

Overlap properties and adsorption transition of two Hamiltonian paths

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Abstract. We consider a model of two (fully) compact polymer chains, coupled through an attractive interaction. These compact chains are represented by Hamiltonian paths (HP), and the coupling favors the existence of common bonds between the chains. We use a ($n = 0$ component) spin representation for these paths, and we evaluate the resulting partition function within a homogeneous saddle point approximation. For strong coupling (*i.e.* at low temperature), one finds a phase transition towards a “frozen” phase where one chain is completely adsorbed onto the other. By performing a Legendre transform, we obtain the probability distribution of overlaps. The fraction of common bonds between two HP, *i.e.* their overlap q , has both lower (q_m) and upper (q_M) bounds. This means in particular that two HP with overlap greater than q_M coincide. These results may be of interest in (bio)polymers and in optimization problems.

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1 Introduction

The study of two coupled identical systems is a familiar topic in Statistical Physics, both in equilibrium [1] and non equilibrium contexts [2]. It is commonly considered in the physics of glassy systems [3,4], where it is a substitute to the time honored conjugate field in the exploration of phase space. In this note, we wish to extend these studies to the case of two compact polymer chains. The coupling between the chains is chosen as an attractive term which favors the existence of common monomers (bonds); in other words, we consider the “adsorption” of a chain onto the other. By a Legendre transform, this model maps onto the overlap probability distribution of the chains.

For simplicity, we will consider fully compact chains. This allows us to use a simple spin representation [5] to describe the chain properties through Hamiltonian paths. Beside its interest in homopolymer physics, this model may yield some insight in the sequence-structure relationship in proteins, or in some related optimization problems such as the traveling salesman. The outline of the paper is as follows: we briefly recall in Section 2 the connection between a single polymer chain and an n -component spin system, in the limit $n = 0$. The extension to the problem of two interacting chains (Sect. 3) is then straightforward, and will be solved at a mean field level in Section 4. We finally mention some possible consequences of the model.

2 The single chain problem

The connection between polymer physics and spin systems may be presented as follows [6]. Let us consider, on each site \mathbf{r} of a d -dimensional cubic lattice, a spin variable \mathbf{S}_r , with n components. The normalization is such that $\mathbf{S}_r^2 = n$. Consider the sum:

$$Z(K) = \int \prod_{\mathbf{r}} d\mu(\mathbf{S}_r) \prod_{\{\mathbf{r}, \mathbf{r}'\}} (1 + K \mathbf{S}_r \mathbf{S}_{r'}) \quad (1)$$

where the variable K denotes the fugacity of a monomer, and the product runs over neighboring pairs of sites (*i.e.* bonds) of the lattice. In equation (1), $d\mu$ is the normalized integration measure on the $(n - 1)$ dimensional sphere of radius \sqrt{n} .

Due to the normalization of \mathbf{S}_r , it is easy to see that

$$\int d\mu(\mathbf{S}_r) \exp(\mathbf{H}_r \mathbf{S}_r) = 1 + \frac{\mathbf{H}_r^2}{2} + O(n) \quad (2)$$

so that, by taking derivative with respect to H_r^α ($\alpha = 1, \dots, n$), we obtain:

$$\int d\mu(\mathbf{S}_r) 1 = 1; \quad \int d\mu(\mathbf{S}_r) (S_r^\alpha)^2 = 1.$$

All higher powers of \mathbf{S}_r are at least of order n .

Expanding equation (1) in powers of K , and using the previous remark, we see that $Z(K)$ can be viewed as a sum over all closed loops, each closed loop of length l contributing a weight nK^l . In the limit $n \rightarrow 0$, only the single

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connected loops survive, hence the possibility to represent self-avoiding walks (SAW) on the lattice by equation (1). A very useful rewriting of equation (1) is

$$Z(K) = \int \prod_{\mathbf{r}} d\mu(\mathbf{S}_r) e^{\frac{1}{2} \sum_{(\mathbf{r}, \mathbf{r}')} K \mathbf{S}_r \Delta_{\mathbf{r}\mathbf{r}'} \mathbf{S}_{r'}} \quad (3)$$

