Simulations of ground state fluctuations in mean-field Ising spin glasses

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Abstract. The scaling of fluctuations in the distribution of ground state energies or costs with the system size $N$ for Ising spin glasses is considered using an extensive set of simulations with the extremal optimization heuristic across a range of different models on sparse and dense graphs. These models exhibit very diverse behaviors, and an asymptotic extrapolation is often complicated by higher-order corrections in size. The clearest picture, in fact, emerges from the study of graph bipartitioning, a combinatorial optimization problem closely related to spin glasses. Asides from two-spin interactions with discrete bonds, we also consider problems with Gaussian bonds and three-spin interactions, which behave quite differently.

Keywords: spin glasses (theory), fluctuations (theory), heuristics
1. Introduction

Ising spin glasses are the paradigmatic model for disorder not only in materials [1], but provide the archetype for complex behavior in many contexts, such as hard combinatorial problems [2, 3], information theory [4] and learning [5, 6]. An Ising spin glass is generally described by the Hamiltonian

\[ H = - \sum_{i,j} J_{i,j} \sigma_i \sigma_j \]  

(1)

with \( N \) Ising spins \( \sigma_i \in \{\pm 1\} \) and quenched random bonds \( J_{i,j} \). The bonds are chosen from a distribution, here, of zero mean and width \( \sqrt{\langle J^2 \rangle} = J_0 \) that is either bimodal (\( J_{i,j} \in \{\pm J_0\} \)) or Gaussian. The sum parses over all extant bonds \( \langle i, j \rangle \) between any pair of spins \( \sigma_i \) and \( \sigma_j \). The Sherrington–Kirkpatrick model (SK) [7] is the mean-field limit of
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Ising spin glasses, in which each spin is coupled to every other spin in the system. To keep the energies \( E \) of an equilibrium spin configuration in SK extensive, we set \( J_0 = 1/\sqrt{N} \); the other models discussed here are defined on sparse graphs and require \( J_0 = 1 \).

It is surprising to still find new features of such a well-studied model after some 30 years. Therefore, the unusual behavior of the distribution of ground state energies \( E_0 \) over the bond disorder in SK has raised significant interest in recent years. This interest is further elevated by its close connection with the statistics of extremely rare events, that in many jammed, disordered systems can become the controlling feature of the dynamics. It was found [8]–[12] that the fluctuations in \( E_0 \) behave in a highly non-normal fashion and rather resemble distributions found in extremal-value statistics [13]. This connection becomes rigorous for the fluctuations of the random-energy model (REM) [14], for which a Gumbel distribution can be derived exactly. The shape in SK shares similarities with a higher-order Gumbel distribution [8,11,15] but its precise functional form remains unknown. There exists a high degree of universality in the extreme-value statistics of intrinsically uncorrelated states, but in long-range connected systems with quenched disorder such an assumption may fail. A general discussion of the ordinary versus extreme fluctuations in SK and other disordered models is provided in [16].

Of special interest for the energy fluctuations is the variation in width of the distribution with the system size, as it provides important clues to the structural properties of the ground states (or low-temperature states generally) [9,17,18]. A number of arguments regarding the system-size scaling of the standard deviation for the ground state energy densities \( e_0 = E_0/N \):

\[
\sigma (e_0) = \sqrt{\langle e_0^2 \rangle - \langle e_0 \rangle^2} \sim AN^{-\rho} + BN^{-a} + \cdots \quad (a > \rho), \tag{2}
\]

for \( N \to \infty \) have been put forward, leading to values of either [9,19] \( \rho = \frac{3}{4} \) or [20]–[25] \( \rho = \frac{5}{6} \). Both conjectures predict decay that is faster than for normal fluctuations \( \rho = \frac{1}{2} \), which would be obtained from the central limit theorem under the assumption of negligible correlations between individual terms of the spin glass Hamiltonian in equation (1). While a bound of \( \rho \geq \frac{3}{4} \) has been shown [17,18] for SK, Gaussian behavior is indeed found for spin glasses on a finite-dimensional lattice [26] and has also been observed on sparse random graphs [9]. Exact values different from any of these are known for the replica symmetric spherical spin glass (\( \rho = \frac{2}{3} \)) and proposed for the \( m \)-vector spin glass for \( m \to \infty \) (\( \rho = \frac{4}{5} \)) [27,28].

