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

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Supplementary text

This supplementary text contains the technical details of the article.

We first derive Eq. (2), Eq. (3), and Eq. (4). In what follows, we focus on one macroscopic state α of ground–state energy. When we mention that a vertex is unfrozen (or frozen), what it really means is that this vertex is unfrozen (or frozen) in state α.

Consider the minimal vertex cover problem on a random graph $G(N, c)$. The fraction of unfrozen, positively frozen, and negatively frozen vertices of this graph G is respectively q_0, q_+, and q_- in state α. As one way of deriving Eqs. (2), (3), and (4), we proceed by adding a new vertex i into the system and connecting it to k randomly chosen vertices of graph G, where k is a random integer following the Poisson distribution $P_c(k)$ with mean c. The enlarged graph is denoted as G', and the set of nearest neighbors of vertex i is denoted as V_i.

In the original graph G and in state α, the number of unfrozen, positively frozen, and negatively frozen vertices is denoted as N_0, N_+, and N_-, respectively. When N is large, to leading order of N we have

$$
\begin{aligned}
N_0 &= N q_0 + o(N) \ , \\
N_+ &= N q_+ + o(N) \ , \\
N_- &= N q_- + o(N) \ .
\end{aligned}
\tag{S1}
$$

Since the k vertices in set V_i are randomly chosen from the N vertices of graph G, the probability that in graph G k_0 of them are unfrozen, k_+ of them are positively frozen, and k_- of them are negatively frozen is equal to

$$
\frac{C_{N_0}^{k_0} C_{N_+}^{k_+} C_{N_-}^{k_-}}{C_N^k} \delta_{k_0+k_++k_-}^{k} \ , \tag{S2}
$$

where $C_k^l = k!/(l!(k-l)!)$ is the Binomial coefficient and δ is the Kronecker symbol. When N is sufficiently large, we can insert Eq. (S1) into Eq. (S2) and then use Stirling's formula to rewrite Eq. (S2) in the following form:

$$\frac{k!}{k_0!k_+!k_-!} q_0^{k_0} q_+^{k_+} q_-^{k_-} \delta_{k_0+k_++k_-}^{k} \ . \tag{S3}$$

Since the newly added vertex i has probability $P_c(k)$ to have k nearest neighbors, then based on Eq. (S3) we know that the probability of vertex i to be connected to k_0 unfrozen, k_+ positively frozen, and k_- negatively frozen vertices of graph G is equal to

$$\frac{e^{-cq_0}(cq_0)^{k_0}}{k_0!} \frac{e^{-cq_+}(cq_+)^{k_+}}{k_+!} \frac{e^{-cq_-}(cq_-)^{k_-}}{k_-!} = P_{cq_0}(k_0)\ P_{cq_+}(k_+)\ P_{cq_-}(k_-) \ , \tag{S4}$$

where, as before, $P_\lambda(m)$ is the Poisson distribution with mean λ: $P_\lambda(m) = e^{-\lambda}\lambda^m/m!$.

A randomly chosen unfrozen vertex has probability R to be type-I unfrozen. Among the k_0 unfrozen vertices that are connected to vertex i, the probability that k_0' of them are type-I unfrozen and k_0'' of them are type-II unfrozen is equal to

$$\frac{k_0!}{k_0'!k_0''!} R^{k_0'}(1-R)^{k_0''} \delta_{k_0'+k_0''}^{k_0} \ . \tag{S5}$$

Combining Eqs. (S4) and (S5), we know the probability $P^{(i)}(k_0', k_0'', k_+, k_-)$ that vertex i is connected to k_0' type-I unfrozen, k_0'' type-II unfrozen, k_+ positively frozen, and k_- negatively frozen vertices of graph G is

$$P^{(i)}(k_0', k_0'', k_+, k_-) = P_{cq_0R}(k_0')\ P_{cq_0(1-R)}(k_0'')\ P_{cq_+}(k_+)\ P_{cq_-}(k_-) \ . \tag{S6}$$

In the case that $k_0' \geq 1$ for vertex i, these k_0' type-I unfrozen vertices of graph G could be divided into two subgroups: the vertices in each subgroup can take the spin value -1 simultaneously in state α; while if any vertex in one subgroup is taking the spin value -1, then *all* the vertices in the other subgroup must take the spin value $+1$. The probability that one of these two subgroups is empty, namely the probability that all these k_0' type-I unfrozen vertices take the spin value -1 simultaneously in some configurations of state α, is equal to

$$\delta_{k_0'}^{1} + (1-\delta_{k_0'}^{1}) \frac{1}{2^{k_0'-1}} \ ; \tag{S7}$$

similarly, the probability that one of these two subgroup contains $k_0' - 1$ vertices while the other subgroup contains just one vertex, namely the probability that $k_0' - 1$ of these type-I unfrozen vertices (but not all of them) take the spin value -1 simultaneously in some configurations of state α, is equal to

$$\delta_{k_0'}^2 \frac{1}{2} + (1 - \delta_{k_0'}^1 - \delta_{k_0'}^2) \frac{k_0'}{2^{k_0'-1}} \ . \tag{S8}$$