where the operator $\Delta_{\mathbf{r}\mathbf{r}'}$ is a lattice Δ function ($\Delta_{\mathbf{r}\mathbf{r}'} = 1$, if \mathbf{r} and \mathbf{r}' are neighboring sites, and 0 otherwise). Note that the sum in the exponential term of equation (3) is over the sites of the lattice. Applying the familiar Stratonovich-Hubbard transformation to equation (3), we introduce $n = 0$ component fields ϕ_r and get

$$Z(K) = \int \prod_{\mathbf{r}} d\phi_r e^{-\frac{1}{2} \sum_{(\mathbf{r}, \mathbf{r}')} \phi_r \Delta_{\mathbf{r}\mathbf{r}'}^{-1} \phi_{r'}} \times \int \prod_{\mathbf{r}} d\mu(\mathbf{S}_r) e^{\sqrt{K} \sum_{\mathbf{r}} \mathbf{S}_r \phi_r}. \quad (4)$$

Using equation (2), we get

$$Z(K) = \int \prod_{\mathbf{r}} d\phi_r e^{-\frac{1}{2} \sum_{(\mathbf{r}, \mathbf{r}')} \phi_r \Delta_{\mathbf{r}\mathbf{r}'}^{-1} \phi_{r'}} \times \prod_{\mathbf{r}} \left(1 + \frac{K}{2} \phi_r^2 \right). \quad (5)$$

So far we have not specified the spatial extension of the SAW: $Z(K)$ is the grand partition function of the chain, so that the number M of sites of the lattice is not related to the number N of bonds of the SAW. We now require that fully compact configurations are the only configurations present in equation (5), *i.e.* $M = N$. This full compactness requirement amounts to keep the term proportional to nK^N in equation (5). The coefficient of this term is simply the number \mathcal{N} of self avoiding fully compact configurations (also called Hamiltonian paths or HP), that is

$$\mathcal{N} = K^{-N} \left(\frac{Z(K)}{n} \right)_{\substack{n=0 \\ K=\infty}} = \lim_{n \rightarrow 0} \frac{1}{n} \int \prod_{\mathbf{r}} d\phi_r e^{-\frac{1}{2} \sum_{(\mathbf{r}, \mathbf{r}')} \phi_r \Delta_{\mathbf{r}\mathbf{r}'}^{-1} \phi_{r'}} \prod_{\mathbf{r}} \left(\frac{\phi_r^2}{2} \right). \quad (6)$$

Note that \mathcal{N} is simply the canonical partition function for a HP of N bonds. Performing a homogeneous saddle point approximation on ϕ in equation (6) yields [7]

$$\mathcal{N} = \left(\frac{z}{e} \right)^N \quad (7)$$

where $z = 2d$ is the coordination number of the lattice. Note that in the context of Hamiltonian paths, an homogeneous solution implies that one deals with periodic boundary conditions [8].

Equation (6) holds for an arbitrarily connected graph with adjacency matrix $\Delta_{\mathbf{r}\mathbf{r}'}$, but the saddle point evaluation is *a priori* valid only for large enough z . Indeed, for

the fully connected graph ($z = N$), the number of HP can be directly estimated ($\mathcal{N} = N!/(2N)$), and equation (7) reduces to the Stirling formula. These results can also be obtained through the application of the Bethe approximation to polymers [9].

3 The coupled chains problem

We now extend the above approach to the case of two interacting self avoiding chains. By “interacting chains”, we mean that the presence of common (or doubly occupied) bonds between the chains is thermodynamically favored, and we are interested in counting the number of configurations of two such HP.

Following equation (1), we denote by K the fugacity of a monomer and consider the sum

$$Z_2(K, \lambda) = \int \prod_{\mathbf{r}} d\mu(\mathbf{S}_r) d\mu(\boldsymbol{\sigma}_r) \times \prod_{\{\mathbf{r}, \mathbf{r}'\}} (1 + K(\mathbf{S}_r \mathbf{S}_{r'} + \boldsymbol{\sigma}_r \boldsymbol{\sigma}_{r'}) + \lambda K^2 (\mathbf{S}_r \mathbf{S}_{r'}) (\boldsymbol{\sigma}_r \boldsymbol{\sigma}_{r'})) \quad (8)$$

where $\boldsymbol{\sigma}_r$ has the same properties as \mathbf{S}_r ($\boldsymbol{\sigma}_r^2 = n$), and the parameter λ is a measure of the interaction between the chains (see below). The contribution of doubly occupied bonds to equation (8) is proportional to $\lambda^{N_{12}}$, where N_{12} is the number of these bonds (implying $\lambda > 1$).