Numerically, both conjectures for \( \rho \) in SK have proven difficult to distinguish with any certainty, and while most initial predictions [8]–[11] seem to favor a value close to \( \rho = \frac{3}{4} \), more recently a trend towards \( \rho = \frac{5}{6} \) was found at larger system sizes [12]. That would support the current consensus in the theoretical work [21]–[25]. Such a larger value is also desirable for numerical consistency in relations connecting \( \rho \) to the exponent describing domain wall excitations [19], as found in high dimensions [29].

Here, we report on extensive simulations to clarify this important question regarding the low-temperature properties of spin glasses. The results for SK are at best marginally consistent with any of the theoretical predictions. Since the data analysis proves to be complicated by transient behavior, we have widened the scope of our investigation to incorporate a large number of related models for comparison. For instance, we provide corresponding data for spin glasses on random regular graphs (‘Bethe lattices’) of sparse
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degree, both for two- and three-spin interactions and discrete ($\pm J$) as well as Gaussian bonds. Two-spin-coupled spin glasses on Bethe lattices of degree $r$ provide a convenient one-parameter family of models which smoothly extrapolates to SK for increasing degree, $r \to \infty$ [30, 31]. The results are quite similar to those we find in SK, thus providing a likely trend for the SK behavior itself, but they are equally beset with strong transients. The three-spin model provides data for discrete bonds that is consistent with recent studies [32, 33]. Such a model also highlights the question of universality of the results when continuous bonds are used. As we have noted before [34], on sparse graphs finite-size corrections may already depend on details of the bond distribution; this dependence appears to extend also to ground state deviations.

Alternatively, we study the graph bipartitioning problem (GBP) on these Bethe lattices. We find much diminished transients and a consistent extrapolation for the value of $\rho$. But that value is between—and likely distinct from—$\frac{2}{5}$ and $\frac{5}{6}$. Although it was recently predicted [35] that GBP in the thermodynamic limit is equivalent to the corresponding spin glass at $T = 0$ on those Bethe lattices, it is of course less clear whether such a relation would hold at finite size. Finite-size corrections to the average ground state energies, for instance, already differ significantly between GBP and spin glasses.

This paper is structured as follows: we start with a few remarks about the optimization heuristic used in all of our simulations in section 2.1. Since the clearest case is provided by GBP, we present our data for this problem first in section 3. In section 4, we discuss SK data at length. In section 5, we present the data for the corresponding spin glass problem on Bethe lattices, followed by a similar study on ordinary random graphs in section 6. In section 7, we supplement our investigation with a study of three-spin interactions on a Bethe lattice. We summarize with a few conclusions in section 8.

2. Means and methods

In this section, we introduce the simulation methods and techniques by which the resulting data was analyzed.

2.1. Optimization methods

We have employed the extremal optimization heuristic (EO) [36]–[38] in the implementation described previously for the SK spin glass [11] and those on Bethe lattices [31], with various improvements to attain an order of magnitude in speed-up\(^1\). Resorting to a simple bimodal bond distribution whenever possible allows further an efficient use of integer arithmetic. Discrete bonds provide computational advantages while continuous (Gaussian) bonds also pose significant entropic barriers in addition to the usual complexities faced by local search in a multi-modal energy landscape [39]. To find approximations to GBP ground states, we use EO as described in [35, 40].

Unlike, for instance, the parallel tempering Monte Carlo technique used at larger system sizes for SK in [12], which operates at small but finite temperatures, EO generally performs its local search for minima in the landscape formed by the internal energy itself, with activated spin flips as elementary moves [37]. The only free parameter controlling EO

\(^1\) A sample code of this implementation of EO for SK can be found at http://www.physics.emory.edu/faculty/boettcher/Research/OEO_deno demoSK.c.

