Long–Range Frustrations in a Spin–Glass Model of the Vertex–Cover Problem

Haijun Zhou[1,2]

[1]Max-Planck-Institute of Colloids and Interfaces, 14424 Potsdam, Germany

[2]Institute of Theoretical Physics, the Chinese Academy of Sciences, Beijing 100080, China

November 3, 2004

Abstract

Long–range frustrations among distantly separated vertices are shown to exist in finite–connectivity spin–glass systems. A cavity–field–motivated method is suggested to tackle such long–range frustrations and is applied in studying the NP–complete vertex–cover problem as a spin–glass model. The ground–state energy of this model is analytically predicted; it is in full agreement with known exact enumeration results and with a rigorous mathematical asymptotic formula. A correct mean–field finite-connectivity spin–glass theory should take long–range frustrations into account.

PACS number: 75.10.Nr, 89.75.-k, 05.20.-y, 02.10.Ox

The cavity–field formalism [1] represents a major breakthrough in the mean–field theory of finite–connectivity Viana–Bray spin–glass models [2]. In the cavity–field formalism, microscopic configurations in a spin–glass system are grouped into different macroscopic states (hereafter, a macroscopic state is simply referred as a 'state' and a microscopic configuration as a 'configuration'). In a state α each vertex i feels a cavity field $h_i(\alpha)$, and the fluctuation of this field among all the states is characterized by a probability distribution $P_i(h_i)$. The physical picture behind the cavity–field formalism is simple: the energy landscape of a spin–glass system is far from being smooth. There are exponentially many metastable domains in the configurational space; these domains are mutually separated from each other by high energy barriers that approach infinity for large system size.

The zero–temperature limit of this cavity–field formalism [3] is especially interesting, as it is deeply connected to NP-complete combinatorial optimization problems (COPs) in computer science [4]. Examples of NP-complete COPs include the satisfiability problem, the vertex cover problem, and the graph coloring problem. They are very hard in the sense that finding a solution to such a problem may need a computation time that scales exponentially with the problem size N. Recently, many NP-complete COPs are mapped into some equivalent spin–glass problems and solved to some extent by cavity–field method [5, 6, 7, 8].

However, one fundamental physical point is missing in the cavity–field formalism, namely long–range frustrations among distantly separated vertices. In the cavity–field formalism, in a given state, the cavity fields on randomly chosen vertices of a spin–glass system are assumed to be uncorrelated to each other. However, as we show in this paper, this assumption is physically wrong. There are long–range frustrations among some vertices of a spin–glass system. A correct mean–field spin–glass theory therefore must take these long–range frustrations into account. Consider the zero–temperature cavity–field theory for a spin–glass system. In a given minimum–energy state α, some of the vertices are frozen in the sense that their spin variables are fixed to the same value in in all configurations that belong to α; the remaining vertices are unfrozen, their spins can change values in different configurations of α. When long–range frustration is concerned those frozen vertices are of no interest, since their values are already fixed. However, two unfrozen vertices i and j, even when they are far apart from each other, may have their spin values strongly correlated. For example, it may happen that vertex j

could only take the spin value $\sigma_j = +1$ in *all* those configurations of state α where the spin value of vertex i is $\sigma_i = -1$.

This paper focuses on such long-range frustrations among unfrozen vertices. A *frustration index* R is defined to quantify the above–mentioned physical frustration picture. The calculation is demonstrated by working on an equivalent spin–glass model [8] of the NP-complete vertex–cover problem [9, 10, 11]. For the vertex–cover model, we show that R become positive when the mean vertex–degree c of the underlying random graph exceeds $c = e = 2.7183$. Previously it was already revealed that the condition $c \geq e$ marks the breaking of replica symmetry in this spin–glass system [9, 10, 8]. Here we see that it also marks the onset of long–range frustrations. After including the effect of long–range frustrations, an estimation of the minimal vertex–cover size is made and is found to be in agreement with exact enumeration results of Weigt and Hartmann [9, 10] and with a rigorous asymptotic result of Frieze [12]. The method of this work can be extended to other NP-complete COPs and to finite–connectivity spin–glass systems in general. Results on the random–graph 3–satisfiability problem [13, 5, 6] and the graph coloring problem [7] will be reported elsewhere[14]. The excellent agreement between our analytical result and the exact enumeration results also raises the hope that, an exact mean-field theory for spin–glasses on random-graphs might be achieved by incorporating long-range frustrations into the cavity–field formalism. Efforts along this line are currently being made by the present author.

