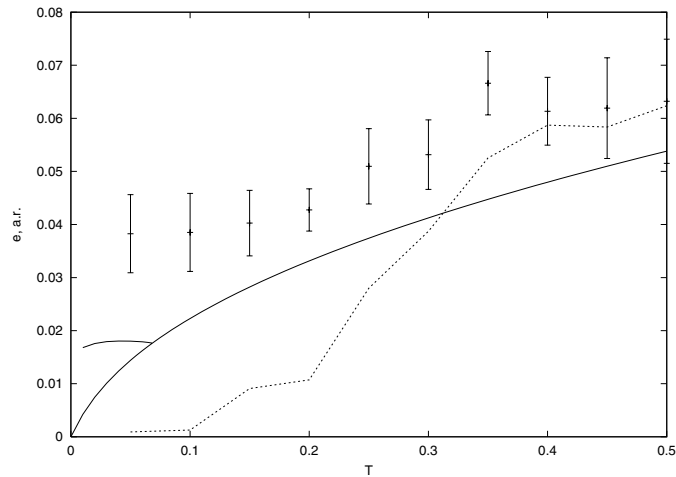
We first note that there are several types of dynamics for monomer sequence evolution. One is to add or remove monomers at the ends or in the middle of a polymer, which changes the length of the polymer. Second is to change the kinds of monomers without changing

the length of the polymer, which may be called a mutation in the biological context. We suppose that this change corresponds to a spin flip in the Ising spin models. If we assume that the binding energy of strong monomer couplings is finite, both kinds of changes should be included for consistency. However, this makes the problem very difficult. In this paper, we restrict ourselves to the changes which correspond to spin dynamics. In the context of the polymer problem, this situation will correspond to an isolated long polymer in a solution which is full of two kinds of free monomers. However, this instance is somewhat unrealistic since free monomers will tend to make dimers or small polymers rather than being isolated. In this sense, the following simulation cannot be related to the evolution directly but gives some idea of low cost states. Accordingly, the monomer temperature  $T$ , which is required to do simulations, is a formal one and is not directly related to real temperature. Note that the rate of monomer change will be controlled not only by binding energy and real temperature but also by the density of free monomers.

With mutation only, double dynamics of polymer chain and monomer sequences goes as follows. As in section 2, we consider a polymer of length  $L - 1$  which is placed in a four-dimensional simple cubic lattice. Initial polymer configurations are generated by a  $(L - 1)$ -step random walk. The initial monomer sequence is given by randomly generated  $S_i$ . The energy function is then given by (1). To avoid the overlapping of monomers, we assume a very high energy when  $|r_i - r_j| = 0$ . In the MC simulation of polymer dynamics, three kinds of one-step change are allowed: end rotation, kink jump and crankshaft [17]. When monomer coordinates are expressed as a summation of  $r_{i+1} - r_i$  ( $i = 1, 2, \dots, L - 1$ ), end rotation is performed by rotation of  $r_1 - r_2$  or  $r_L - r_{L-1}$ , a kink jump is by interchange of  $r_i - r_{i-1}$  and  $r_{i+1} - r_i$ , and crankshaft is by simultaneous rotation of  $r_{i+1} - r_i$  and  $r_{i+3} - r_{i+2}$  when  $r_{i+1} - r_i = -(r_{i+3} - r_{i+2})$ , respectively. Monomers are checked sequentially to find which change is possible. For each change, the change of energy (1), denoted by  $\Delta H_p$ , is evaluated. This change is allowed with probability  $\min[1, \exp(-\beta_p \Delta H_p)]$ . All these processes are performed for a fixed monomer configuration. The change of monomer is assumed to take place every  $M_p$  MC steps of polymer dynamics. For simplicity, we use the expectation value of  $H_p$ , denoted by  $\langle H_p \rangle$ , over  $M_p$  MC steps for the cost function of monomer sequences instead of free energy. This approximation will be good at high enough temperature. With a given monomer sequence  $S_i$ ,  $\langle H_p \rangle$  is evaluated and then after  $S_j \rightarrow -S_j$  for a certain  $j$ ,  $\langle H_p \rangle'$  for the changed monomer sequence is evaluated. This change is allowed with probability  $\min[1, \exp(-\beta(\langle H_p \rangle' - \langle H_p \rangle))]$ . Site  $j$  varies from 1 to  $L$  in one MC step of monomer dynamics.