Following exactly the same steps as in Section 2, we have

$$Z_2(K, \lambda) = \int \prod_{\mathbf{r}} d\mu(\mathbf{S}_r) d\mu(\boldsymbol{\sigma}_r) e^{\frac{1}{2} \sum_{(\mathbf{r}, \mathbf{r}')} \Delta_{\mathbf{r}\mathbf{r}'} G_2(\mathbf{S}, \boldsymbol{\sigma})} \quad (9)$$

with

$$G_2(\mathbf{S}, \boldsymbol{\sigma}) = K(\mathbf{S}_r \mathbf{S}_{r'} + \boldsymbol{\sigma}_r \boldsymbol{\sigma}_{r'}) + (\lambda - 1) K^2 (\mathbf{S}_r \mathbf{S}_{r'}) (\boldsymbol{\sigma}_r \boldsymbol{\sigma}_{r'}). \quad (10)$$

Performing the Stratonovich-Hubbard transformation on equations (9, 10) yields

$$Z_2(K, \lambda) = \int \prod_{\mathbf{r}} d\phi_r d\psi_r \prod_{\alpha\beta} dq_{\alpha\beta}(r) e^{-\frac{1}{2} \sum_{(\mathbf{r}, \mathbf{r}')} \Delta_{\mathbf{r}\mathbf{r}'}^{-1} \mathcal{A}_{\mathbf{r}\mathbf{r}'}} \times \int \prod_{\mathbf{r}} d\mu(\mathbf{S}_r) d\mu(\boldsymbol{\sigma}_r) e^{\sqrt{K} \sum_{\mathbf{r}} \mathcal{B}_r} \quad (11)$$

with

$$\mathcal{A}_{\mathbf{r}\mathbf{r}'} = \phi_r \phi_{r'} + \psi_r \psi_{r'} + \sum_{\alpha\beta} q_{\alpha\beta}(\mathbf{r}) q_{\alpha\beta}(\mathbf{r}') \quad (12)$$

and

$$\mathcal{B}_r = \mathbf{S}_r \phi_r + \boldsymbol{\sigma}_r \psi_r + \sqrt{K} \sqrt{\lambda - 1} \sum_{\alpha\beta} q_{\alpha\beta}(r) S_r^\alpha \sigma_r^\beta. \quad (13)$$

Note that the previous transformations require two n component fields ϕ_r and ψ_r , and an $n \times n$ matrix $q_{\alpha\beta}(r)$, with $n = 0$. One may now perform the integration over the original spin variables \mathbf{S}_r and σ_r in equation (11). We obtain

$$Z_2(K, \lambda) = \int \prod_{\mathbf{r}} d\phi_r d\psi_r \times \prod_{\alpha\beta} dq_{\alpha\beta}(r) e^{-\frac{1}{2} \sum_{(r,r')} \Delta_{rr'}^{-1} \mathcal{A}_{rr'}} \prod_{\mathbf{r}} \mathcal{C}_r \quad (14)$$

where

$$\begin{aligned} \mathcal{C}_r = & 1 + \frac{K}{2}(\phi_r^2 + \psi_r^2) + \frac{K^2}{4}\phi_r^2\psi_r^2 \\ & + K^2\sqrt{\lambda-1} \sum_{\alpha\beta} \phi_r^\alpha q_{\alpha\beta}(r) \psi_r^\beta \\ & + \frac{K^2}{2}(\lambda-1) \sum_{\alpha\beta} q_{\alpha\beta}^2(r). \end{aligned} \quad (15)$$

So far, we have not specified the spatial extension of the chains. The sum $Z_2(K, \lambda)$ is grand canonical with respect to both singly and doubly occupied bonds. Following the previous section, we now enforce the full compactness constraint for both chains, by keeping the term proportional to $n^2 K^{2N}$ in equation (14). Defining by $\mathcal{Z}(\lambda)$, the total number of HP of the two interacting chains, we have

$$\mathcal{Z}(\lambda) = K^{-2N} \left(\frac{Z_2(K, \lambda)}{n^2} \right)_{\substack{n=0 \\ K=\infty}}. \quad (16)$$