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was set to $\tau = 1.25$ for discrete problems and somewhat higher at $\tau = 1.5$ for problems with Gaussian weights, and about $0.1 N^3$ spin flips were executed in each run, restarting from a random initial configuration. At least two such restarts were performed for each instance, and the number of runs is doubled on-the-fly whenever a new optimum is found in the latter half of all runs. For some rare instances, more than 10 runs were required, always ensuring that the latter half of all runs merely confirms the previously found optimum but does not exceed it. In each section, we have listed the number of instances treated at each $N$. Besides trying to reach large sizes, we have often emphasized simulating a very large number of instances on a relatively dense set of intermediate $N$. We have conducted extensive tests for each model to ensure the accuracy of the results. Testing on testbeds of exactly solved instances (using branch-and-bound) typically results in perfect agreement, but system sizes are small ($N \approx 50–70$). On larger systems, we have done sample runs with ten times more updates and found only a few inaccuracies, which lead to systematic errors far below statistical errors (unless otherwise noted).

Although all of the problems in this project could be classified as spin glasses, they stand in for a large class of combinatorial problems. It should be noted that the EO heuristic provides data of great detail with only small changes in the implementation. Only the input for the various graph types needed to be changed. (For GBP, we have to impose the additional constraint of vanishing magnetization.) While we treat only mean-field problems here, pertinent results have been obtained previously for structured instances, such as finite-dimensional lattices [41, 42].

### 2.2. Data analysis

To obtain insights into the finite-size scaling of our observables, we study fits of the data generated in our simulations to a number of asymptotic forms. These forms seem to be the most natural candidates to describe corrections to the leading asymptotic behavior. But there can never be an exhaustive list of all possibilities without any theoretical knowledge a priori. Therefore, we list as many as possible of the data points obtained in the simulations in tables that would allow readers to pursue their own hypotheses.

Any asymptotic ($N \to \infty$) fit bears considerable risks: not only may a presumed asymptotic form be insufficient and may, for instance, miss logarithmic corrections, etc. But even if correct, it would certainly fit data for larger system sizes $N$ better than any transients, raising the question of how many data points for lower $N$ to include. Any of these uncertainties can introduce potentially sizable systematic errors, even if the heuristic had been perfectly accurate. Such errors can only be eliminated fully with a theory to compare with, which at present does not exist. The obtained qualities-of-fit $Q$ have to be seen in this context, and a poor $Q$ value should not be taken immediately as disproving a hypothesis, unless it is seen in relation to alternative fits and a discussion of how much transient data has been included. In fact, to obtain any reasonable $Q$ values, in each fit we have—somewhat arbitrarily—increased the error bars uniformly by a factor of four from the purely statistical errors given as a bracketed uncertainty in the last digit of the simulation data listed in the tables. Such a uniform allowance for systematic errors, either from heuristic inaccuracies or functional uncertainty in the fit, is definitely inadequate and would deserve better consideration in the future.

Thus, we fit the asymptotic extrapolation of the finite-size data towards the thermodynamic limit ($N \to \infty$) for the presumed ground state energy $\langle e_r \rangle_N$ or cost
densities $\langle c_r \rangle_N$ to the following forms, abbreviating $x \in \{c, e\}$:

$$
\langle x_r \rangle_N \sim \langle x_r \rangle_\infty + AN^{-\omega} + \cdots
$$

for just the first-order correction, or

$$
\langle x_r \rangle_N \sim \langle x_r \rangle_\infty + AN^{-\omega} + BN^{-\omega_1} + \cdots
$$

as a second-order correction, where we have to fix the first-order exponent $\omega$ and require $\omega_1 > \omega$ to achieve a stable fit. An alternative second-order logarithmic fit:

$$
\langle x_r \rangle_N \sim \langle x_r \rangle_\infty + AN^{-\omega} + B \ln \frac{N}{N} + \cdots,
$$

with arbitrary $\omega < 1$ also seems conceivable.