We begin with a brief re-introduction of random graph and the vertex–cover problem. A random graph $G(N, c)$ has N vertices $V = \{1, 2, \cdots, N\}$. Between any two vertices an edge is present with probability $c/(N-1)$ and absent with probability $1 - c/(N-1)$. The average number of edges incident to a randomly chosen vertex is c (the mean vertex–degree); and for large graph size N, the number k of edges associated with a given vertex obeys the Poisson distribution $P_c(k) = e^{-c}c^k/k!$ [15]. Denote $E(G)$ as the edge set of graph G. A vertex cover of G consists of a set of vertices $\Lambda = \{i_1, i_2, \cdots, i_m\}$, with the property that if edge $(i, j) \in E(G)$, then either $i \in \Lambda$ or $j \in \Lambda$ or both. The vertex–cover problem consists of finding a vertex cover Λ such that its size $|\Lambda| \leq n_0$, with n_0 being a pre-given integer number. This problem can be mapped to a spin–glass model with an energy functional

$$E[\{\sigma_i\}] = -\sum_{i=1}^{N} \sigma_i + \sum_{(i,j)\in E(G)} (1 + \sigma_i)(1 + \sigma_j). \tag{1}$$

The spin on vertex i takes $\sigma_i = -1$ if $i \in \Lambda$ (covered) or $\sigma_i = +1$ if $i \notin \Lambda$ (uncovered). It was shown in Ref. [8] that the ground–energy configurations of model (1) correspond to vertex cover patterns with the global minimum size.

We now begin to examine long-range frustrations in the ground–energy configurations of Eq. (1). For a random graph of $N \to \infty$, there can exist an exponential number of ground–energy configurations for model (1). Following the cavity–field formalism [3], these configurations are grouped into different states. A state of the system includes many configurations. These configurations all have the same minimum energy; and any two configurations in this state are mutually reachable by flipping a finite number of spins in one configuration and then letting the system relax. Let us focus on one state, say α. In state α, a randomly chosen vertex i may have its spin fixed to $\sigma_i \equiv +1$ in all configurations of α. In this case we say vertex i feels a positive cavity field ($h_i = 1$) [8]. It may happen that $\sigma_i \equiv -1$ in all configurations of α. Then we say that vertex i feels a negative cavity field ($h_i \leq -1$). It may also happen that $\sigma_i = +1$ in *some* configurations of α and $\sigma_i = -1$ in other configurations of α. Then we say that vertex i is unfrozen and feels a zero cavity field ($h_i = 0$). A randomly chosen vertex has probability q_+, q_-, and q_0, respectively, to have positive, negative, and zero cavity field.

Since a unfrozen vertex i will have its spin value fluctuates among configurations of state α, the 'correlation length' of this fluctuation needs to be investigated. Let us ask the following question: if we fix the spin value of vertex i to $\sigma_i = -1$ in all configurations of state α, how many spin values will eventually be fixed as a consequence?

For a random graph with infinite size N, the total number of affected vertices may reach infinity. If this happens, vertex i is referred to as a type-I unfrozen vertex. The probability for this to happen is denoted as R (this is the definition for our frustration index). The total number of affected vertices may also be finite and has probability $f(s)$ to take integer value s. In this case, vertex i is a type-II unfrozen vertex. Obviously, $R = 1 - \sum_{s=0}^{\infty} f(s)$. Based on insights gained from studies on random graphs [15], we know that, if $R > 0$, all those type-I unfrozen vertices will form a *connected* giant percolation cluster and their spin values are therefore strongly correlated. If we randomly choose two type-I unfrozen vertices i and j, then with probability one-half their spin values can be -1 simultaneously in a configuration of state α. however, with probability one-half their spin values could not be -1

simultaneously: if $\sigma_i = -1$, then σ_j must be $+1$; and if $\sigma_j = -1$, then σ_i must be $+1$.

On the other hand, two randomly selected type-II unfrozen vertices are mutually independent, since each vertex can only influence the spin values of $s \sim O(1)$ other vertices [15]. Our frustration index R therefore quantifies how strongly correlated are two randomly selected unfrozen vertices.