Technically, the extraction of the term proportional to K^{2N} in $Z_2(K, \lambda)$, amounts to keep on each site \mathbf{r} the terms proportional to K^2 in equations (14, 15). We may therefore write

$$\begin{aligned} \mathcal{Z}(\lambda) = & \lim_{n \rightarrow 0} \frac{1}{n^2} \int \prod_{\mathbf{r}} d\phi_r d\psi_r \\ & \times \prod_{\alpha\beta} dq_{\alpha\beta}(r) e^{-\frac{1}{2} \sum_{(r,r')} \Delta_{rr'}^{-1} \mathcal{A}_{rr'}} \prod_{\mathbf{r}} \mathcal{D}_r \end{aligned} \quad (17)$$

where $\mathcal{A}_{rr'}$ is given in equation (12) and

$$\begin{aligned} \mathcal{D}_r = & \frac{\phi_r^2 \psi_r^2}{4} + \sqrt{\lambda-1} \sum_{\alpha\beta} \phi_r^\alpha q_{\alpha\beta}(r) \psi_r^\beta \\ & + \frac{1}{2}(\lambda-1) \sum_{\alpha\beta} q_{\alpha\beta}^2(r). \end{aligned} \quad (18)$$

Note that $\mathcal{Z}(\lambda)$ is still grand canonical with respect to the number N_{12} of common bonds between the two HP, since, as mentioned above, the term with N_{12} common bonds in $\mathcal{Z}(\lambda)$ yields a contribution proportional to $\lambda^{N_{12}}$.

One may also interpret equation (16) as giving the partition function of two HP of N bonds, with an attractive interaction energy ε favoring common bonds, at temperature T , that is

$$Z(\varepsilon) = \sum_{(HP_1, HP_2)} e^{\beta\varepsilon N_{12}} \quad (19)$$

with $\beta = \frac{1}{T}$. The identity between equations (16, 19), *i.e.* between $\mathcal{Z}(\lambda)$ and $Z(\varepsilon)$, yields the familiar result $\lambda = e^{\beta\varepsilon}$. Moreover, equation (19) allows us to derive bounds for the partition function $Z(\varepsilon)$ (or $\mathcal{Z}(\lambda)$), namely

$$\mathcal{N} e^{\beta\varepsilon N} \leq Z(\varepsilon) \leq \mathcal{N}^2 \quad (20)$$

where \mathcal{N} is given in equation (7). From now on, we will set $\varepsilon = 1$.

4 Saddle point approximation and phase transitions

Since an exact evaluation of equations (17, 18) seems to be out of reach, we will use a saddle point approximation with respect to the variables ϕ_r , ψ_r , and $q_{\alpha\beta}(r)$. This saddle point will be further restricted to be space independent ($\phi_r = \phi$, $\psi_r = \psi$, $q_{\alpha\beta}(r) = q_{\alpha\beta}$), again implying periodic boundary conditions. Setting $\mathcal{Z}(\lambda) = e^{-N\omega(\lambda)}$, we get

$$\omega(\lambda) = \text{Min}_{(\phi, \psi, q_{\alpha\beta})} \left(\frac{1}{4d}(\phi^2 + \psi^2 + \sum_{\alpha\beta} q_{\alpha\beta}^2) - \text{Log} \mathcal{D} \right) \quad (21)$$

where

$$\begin{aligned} \mathcal{D} = & \frac{\phi^2 \psi^2}{4} + \sqrt{\lambda-1} \sum_{\alpha\beta} \phi^\alpha q_{\alpha\beta} \psi^\beta \\ & + \frac{1}{2}(\lambda-1) \sum_{\alpha\beta} q_{\alpha\beta}^2. \end{aligned} \quad (22)$$