In the simulated annealing of monomer sequences, monomer temperature  $T$  decreases step by step with fixed polymer temperature  $T_p$ . For the sampling of polymer configurations, we are obliged to take small  $L$ . In figure 2, we present the  $T$ -dependence of  $\langle H_p \rangle/L + 0.5$  by simulated annealing, where  $l_0 = 40$ ,  $L = 50$ ,  $M_p = 20$ , and  $T_p = 5.0$ . The acceptance rate of polymer dynamics for this  $T_p$  is more than 50% irrespective of  $T$ . The number of MC steps of monomer dynamics is 10 for each  $T$ . The qualitative behaviour of the energy seems consistent with that of the spin model in figure 1. The acceptance rate of monomer changes becomes zero rapidly for  $T \lesssim 0.1$ , where  $\langle H_p \rangle/L$  also ceases to decrease. Although this is consistent with the existence of a glass transition, the scale of simulation is too small to give any conclusion on the phase transition.

The monomer dynamics presented in this section is made to correspond to spin dynamics of the effective AF spin model, which will be achieved in the  $M_p \rightarrow \infty$  limit. We implicitly made an assumption that  $T$  is controlled by the monomer binding energy and the density of free monomers. If we start with finite binding energy, we are obliged to take into account breaking and binding of polymers. In this sense, the dynamics studied in this section may



**Figure 2.** Dots with error bars represent the  $T$ -dependence of  $\langle H_p \rangle / L + 0.5$  of double dynamics for the polymer model for five runs. See the text for the values of parameters. Theoretical results for the AF spin model are also depicted for reference. The dotted line shows the averaged acceptance rate of monomer dynamics. The vertical axis is common to all data. Although the averaged acceptance rate is not zero for  $T = 0.05$ , the original values are zero for most runs.

have limited relevance in understanding the monomer sequence evolution. However, monomer configurations with low cost function value are those which should be achieved by any kind of descent dynamics controlled by the cost function. The simulations for a polymer imply that, as far as the monomer interaction energy is concerned, the polymer problem seems to be well described by the effective spin model.

## 5. Discussion

In this paper, we introduced and discussed the cost function of monomer sequences by assuming that evolution occurs in the high temperature random coil phase. This is motivated by the naive idea that rearrangement of the strong monomer bonds will take place mainly in the high temperature random coil phase and the resulting monomer sequences are tested in the same environment. The cost function for monomer sequences becomes the energy function of the long range AF spin model if the kinds of monomers are regarded as spin variables. Like the AF spin models studied before, this model has a glass transition, which is found by the replica method with the marginality condition. The MC simulation for the spin model is qualitatively in agreement with the replica theory, although the energy values of simulation are systematically higher than the results of replica theory. We suppose that this is due to non-zero  $J(k)$  for  $k \sim \pi$ . It is desirable to make a more sophisticated study of this situation.

Having the effective AF spin model, we have directly studied the monomer dynamics by double MC dynamics, assuming a monomer change takes place every  $M_p$  MC steps of high temperature polymer dynamics. The energy range of the polymer simulation is found to be consistent with that of the effective spin model. Around  $T_g$ , monomer dynamics becomes very slow, which implies a qualitative change of the dynamics. This is also consistent with the glass transition suggested by the effective AF spin model.

Let us make some remarks on the modification of the cost function. The interaction studied in this paper simply gives an AF order for an absolute minimum state. This may

change by including another interaction term. Here we consider the effect of suppressing nearest neighbour AF interactions. In the Fourier representation, the additional cost function takes the form  $-a \sum_k \cos(k) |S(k)|^2$  with a positive  $a$ . For suitable  $a$ , this term makes  $J(k)$  non-monotonic for  $k$  close to  $\pi$ , implying that AF order is no longer an absolute minimum state. When some  $J(k)$  are negative, interactions  $J_{ij}$  can be regarded as a mixture of Hebbian and anti-Hebbian type amplitudes. According to the replica study [15], even only Hebbian type does not allow the condensation of a certain mode due to quenched noises created by other modes, if the number of modes is not small enough. We think that this is the case in our modified model. An interesting possibility is that the glass transition is replaced by the usual spin-glass transition, which can be identified by the appearance of a non-trivial RS solution. This also implies that a several-steps RSB solution is required to describe the low temperature phase correctly, giving the hierarchical organization [18] of monomer sequences. However, the situation with partly negative  $J(k)$  is not so clear since the Gaussian approximation for the replicated partition function is not necessarily suitable for partly negative  $J(k)$ .

An analogy to spin models is illuminating in describing the states of monomer sequences. As discussed in section 3, using the terminology of spin models, we say that a monomer is right if the corresponding spin is parallel to the local field and wrong if not. In the polymer problem, there are two factors which encourage the replacement of wrong monomers; one is of course that the local field by other monomers favours a right monomer and another is that the wrong monomer itself attracts a right monomer. We thus expect that wrong monomers on the sequences are strong attractive spots for free monomers. Below the glass transition temperature, there are many kinds of polymers which have almost all right monomers. In this sense, the concept of glassy states seems suitable to explain the stability and diversity of biological polymers, as was suggested in the literature. However, we should note that glassy states are not in equilibrium, which will make further evolution.