The task now is to find an expression for R. In our present vertex–cover problem, we can proceed according to the following way. Suppose vertex i is type-II unfrozen, and denote V_i as the set of its nearest-neighbors. There are two possibilities concerning vertices in V_i: (i) all of these vertices have cavity fields $h \leq 0$ [1] two or more of them are type-I unfrozen, among which one vertex j_1 is in conflict with all the other vertices j_2, i.e., $\sigma_{j_1}\sigma_{j_2} = -1$ in all configurations of state α. (ii) one vertex has positive cavity field, and all the others have non-positive cavity fields and no long–range frustrations among them. Situation (i) occurs with probability p_1, with p_1 being expressed as

$$\begin{aligned} p_1 &= \frac{1}{q_0}\sum_{k=2}^{\infty} P_c(k) \sum_{l=2}^{k} C_k^l (q_0 R)^l (q_- + q_0(1-R))^{k-l} \left(\frac{1}{2}\delta_l^2 + \frac{l}{2^{l-1}}(1-\delta_l^2)\right) \\ &= cR\exp(-c(q_+ + q_0 R))(\exp(cq_0R/2) - 1 - cq_0R/4), \end{aligned} \tag{2}$$

where $C_k^l = k!/[l!(k-l)!]$ is binomial coefficient.

On the other hand, for a vertex i that is frozen to $\sigma_i \equiv +1$ and therefore $h_i > 0$, the probability p_2 for *all* its nearest–neighbors not to be type-I unfrozen is

$$\begin{aligned} p_2 &= \frac{\sum\limits_k P_c(k)(q_- + q_0(1-R))^k}{\sum\limits_k P_c(k)\sum\limits_{l=0}^{k} C_k^l (q_0R)^l (q_- + q_0(1-R))^{k-l}(\delta_l^0 + \frac{1}{2^{l-1}}(1-\delta_l^0))} \\ &= (2\exp(cq_0R/2) - 1)^{-1}. \end{aligned} \tag{3}$$

With these preparations, one can derive the following self-consistent equation for the probability distribution $f(s)$ of the number of affected vertices:

$$f(s) = p_1\delta_s^1 + (1-p_1)\sum_{l=0} P_{c'}(l) \sum_{s_1,\ldots,s_l} f(s_1)\ldots f(s_l)\delta_{s_1+\ldots s_l}^{s-2}. \tag{4}$$

[1] Notice that the cavity field on a nearest–neighboring vertex of vertex i is calculated by first removing i and all its incident edges from the network.

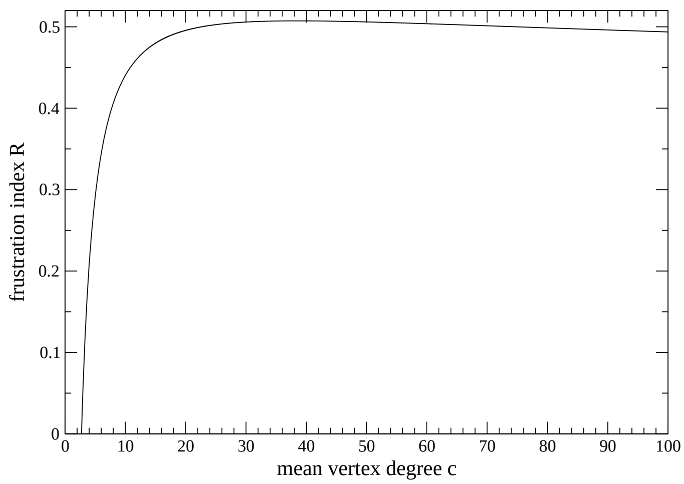

Figure 1: The frustration index R as a function of mean vertex degree c calculated according to Eq. (5).

In Eq. (4), $c' = cq_0(1-R)$. c' is the mean number of nearest–neighboring type-II unfrozen vertices that are reachable from a vertex of positive cavity field.

Since $R = 1 - \sum_{s=0}^{\infty} f(s)$, from Eq. (4) we know that the frustration index R is determined by the following self-consistent equation:

$$R = (1-p_1)(1-\exp[-cq_0 R(1-R)]). \tag{5}$$

Equation (5) is the main result of this paper. A positive R signifies the appearance of a percolation cluster of vertices whose spin values are strongly correlated.