The saddle point equations are easily solved, by introducing the quantities $\Phi = \phi^2$, $\Psi = \psi^2$, $\mathbf{R} = \sum_{\alpha\beta} \phi^\alpha q_{\alpha\beta} \psi^\beta$, and $\mathbf{Q} = \sum_{\alpha\beta} q_{\alpha\beta}^2$. Denoting the saddle point values with a subscript 0, we obtain

$$\frac{\Phi_0}{2d} = \frac{\frac{1}{2}\Phi_0^2 + \sqrt{\lambda-1}\mathbf{R}_0}{\mathcal{D}_0} \quad (23)$$

$$\frac{\mathbf{R}_0}{2d} = \frac{(\lambda-1)\mathbf{R}_0 + \sqrt{\lambda-1}\Phi_0^2}{\mathcal{D}_0} \quad (24)$$

$$\frac{\mathbf{Q}_0}{2d} = \frac{(\lambda-1)\mathbf{Q}_0 + \sqrt{\lambda-1}\mathbf{R}_0}{\mathcal{D}_0} \quad (25)$$

together with $\Phi_0 = \Psi_0$. In equations (23–25), the denominator is given by

$$\mathcal{D}_0 = \frac{\Phi_0^2}{4} + \sqrt{\lambda-1}\mathbf{R}_0 + \frac{(\lambda-1)}{2}\mathbf{Q}_0. \quad (26)$$

One then gets

$$\omega_0(\lambda) = \frac{\Phi_0}{2d} + \frac{\mathbf{Q}_0}{4d} - \text{Log} \mathcal{D}_0. \quad (27)$$

At this point, one has to resort to a numerical solution of the saddle point equations. Note that the possible solutions obey simple equalities or inequalities, such as: $\Phi_0, \mathbf{Q}_0 > 0$, $\Phi_0 + \mathbf{Q}_0 = 4d$, $\mathbf{R}_0^2 = \mathbf{Q}_0 \Phi_0^2$.

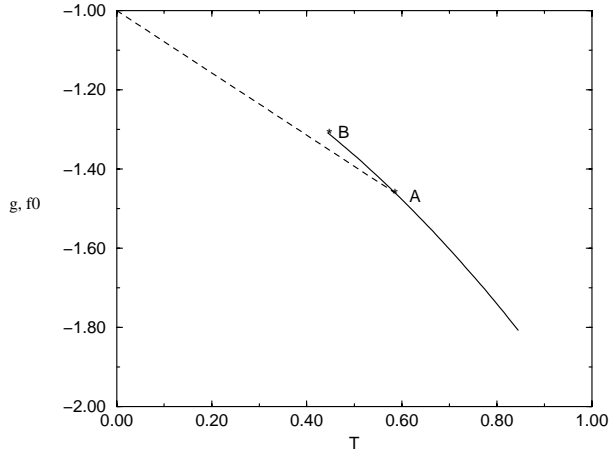


Fig. 1. The free energy f as a function of temperature. The saddle point result f_0 (full line) crosses the free energy g of the fully adsorbed phase (hatched line) at point A ($T = T_3 \sim 0.58$). Branch AB is metastable (see text).

Our results can be interpreted in two ways. They first describe the (thermal) properties of two HP coupled *via* equation (19): $\text{Log}\mathcal{Z}(\lambda) = -N\omega(\lambda)$ is then, up to a temperature factor, the free energy (with $\lambda = e^\beta$). On the other hand, a Legendre transformation with respect to $\text{Log}\lambda$, gives information on the number N_{12} of common bonds between the HP, *i.e.* on their overlap properties. For convenience, we define $N_{12} = Nq$, and

$$\Theta(q) = \oint \frac{d\lambda}{2i\pi\lambda} \mathcal{Z}(\lambda) \lambda^{-Nq}. \quad (28)$$

A saddle point evaluation of equation (28) gives

$$q = -\frac{\partial\omega(\lambda)}{\partial\text{Log}\lambda}. \quad (29)$$

Using equations (23–27), we obtain

$$q_0 = \frac{\lambda}{\lambda - 1} \frac{Q_0}{4d}. \quad (30)$$

We now present our results along both ways.

4.1 Thermal properties of the coupled Hamiltonian paths

Unless otherwise specified, our results are given for $d = 3$, and the main parameter of this section is the temperature T ($T = \frac{1}{\text{Log}\lambda}$). The saddle point equations (23–27) yield the free energy $f_0(T) = T\omega_0(e^{\frac{1}{T}})$ as a function of T (see Fig. 1).