An analogy to spin models also reveals the limit of spin models in understanding polymer evolution. Although mutation is a suitable operation to achieve the right monomer sequence, evolution only by mutation sounds unrealistic if monomer binding energy is finite. Mutation requires successive changes of two bonds and a finite density of free monomers in the solution. This situation will make the evolution very complicated since it induces various other processes which change the length of polymers. In addition, finite free monomer density will encourage the formation of small polymers. Thus the density of free monomers will be very small, which may suppress mutation greatly. For these reasons, we think that evolution which includes the change of polymer length will mainly control the evolution in a system with finite monomer binding energy.

With combination, crossover and breaking of polymers, we should consider not a single polymer but an ensemble of polymers, which may be studied by methods similar to genetic algorithms [19], although making copies is far from trivial in the polymer evolution problem. An interesting question is whether these processes create lower cost states than the states at glass transition or not. We expect that the processes which include the simultaneous change of many monomers will have a chance to give lower cost states than only by mutation. Another interesting aspect of an ensemble of polymers is that interactions among polymers may work in a certain biased direction in polymer evolution. If there are strong attractive interactions between polymers, the probability of combination and crossover will be larger than the case of weak interactions. This may imply that interactions among polymers become weak as combination and crossover proceed. Remaining interactions among polymers will be a very interesting subject in the study of prebiotic evolution.

To summarize, I have shown that the polymer evolution problem in the high temperature random coil phase is related to the one-dimensional long range AF spin models, which have

low energy glassy states. An important finding may be that monomer sequences of binary polymers have the ability to achieve stability and diversity by themselves even in the random coil phase. Of course, this does not necessarily imply that life started in this situation. However, our study implies that some interesting order may arise among evolving polymers in this seemingly simple situation.

### Appendix A

In this appendix, we discuss the properties of the Fourier representation of  $J_{ij}$ , which is defined by

$$J(k) = \sum_{l=0}^{L-1} \frac{l_0^2}{(l_0 + l)^2} (e^{ikl} + e^{-ikl}) - 1. \quad (\text{A.1})$$

With the integral representation for  $(l_0 + l)^{-2}$ , we obtain

$$J(k) = l_0^2 \int_0^\infty \frac{t(e^t - e^{-t})}{e^t + e^{-t} - 2\cos(k)} \exp(-l_0 t) dt. \quad (\text{A.2})$$

This expression implies that  $J(k)$  is a positive decreasing function of  $k$ . The values of  $J(k)$  at  $k = 0$  and  $k = \pi$  are given by

$$J(0) = l_0^2 \int_0^\infty \frac{t(e^{t/2} + e^{-t/2})}{(e^{t/2} - e^{-t/2})} \exp(-l_0 t) dt$$

$$J(\pi) = l_0^2 \int_0^\infty \frac{t(e^{t/2} - e^{-t/2})}{(e^{t/2} + e^{-t/2})} \exp(-l_0 t) dt.$$

For large  $l_0$ , these expressions give  $J(0) \sim 2l_0$  and  $J(\pi) \sim 1/l_0$ .

To have an idea of the  $k$ -dependence of  $J(k)$ , we consider the limit  $l_0 \rightarrow \infty$ , where contributing  $t$  is very small. Then,

$$\begin{aligned} J(k) &\sim l_0^2 \int_0^\infty \frac{2t^2}{t^2 + 2(1 - \cos(k))} \exp(-l_0 t) dt \\ &= 2l_0 \int_0^\infty \frac{s^2}{s^2 + 2l_0^2(1 - \cos(k))} \exp(-s) ds. \end{aligned}$$

The last expression implies that the characteristic  $k$  is  $l_0^{-1}$ , beyond which  $J(k)$  becomes of order  $l_0^{-1}$ .