When the new vertex i is connected to the set V_i of vertices of graph G, to lower the energy of the enlarged graph G', the spin values on some vertices in the set V_i may have to be changed. These spin flips may in turn cause the spin flips of some next-to-nearest neighbors of vertex i, and so on. However, since the original system is in state α and the addition of vertex i is only a local perturbation, this perturbation will not cause the system to overcome the large energy barrier and jump to another macroscopic state. Therefore, when the original system on graph G is in state α, for each vertex in graph G', we can determine whether it is unfrozen or (positively or negatively) frozen by studying the perturbation effect of the new vertex i on state α of graph G.

For the newly added vertex i to be positively frozen, it must have no nearest neighbors that are positively frozen in graph G (that is, $k_+ = 0$); and furthermore, all its k_0' nearest neighbors that are type-I unfrozen in graph G must be in the same subgroup (capable of taking the spin value -1 simultaneously in graph G). Therefore, based on Eqs. (S6) and (S7), we know that the probability for vertex i to be positively frozen in graph G' is

$$\begin{aligned} q_+(i) &= P_{cq_+}(0) P_{cq_0 R}(0) + P_{cq_+}(0) \sum_{k_0'=1}^{\infty} P_{cq_0 R}(k_0') \big(\delta_{k_0'}^1 + (1 - \delta_{k_0'}^1) \frac{1}{2^{k_0'-1}} \big) \\ &= 2 e^{-cq_+ - cq_0 R/2} - e^{-cq_+ - cq_0 R} \ . \end{aligned} \tag{S9}$$

Similarly, for the newly added vertex i to be unfrozen in graph G', its nearest neighbors must fulfill either one of the following constraints: (a) one of its nearest neighbors are positively frozen in graph G ($k_+ = 1$), and all of its k_0' nearest neighbors that are type-I unfrozen in graph G belong to the same subgroup (capable of taking the spin value -1 simultaneously in graph G); or (b) none of its nearest neighbors are positively frozen in graph G ($k_+ = 0$)

and there are $k'_0 \geq 2$ nearest neighbors that are type-I unfrozen in graph G, $k'_0 - 1$ of which belong to the same subgroup and the remaining one belongs to the other subgroup ($k'_0 - 1$ of these vertices (but not all of them) are capable of taking the spin value -1 simultaneously in graph G). Therefore, based on Eqs. (S6), (S7), and (S8), we know that the probability for vertex i to be unfrozen in graph G' is

$$\begin{aligned} q_0(i) =& P_{cq_+}(1) P_{cq_0 R}(0) + P_{cq_+}(1) \sum_{k'_0=1}^{\infty} P_{cq_0 R}(k'_0) \big(\delta^1_{k'_0} + (1 - \delta^1_{k'_0}) \frac{1}{2^{k'_0 - 1}} \big) \\ &+ P_{cq_+}(0) \sum_{k'_0=2}^{\infty} P_{cq_0 R}(k'_0) \big(\delta^2_{k'_0} \frac{1}{2} + (1 - \delta^2_{k'_0}) \frac{k'_0}{2^{k'_0 - 1}} \big) \\ =& \big(2cq_+ + cq_0 R \big) e^{-cq_+ - cq_0 R/2} - \big(cq_+ + cq_0 R + (cq_0 R)^2/4 \big) e^{-cq_+ - cq_0 R} \ . \end{aligned} \tag{S10}$$

In the limit of $N \to \infty$, we assume that the unfrozen/frozen probabilities of a vertex in graph G' will converge to those of a vertex in graph G; in other words, we assume that

$$\begin{aligned} \lim_{N \to \infty} q_0(i) = q_0 \ , \\ \lim_{N \to \infty} q_+(i) = q_+ \ . \end{aligned} \tag{S11}$$

Then we get two self-consistent equations, Eqs. (2) and (3) of the main text, for q_0 and q_+.

For the long range frustration order parameter R, we proceed as follows. Suppose the newly added vertex i is unfrozen in graph G'. Now flip the spin of vertex i to $\sigma_i = -1$, how many unfrozen vertices in graph G' will have their spin values be fixed as a consequence? For the number s of affected other unfrozen vertices to be finite, there are the following two different situations.

