Comment on "Glassy Transition in a Disordered Model for the RNA Secondary Structure"

In a recent, very interesting paper, Pagnani, Parisi and Ricci-Tersenghi [1] have studied the low-temperature behavior of a model for RNA secondary structure. They claim that the model exhibits a breaking of the replica symmetry, since the width of the distribution $P(q)$ of overlaps may converge to a finite value at $T = 0$. The authors used an exact enumeration method to obtain all ground states for a given RNA sequence. Because of the exponential growing degeneracy, only sequences up to length $L = 256$ could be studied.

Here it is shown that, in contrast to the previous results, by going to much larger sizes as $L = 2000$ the variance $\sigma^2(q) \propto L^{-0.5}$. This means that $P(q)$ becomes a delta function in the thermodynamical limit at $T = 0$. The method used here combines the ideas presented in [1] and [2]. The method is faster than the algorithm of [2] because no floating-point arithmetic is necessary. Furthermore, the algorithm of [2] is not exact, although usually true ground states are obtained. The technique of [1] guarantees exact ground states but is restricted to small sizes.

Here, a finite number of exact ground states is selected randomly from the set of all ground states which is represented by a graph. Similar to an ordinary Monte-Carlo simulation it has to be guaranteed that each ground state appears with the proper weight, i.e. with the same probability, since all ground states have exactly the same energy. This is ensured by the following technique: Let now $G_{i,j}$ denote the set of ground states for the sequence $[r_i, \ldots, r_j]$. Similar to the representation of the partition function applied in [2,1], $G_{i,j}$ can be expressed in terms of ground states for smaller sequences: a ground state for the sequence $[r_i, \ldots, r_j]$ can either be a ground-state of $[r_{i+1}, \ldots, r_j]$ (if the energy is low enough), or it is a combination of a pair (i, k) $(k \in (i + 1, \ldots, j))$ with an arbitrary ground state of $[r_i, \ldots, r_{k-1}]$ and an arbitrary ground state of $[r_{k+1}, \ldots, r_j]$ (if the energy is low enough).

The calculation of all ground states proceeds as follows: $G_{i,i} = G_{i,i+1} = \emptyset$ for all feasible i holds. Starting with $G_{i,i+2} = \{(i, i + 2)\}$ $(i = 1, \ldots, L - 2)$ the complete set of ground states can be calculated recursively. The result is stored as a acyclic directed graph with $G_{i,j}$ $(1 \leq i \leq j \leq L)$ being the nodes and $G_{1,L}$ the root. At each node, edges pointing to to the descendant sets $G_{i+1,j}$, $G_{i+1,k-1}$ and $G_{k+1,1}$ are stored instead of enumerating the states. Additionally, along with each node the ground-state energy $E_0(i, j)$ and the number of ground states $d_{i,j}$ is kept. The degeneracy $d_{i,j}$ can be calculated recursively as well.

The selection of a ground state is performed by a steepest descent into the graph. Each ground state consists of the pairs encountered during the descent. At each node the steepest descent continues either into one descendant $G_{i+1,j}$ or into two descendant $G_{i+1,k-1}, G_{k+1,j}$, the alternative for proceeding being chosen randomly. The probability for each choice is proportional to the number of ground states found in the corresponding branch(s). For that purpose the degeneracy values $d_{i,j}$ are used. It means that a path which contains twice the number of ground states of another path is selected on average twice as often. Therefore, it is guaranteed that each single ground state contributes with the same weight and a statistical correct $T = 0$ average is obtained.

For each sequence length the calculations were performed for 8000 independent realizations of the disordered, except for $L = 2000$ where only 1800 random sequences were generated. For each realization 100 ground states were selected randomly and stored for further evaluation. It was tested that by increasing this number the results do not change significantly.

The resulting values $\sigma^2(q)$ are shown in Fig. 1 using a double logarithmic scale. Clearly, the function converges towards zero, thus $P(q) \to \delta(q)$ for $L \to \infty$, a similar result was found [3] for the model presented in [2]. For small sizes, this convergence is much smaller due to finite-size effects. This may be the reason that in [1] no decision about the behavior of the width of $P(q)$ could be taken.

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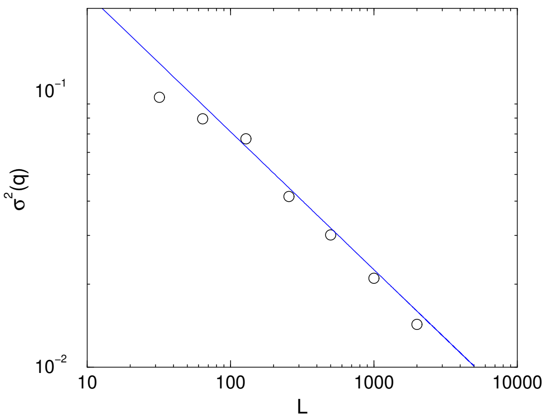

FIG. 1. Variance $\sigma^2(q)$ of the distribution of overlaps as a function of system size L. The line represents the function $0.71L^{-0.5}$. Please note the double logarithmic scale.

[1] A. Pagnani, G. Parisi and F. Ricci-Tersenghi, Phys. Rev. Lett. **84**, 2026 (2000)
[2] P.G. Higgs, Phys. Rev. Lett **76** (1996)
[3] A.K. Hartmann, unpublished