Figure 1 shows the value of the frustration index R as a function of the mean vertex-degree c. When the mean vertex-degree $c \leq e = 2.7183$, one finds that $R \equiv 0$, and the system is not frustrated. This is consistent with the work of Bauer and Golinelli [16] that a minimal vertex cover pattern can be found by an polynomial leaf-removal algorithm. When $c > e$, a finite fraction of the unfrozen vertices vertices are frustrated. At mean vertex degree $c \simeq 40$, the frustration index reaches a maximal value that slightly exceeds 0.5; then it gradually decays to zero as $c \to \infty$. This behavior is consistent with the intuition that long-range frustrations are caused by the formation of long-

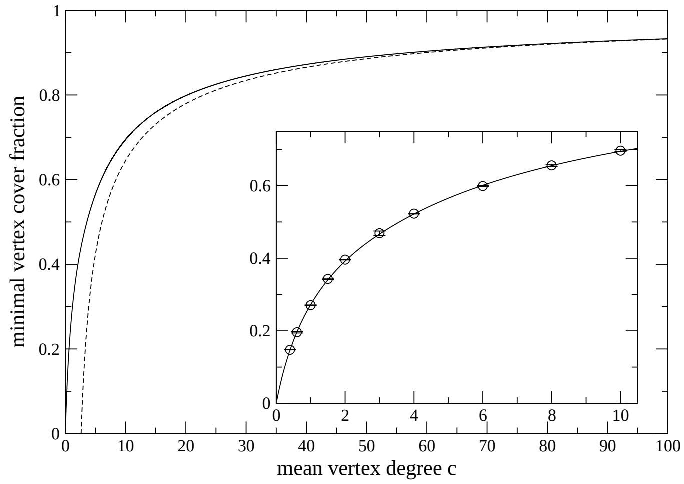

Figure 2: The minimal vertex cover fraction X_{min} (solid line) as a function of mean vertex degree c predicted by Eq. (8) and the comparison with the asymptotic relationship given in Ref. [12] (dashed line). (Inset) The solid line corresponds to Eq. (8) and the circular symbols are exact enumeration results of Weigt and Hartmann [9, 10].

distance loops, and for an infinitely connected graph there is no such loops as the geodesic distance between any two vertices is of order unity.

After taking into account this kind of long-range frustrations, the expressions for q_+ and q_0 can also be easily obtained, and $q_- = 1 - q_+ - q_0$. The expressions for q_+ and q_0 are

$$q_+ = 2\exp(-c(q_+ + q_0 R/2)) - \exp(-c(q_+ + q_0 R)), \tag{6}$$

$$q_0 = c\exp(-c(q_+ + q_0 R))((2q_+ + q_0 R)\exp(\frac{c q_0 R}{2}) - q_+ - q_0 R - \frac{c q_0^2 R^2}{4})) \tag{7}$$

The fraction of vertices that are covered in a minimal vertex cover is expressed as

$$X_{\mathrm{min}} = 1 - q_+ - \frac{q_0}{2}. \tag{8}$$

Figure 2 shows the relationship between X_{min} and mean vertex degree c. At large c values, Eq. (8) is in agreement with a rigorous asymptotic expression given by Frieze [12]. At low values of mean vertex degree c, Eq. (8)

is in agreement with the exact enumeration results of Weigt and Hartmann [9, 10]. These excellent agreements indicate that the present analytical prediction Eq. (8) might be exact for the vertex–cover problem. If long–range frustrations were not taken into account, we know [8] that the cavity–field method could not predict the correct minimal vertex–cover size, even when the appearance of many minimum–energy states were considered.

In summary, in this paper we suggested that long–range frustrations are important in understanding the statistical physics of finite–connectivity spin glasses. We were able to integrate the effects of such long–range frustrations into a frustration index R of positive value. The essence of our method to focus on those vertices that are unfrozen in a given macroscopic state of a spin–glass system. As a simple application of our method, the NP-complete vertex–cover problem on random graphs was studied as a spin–glass model; our analytical results were in exciting agreement with known numerical and mathematical results. Our method is of cause applicable to other finite–connectivity spin–glass models. In another manuscript [14] we report our calculations on long–range frustrations in the random K-satisfiability problem [13, 5, 6] and in the $\pm J$ finite–connecivity Viana–Bray spin glass model [2].

We emphasize that the appearance of many macroscopic states in the energy landscape of a system not necessarily mean that there exist long–range frustrations in a single macroscopic state. As an counter–example, in the matching problem studied in [17] there is no long–range frustrations ($R \equiv 0$) but there exist an exponential number of macroscopic states. It is interesting to notice that the matching problem is not NP-complete. Might the existence of long–range frustrations be a necessary (and sufficient) condition for NP-completeness? We believe that the present work will stimulate the designing of better algorithms for NP-complete combinatorial optimization problems.

On the other hand, we believe that the existence of long–range frustrations will always mean the existence of many macroscopic states. The proof of this conjecture, however, may be extremely challenging.