Solving numerically the above equations, we get the following results

$$1) T_1 = \infty$$

In this case, we find a finite fraction of common bonds $q_0^{(1)} = \frac{1}{d} = \frac{1}{3}$. This value corresponds to a random choice

of a common bond among the $d = 3$ lattice dimensions, and is the smallest possible value q_m of the overlap.

$$2) T_2 = \frac{1}{\text{Log}(d+1)} \simeq 0.7213$$

One then has $\Phi_0 = Q_0 = 2d = 6$. This point is in some sense a disorder point [10] where the values of Φ_0 (linked to the entropy of a single HP) and Q_0 (linked to the overlap of the two HP) cross. It corresponds to an overlap $q_0^{(2)} = \frac{d+1}{2d} = \frac{2}{3}$.

$$3) T_3 \simeq 0.5846: \text{ the complete adsorption transition.}$$

At this point, the two HP system “freezes” into a single HP: one may also say that one chain gets fully adsorbed onto the other. This total adsorption is due to the strong topological constraints imposed by the chain connectivity and the full compactness of the HP. As a result, it is impossible for two chains to have a large overlap and differ only by small “bubbles” while filling up the whole space.

Of course, the entropy does not vanish below T_3 , but becomes equal to the entropy of a single HP, see equation (7). Note that this solution is not a saddle point solution. It must nevertheless be taken into account, since its free energy per monomer which reads

$$g(T) = -1 - T \text{Log} \left(\frac{z}{e} \right) \quad (31)$$

is an upper bound (see Eq. (20)). The transition temperature T_3 is thus defined by $g(T_3) = f_0(T_3)$ (see point A of Fig. 1). The mechanism of this first order freezing transition is analogous to the one studied in reference [11], in the context of polymer crystallization. Note that q jumps from $q_0^{(3)} \simeq 0.7572$ to $q = 1$ across the transition. From a thermodynamic point of view, we have thus found that the overlap fraction of two HP has a maximum value $q_M \simeq 0.7572$, beyond which the two HP coincide. The intuitive image of two HP differing by finite independent “bubbles” does not hold, due to the topological frustration.

Note that, as the space dimension d increases, the adsorption temperature T_3 decreases. In particular, the transition does not occur for the fully connected graph ($d \rightarrow \infty$).

4) In the present mean field description, one may continue the high temperature branch of the free energy $f_0(T)$ beyond the full adsorption point. This continuation implies the existence of a metastable state. As in reference [11], a particular temperature T_4 may be defined, where the entropy $s_0(T) = -\frac{\partial f_0(T)}{\partial T}$ equals that of a single HP

$$s_0(T_4) = \text{Log} \left(\frac{z}{e} \right) \quad (32)$$

leading to $T_4 \simeq 0.4350$, and in turn to $q_0^{(4)} \simeq 0.9627$. From a physical point of view, one can argue that the entropy of the two coupled HP system is bounded by the entropy of a single HP: temperature T_4 (*i.e.* point B of Fig. 1) can then be identified to a limit of metastability. We do not have a clear understanding of the metastable branch (note in particular that $q_0^{(4)} \neq 1$), and more work is needed on this point.

4.2 Overlaps and Legendre transform

As previously mentioned, our results can also be interpreted in terms of the overlap properties of the two HP. A convenient function to characterize these properties is the overlap probability distribution $\mathcal{P}(q)$ defined as

$$\mathcal{P}(q) = \frac{1}{\mathcal{N}^2} \sum_{(HP_1, HP_2)} \delta(N_{12} - Nq) \quad (33)$$

where \mathcal{N} is given in equation (7) and N_{12} is the number of common bonds of the HP. Equations (28, 33) imply that

$$\mathcal{P}(q) = \frac{1}{\mathcal{N}^2} \Theta(q). \quad (34)$$

From a strictly thermodynamic point of view, we have the result that the overlap probability distribution $\mathcal{P}(q)$ is defined only for $q_m < q < q_M$, and for $q = 1$. The existence of a metastable branch beyond q_M is not easy to interpret: the saddle point evaluation (29) of the Legendre transform (28) then becomes ill-defined, since $\lambda(q)$ becomes a multi-valued function.

For $q_m < q < q_M$, the relation between λ (*i.e.* temperature) and q (*i.e.* overlap) can be inverted through equation (29). There is thus a one to one correspondence between overlap and temperature in the region $1 < \lambda < \lambda_3 = e^{\frac{1}{73}} \simeq 5.532$. The thermal properties of the coupled system imply that, for $1 < \lambda < \lambda_3$, we have $\mathcal{P}(q) = \delta(q_0 - q)$, where q_0 is given by equation (30). On the other hand, for $\lambda > \lambda_3$, we have $\mathcal{P}(q) = \delta(1 - q)$.