### Appendix B

In this appendix, we review the mean-field replica theory of the long range AF model, whose energy function is given by

$$H\{S_i\} = \frac{1}{2} \sum_k J(k) |S(k)|^2 \quad (\text{B.1})$$

where  $S(k)$  are Fourier components of  $S_i$ . By the argument in the previous papers, the replicated partition function is defined by

$$Z^n = \frac{1}{2^L} \sum_{\{\eta, S\}} \exp \left( -\beta \sum_{\rho=1}^n H\{\eta_i S_i^\rho\} \right). \quad (\text{B.2})$$

By introducing Gaussian variables  $\phi_k^\rho$  and performing the  $\eta$ -sum, we obtain

$$Z^n = \sum_{\{S\}} \int \exp \left( -\frac{1}{2} \sum_{\rho, |k|} |\phi_k^\rho|^2 + \sum_j \ln \cos \left( \frac{\sqrt{\beta}}{\sqrt{2L}} \sum_{\rho, k} \sqrt{J(k)} \phi_k^\rho e_j^k S_j^\rho \right) \right) \prod_{\rho, |k|} \frac{d\phi_k^\rho}{2\pi} \quad (\text{B.3})$$

where  $e_j^k = \exp(ikj)$ ,  $d\phi_k^\rho = d \operatorname{Re} \phi_k^\rho d \operatorname{Im} \phi_k^\rho$ , and  $\sum_{|k|}$  means a sum over  $k = 2\pi\mu/L$  ( $\mu = 0, 1, \dots, L/2$ ). To integrate over  $\phi_k^\rho$ , we make an approximation  $\ln \cos(x) \sim -x^2/2$ , i.e., a Gaussian approximation, which will be justified for small  $l_0^{-1}$ . Then we have

$$Z^n = \sum_{\{S\}} \exp(-\operatorname{Tr} g(\beta q)) \quad (\text{B.4})$$

where  $q$  is a matrix defined by  $q_{\rho\sigma} = \sum_i S_i^\rho S_i^\sigma / L$  with  $q_{\rho\rho} = 1$  and

$$g(x) = \frac{1}{2} \int_{-\pi}^{\pi} \ln(1 + xJ(k)) \frac{dk}{2\pi} \quad (\text{B.5})$$

$Z^n$  is evaluated by the saddle-point approximation by introducing an integral representation for the delta-function  $\delta(Lq_{\rho\sigma} - \sum_i S_i^\rho S_i^\sigma)$ . At the saddle point,

$$Z^n = \exp(-\beta n f(\lambda_{\rho\sigma}, q_{\rho\sigma})) \quad (\text{B.6})$$

where

$$\beta n f(\lambda_{\rho\sigma}, q_{\rho\sigma}) = \operatorname{Tr} g(\beta q) + \frac{1}{2} \sum_{\rho \neq \sigma} \lambda_{\rho\sigma} q_{\rho\sigma} - \ln \sum_{\{S\}} \exp \frac{1}{2} \sum_{\rho \neq \sigma} \lambda_{\rho\sigma} S^\rho S^\sigma \quad (\text{B.7})$$

where  $q_{\rho\sigma}$  and  $\lambda_{\rho\sigma}$  are the solutions of the saddle-point equations. The result for the high temperature phase is obtained by setting  $n = 1$ , which is given in section 3.

The RS solution is defined by  $q_{\rho\sigma} = q$ ,  $\lambda_{\rho\sigma} = \lambda$  for all  $\rho \neq \sigma$ , which gives

$$\beta f = \beta q g'(\beta(1-q)) + g(\beta(1-q)) + \frac{1}{2} \lambda(1-q) - \int \ln 2 \cosh(\sqrt{\lambda}x) Dx \quad (\text{B.8})$$

yielding a saddle-point equation,  $q = \int \tanh^2(\sqrt{\lambda}x) Dx$ ,  $\lambda = -2\beta^2 q g''(\beta(1-q))$ . The solution continuously appears at the temperature given by  $1 = -\beta^2 2g''(\beta)$ .

The one-step RSB solution with zero off-diagonal blocks is defined by setting  $q_{\rho\sigma} = q_1$  for diagonal blocks with size  $m \times m$  and zero elsewhere and the same for  $\lambda_{\rho\sigma}$ . With this ansatz, matrix  $q$  has eigenvalue  $x_m = 1 - q_1 + mq_1$  with degeneracy  $n/m$  and eigenvalue  $x_0 = 1 - q_1$  with degeneracy  $n - n/m$ . We then obtain

$$\beta f = \frac{1}{m} g(\beta x_m) + \left(1 - \frac{1}{m}\right) g(\beta x_0) + \frac{1}{2}(m-1)\lambda_1 q_1 + \frac{1}{2}\lambda_1 - \frac{1}{m} \ln \int 2^m \cosh^m(\sqrt{\lambda_1}z) Dz. \quad (\text{B.9})$$

The marginally stable solution is defined by  $\partial f / \partial q_1 = 0$ ,  $\partial f / \partial \lambda_1 = 0$ , and the marginally stable condition, which is obtained by studying the change of (B.7) to the second order of small changes of order parameters. This gives (19).

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