This paper focuses on long-range frustrations and therefore pays no attention to the fact that the energy landscape of a spin–glass system is actually multi–valleyed with high energy barriers. Therefore, it can not correctly predict all the behavior of a spin–glass system. In the vertex–cover problem, for example, Fig. 3 shows the comparison of the analytical backbone size of a minimal

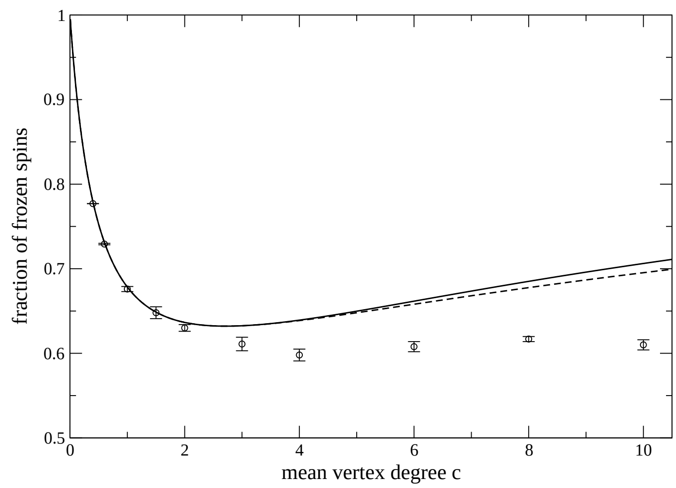

Figure 3: Fraction of frozen vertices in *one* ground–energy macroscopic state of the vertex–cover problem (the solid line) and the fraction of vertices that are frozen in *all* ground-energy macroscopic state. Dashed line corresponds the case when the frustration index R is set to $R = 0$.

vertex cover, $q_+ + q_-$, with simulation results of Weigt and Hartmann [10]. The apparent disagreement is due to the fact that, in the present work only one ground–energy macroscopic state is considered, while in the simulation all the ground–energy macroscopic states are considered. A vertex that is covered in one macroscopic state may be uncovered or unfrozen in another macroscopic state. A full mean–field theory of finite–connectivity spin–glass theory needs to combine long–range frustrations of each macroscopic state with the existence of (exponentially) many macroscopic states. In principle this task should be achievable under the framework of the cavity–field formalism. Such a program is currently under investigation by the present author. A systematic report on this combination will be reported elsewhere.

The author is deeply grateful to Reinhard Lipowsky, Zhong-Can Ou-Yang, and Lu Yu for their encouragement and kind support. This work benefits from a stimulating discussion with Lu Yu on spin glasses and from many helpful discussions with Reinhard Lipowsky on complex networks.

References

[1] Mézard, M & Parisi, G. (2001) *Eur. Phys. J. B* **20**, 217–233.

[2] Viana, L & Bray, A. J. (1985) *J. Phys. C: Solid State Phys.* **18**, 3037–3051.

[3] Mézard, M & Parisi, G. (2003) *J. Stat. Phys.* **111**, 1–34.

[4] Garey, M & Johnson, D. S. (1979) *Computers and Intractability: A Guide to the Theory of NP-Completeness.* (Freeman, San Francisco).

[5] Mézard, M, Parisi, G, & Zecchina, R. (2002) *Science* **297**, 812–815.

[6] Mézard, M & Zecchina, R. (2002) *Phys. Rev. E* **66**, 056126.

[7] Mulet, R, Pagnani, A, Weigt, M, & Zecchina, R. (2002) *Phys. Rev. Lett.* **89**, 268701.

[8] Zhou, H. (2003) *Eur. Phys. J. B* **32**, 265–270.

[9] Weigt, M & Hartmann, A. K. (2000) *Phys. Rev. Lett.* **84**, 6118–6121.

[10] Weigt, M & Hartmann, A. K. (2001) *Phys. Rev. E* **63**, 056127.

[11] Hartmann, A. K & Weigt, M. (2001) *Theo. Comput. Sci.* **265**, 199–225.

[12] Frieze, A. M. (1990) *Discrete Math.* **81**, 171–175.

[13] Biroli, G, Monasson, R, & Weigt, M. (2001) *Eur. Phys. J. B* **14**, 551–568.

[14] Zhou, H. (2004) Long range frustration in finite–connectivity spin glasses: Application to the random k-satisfiability problem (submitted to New Journal of Physics on November 03, 2004).

[15] Bollobás, B. (1985) *Random Graphs.* (Academic Press, Landon).

[16] Bauer, M & Golinelli, O. (2001) *Eur. Phys. J. B* **24**, 339–352.

[17] Zhou, H & Ou-Yang, Z.-C. (2003) Maximum matching on random graphs (e-print: cond-mat/0309348).