The asymptotic scaling for the respective deviation exponent $\rho$ proceeds either through a direct fit (to first or second order) to equation (2), or by the corresponding extrapolated form

$$
-\frac{\log \sigma}{\log N} \sim \rho - \frac{\log A}{\log N} + O \left( \frac{N^{-(a-\rho)}}{\log N} \right).
$$

Either method has its advantages and disadvantages. A direct fit, plotted on a double-logarithmic scale, provides easier convergence when higher-order terms are included. But the logarithmic scale smooths out variability or transients in a dataset. In turn, the extrapolated form in equation (6) is far less forgiving and provides significantly more insight into fluctuations in the dataset. When plotted on a $1/\log N$ scale, data that extends over decades is squashed into a relatively small space. But if a solid linear regime emerges, it provides stronger evidence for the existence and value of an exponent than a double-logarithmic plot. The slope of this extrapolation is arbitrary, though, as we could multiply $\sigma$ by any constant factor without affecting the scaling. We may choose to fix this factor in a way (such as for the spin glasses below) that the $\log C$ term in equation (6) vanishes, or (such as for the GBP below) to splay out several plots into one graph. Clearly, such a choice does not alter any linear regime, if it exists. Without such a linear regime, as we will see, it is very difficult to extract satisfactory information from such a fit, even when higher-order (and strongly non-polynomial) corrections are taken into account.

As we have argued in [34], under certain circumstances it is necessary to consider the cost of frustration (the sum of all violated bonds) in a ground state, instead of its energy (the difference between all violated and all unviolated bonds). We will switch in our discussion between cost and energy repeatedly. There is a simple linear relation between their average densities:

$$
\langle e_0 \rangle_N = 2 \langle c_0 \rangle_N - \frac{r}{p} \langle |J| \rangle_N,
$$

where $r$ is the (average or fixed) degree and $p$ refers to the number of spins coupled via a single bond. The average absolute bond weight for the Gaussian distribution of zero mean and standard width ($J_0^2 = 1$ on sparse graphs, $J_0^2 = 1/N$ for SK) is given by $\lim_{N \to \infty} \langle |J| \rangle_N = \sqrt{2/\pi}$, whereas it is simply $\langle |J| \rangle_N = 1$ for a bimodal distribution on a sparse graph. While there is no difference between cost and energy at the level of averages, the corresponding relation of the (co-)variances mixes the fluctuations in
cost and energy with those of the absolute bond weights. If in each instance the absolute sum of all bond weights is the same, i.e. a δ peak without fluctuations, cost and energy fluctuations are proportional. But if the absolute bond-weight sum fluctuates (independently) from instance to instance, either energy or cost fluctuations will become equally normal distributed, which leaves at most one of them non-trivial. Typically, for SK, cost fluctuations are trivial (i.e. normal) and energy fluctuations are interesting, while for sparse graphs with variable degree and/or continuous bonds the role reverses. Only for Bethe lattices (of fixed degree) with bimodal bonds are cost and energy fluctuations proportional. When \( r \gg 1 \) and each spin acquires a nearly extensive number of neighbors, matters get more complicated.

3. Graph bipartitioning on Bethe lattices

In GBP, a graph of (even) \( N \) vertices and a certain number of edges is divided into two sets of equal size \( N/2 \) such that the number of edges connecting both sets, the ‘cutsize’, is minimized. (Requiring an equal balance between up- and down-spins, GBP in physics corresponds to a ferromagnetic system held at zero magnetization.) The global constraint of an equal division places the GBP among the hardest problems in combinatorial optimization, since determining the exact solution with certainty would, in general, require a computational effort growing faster than any power of \( N \) [43]. Applications of graph partitioning reach from the design of integrated circuits (VLSI) [44] to the partitioning of sparse matrices [45], leading to very different requirements regarding the mix of speed and accuracy in a heuristic [46]. In [47,48], we have considered a range of different graph ensembles, which can affect characteristics of GBP drastically. In [40], the SAT/UNSAT transition of GBP on ordinary random graphs was investigated analytically and numerically. Here, as in [35], we merely focus on Bethe lattices, which are regular and locally tree-like such that some analytical results have been derived [49–52]. These Bethe lattices are also known as \( r \)-regular graphs and are generated by fixing the degree \( r \) at each vertex, which in turn is connected to other vertices at random.