If the unfrozen vertex i has no nearest neighbors that are positively frozen in graph G ($k_+ = 0$), then it must have $k'_0 \geq 2$ nearest neighbors that are type-I unfrozen in graph G, $k'_0 - 1$ of which are capable of taking the spin value -1 simultaneously except the remaining one. In this situation, an unfrozen vertex in graph G is also an unfrozen vertex in graph G'. When σ_i is set to $\sigma_i = -1$, none of the unfrozen vertex of graph G will be forced to fix their spins. Therefore, the number of affected unfrozen vertices is $s = 0$ in this situation. The probability for this situation to occur is

$$p_1 = \frac{1}{q_0} P_{cq_+}(0) \sum_{k_0'=2}^{\infty} P_{cq_0R}(k_0') \big(\delta_{k_0'}^2 \frac{1}{2} + (1 - \delta_{k_0'}^2) \frac{k_0'}{2^{k_0'-1}} \big) \tag{S12}$$

$$= 1 - \frac{c q_+^2}{q_0} \; . \tag{S13}$$

In writing down Eq. (S13) we have used Eqs. (2) and (3) of the main text.

The other situation is that the unfrozen vertex i has one ($k_+ = 1$) nearest neighbor vertex j that is positively frozen in graph G. In the new graph G', this vertex j becomes unfrozen; furthermore, those vertices that are unfrozen in the graph $G \backslash j$ (that is, the graph produced by removing vertex j and its all attached edges from graph G) are also unfrozen in graph G'. In this situation, when σ_i is set to $\sigma_i = -1$, the spin of vertex j (which is unfrozen in graph G') will be fixed to $\sigma_j = +1$. In turn, vertex j may be connected to some vertices that are unfrozen in $G \backslash j$ (which are also unfrozen in G'). When σ_j is set to $\sigma_j = +1$, these unfrozen vertices all will be forced to take the spin value -1. Then, flipping these spins to the -1 value may then cause the fixation of further spin values on other unfrozen vertices, and so on. Since we assume that the initially flipped vertex i is *type-II* unfrozen, there is one crucial point here: the nearest neighboring vertex j should not be connected to any vertices that are type-I unfrozen in graph $G \backslash j$. For if otherwise, fixing $\sigma_i = -1$ (and hence $\sigma_j = +1$) will cause the fixation of the spins on a total number of $O(N)$ unfrozen vertices, in contradiction with the original assumption that vertex i is type-II unfrozen.

As is defined in the main text, $f(s)$ is the probability that flipping the spin value of an unfrozen vertex to the -1 value will cause the fixation of spin values on other $s \sim O(1)$ unfrozen vertices. The analysis described in the preceding two paragraphs leads to the following self-consistent equation for this probability distribution:

$$
\begin{aligned}
f(s) =& p_1 \delta_s^0 + \\
& + (1-p_1) P_{cq_0(1-R)}(0) \delta_s^1 + \\
& + (1-p_1) \sum_{k_0''=1}^{\infty} P_{cq_0(1-R)}(k_0'') \sum_{\{s_m\}} \prod_{m}^{k_0''} f(s_m) \delta_{s-1}^{s_1+\ldots+s_{k_0''}} \ .
\end{aligned}
\tag{S14}
$$

Equation (S14) is the same as Eq. (4) of the main text. In Eq. (S14), the random integer k_0'' is the number of nearest neighbors of vertex j that are type-II unfrozen in graph $G\backslash j$. In writing down Eq. (S14), we have used the mathematical insight that in the $N \to \infty$ limit, the cluster [with size $s \sim O(1)$] of affected vertices due to flipping the spin of vertex i to $\sigma_i = -1$ is a tree; in other words, there is no loops in this cluster.

We now give further explanation of Eq. (6). This equation is equivalent to saying that

$$
X_{\min} = q_- + \frac{1}{2} q_0 \ . \tag{S15}
$$

The first term on the right hand side of Eq. (S15) is easy to understand: a negatively unfrozen vertex contribute 1 to the size of a minimal vertex cover Λ_{mvc}. The factor 1/2 in Eq. (S15) can be understood by the following observation: When an unfrozen vertex i is in the spin state $\sigma_i = +1$, it does not directly contribute to the size of Λ_{mvc}. When it is flipped to spin state $\sigma_i = -1$, it contributes 1 to the size of Λ_{mvc}; however, as vertex i is flipped from $\sigma_i = +1$ to $\sigma_i = -1$, one of its nearest-neighboring unfrozen vertex j must also flip its spin from $\sigma_j = -1$ to $\sigma_j = +1$. Therefore, an unfrozen vertex contributes 1/2 to the size of Λ_{mvc}.

Finally we explain Eq. (7) in a little bit detail. The first term on the right hand size of Eq. (7) is just the fraction of positively frozen vertices. The term $1 - e^{-cq_+} - cq_+ e^{-cq_+}$ in Eq. (7) is the fraction of vertices that are connected to two or more positively frozen ones, as could be easily derived from Eq. (S6).