Another quantity of interest is the entropy, considered as a function of the overlap q . It is given by

$$s(q) = \frac{1}{N} \text{Log} \Theta(q). \quad (35)$$

Performing the saddle point evaluation on λ in equation (28), we get

$$s_0(q) = -\omega_0(\lambda) - q \text{Log} \lambda \quad (36)$$

where $\lambda = \lambda(q)$ is given by equation (30). The phase transition for $q = q_M$ can be interpreted (see Fig. 2) as a Maxwell construction since the results of the previous section can be rewritten as

$$s_0(q_M) - s_0(1) = (1 - q_M) \text{Log} \lambda_3. \quad (37)$$

Beyond the homogeneous saddle point approximation, our results in the region $q_M < q < 1$ are coherent with a phase coexistence picture between a fraction x of the phase $q = q_M$ and a fraction $1 - x$ of the fully adsorbed phase $q = 1$. Such a phase coexistence will give rise to an effective overlap $q_M < q_{\text{eff}} = xq_M + (1 - x) < 1$. Note that this picture is different from that of finite bubbles mentioned in Section 4.1: here, the phase coexistence involves macroscopic domains of overlap 1 and q_M .

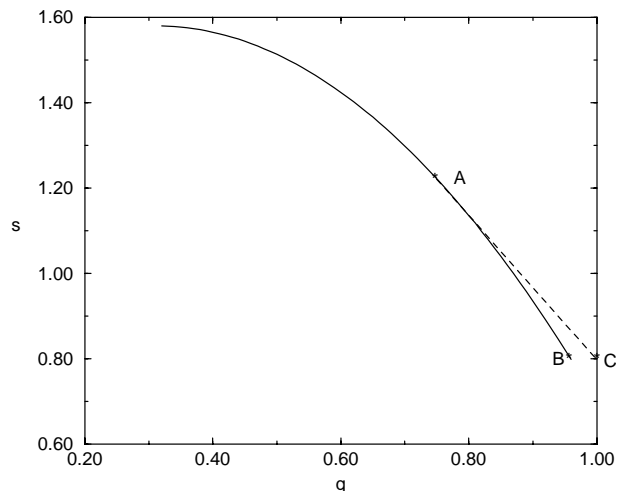


Fig. 2. The entropy $s(q)$ as a function of the overlap q . The full line denotes the saddle point result $s_0(q)$; the hatched line is the result of the Maxwell construction with the fully adsorbed state. Note that AB corresponds to the metastable branch of Figure 1.

5 Conclusion

We have considered the overlap and/or thermal properties of two coupled Hamiltonian paths (HP), in a homogeneous saddle point approximation. We have found (for $d = 3$) a discontinuous phase transition at finite coupling, between an entropy dominated phase and a completely adsorbed phase. At the transition, the overlap between the HP jumps from $q_M \simeq 0.7572$ to $q = 1$. Our results may be relevant in a proteic context (NMR, structure alignment). If the number of constraints exceeds a certain threshold, the existence of q_M suggests that a single spatial structure may survive. For longer polymers, the existence of a first order transition, raises many questions (metastability, glass transition...).

The influence of the fluctuations on these results is difficult to assess, and we appeal to a related problem. In reference [11], we have studied the crystallization transition of a semi-flexible HP using (i) a homogeneous saddle point (ii) a low temperature expansion. Approximation (i) yields a first order transition between a liquid phase and a frozen solid (with zero entropy per monomer), quite reminiscent of the full adsorption transition that we find here for $T = T_3$. On the other hand, approximation (ii) leads to an almost frozen solid (with an exponentially small, albeit finite, entropy per monomer). The critical temperature is also slightly changed, but the liquid-solid transition remains discontinuous. A naive transposition of the results of (ii) to the present model would give a first order transition (*i.e.* with a jump in the overlap q) towards a non fully adsorbed low temperature phase (q exponentially close to 1). This point is currently under study.

Finally, we remark that the coupled chains system of this paper undergoes a phase transition at a finite value of the coupling constant λ , whereas in spin glasses, the two

replica system undergoes a (spin glass) transition when the coupling constant vanishes [3,4].

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