3.1. Average ground state costs

In table 1, we have obtained approximate optima in the cutsize per vertex \( \langle c_r \rangle_N \) on Bethe lattices for degrees \( r \) between 3 and 10, and graph sizes between \( N = 32 \) and 2048. Statistical errors of our averages have been kept small by generating a large number of instances for each \( N \) and \( r \), typically \( n_I \approx 10^6 \) for \( N \leq 200 \) and \( n_I \approx 10^5 \) for \( N \geq 256 \). Reference [35] described the implementation of the \( \tau \)-EO heuristic used to obtain the ground state approximations for GBP. We have presented some of the most salient results of the extrapolation to the thermodynamic limit there.

In [35], we used a fit with first-order corrections according to equation (3) alone, see table 1 and figure 2 there. Such a first-order fit to the data from the largest system sizes only is discussed in table 2. While the fits produce rather consistent results, with very similar values for \( \omega \), there is clearly a distinction between even and odd \( r \) in the quality of the fits, indicative of parity effects typical of regular graphs already noted earlier [30,35].

A surprising feature of these fits are the values for the finite-size scaling exponent \( \omega \). In our previous studies [30,31] of bimodal spin glasses on Bethe lattices we found throughout

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Table 1. Average cost per spin $\langle c_r \rangle_N$ for approximate ground states of GBP on Bethe lattices of degree $r = 3, \ldots, 10$. The given errors, in parentheses after each average, denote the uncertainty in the last given digit of that average. This uncertainty is solely based on the statistical error. Fits of this data and their plots were discussed previously in [35] (see figure 2 there).

| $N$  | $\langle c_3 \rangle_N$ | $\langle c_4 \rangle_N$ | $\langle c_5 \rangle_N$ | $\langle c_6 \rangle_N$ | $\langle c_7 \rangle_N$ | $\langle c_8 \rangle_N$ | $\langle c_9 \rangle_N$ | $\langle c_{10} \rangle_N$ |
|------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|------------------------|
| 32   | 0.19495(3)             | 0.35652(4)             | 0.53893(5)             | 0.71445(5)             | 0.91552(6)             | 1.09781(6)             | 1.31056(6)             | 1.49700(7)             |
| 40   | 0.18161(3)             | 0.34104(3)             | 0.51730(4)             | 0.69348(4)             | 0.88800(5)             | 1.07190(5)             | 1.27774(5)             | 1.46657(6)             |
| 50   | 0.16627(2)             | 0.32820(3)             | 0.49487(3)             | 0.67581(4)             | 0.85919(4)             | 1.05003(4)             | 1.24320(5)             | 1.44071(5)             |
| 64   | 0.15822(2)             | 0.31632(2)             | 0.48312(3)             | 0.65972(3)             | 0.84438(3)             | 1.02997(4)             | 1.22578(4)             | 1.41715(4)             |
| 80   | 0.15042(1)             | 0.30750(2)             | 0.47119(2)             | 0.64753(3)             | 0.82899(3)             | 1.01495(3)             | 1.20743(3)             | 1.39936(3)             |
| 100  | 0.14406(2)             | 0.30016(2)             | 0.46138(3)             | 0.63749(3)             | 0.81632(3)             | 1.00232(4)             | 1.19222(4)             | 1.38449(4)             |
| 128  | 0.13825(2)             | 0.29350(1)             | 0.45240(2)             | 0.62822(2)             | 0.80481(3)             | 0.99082(3)             | 1.17837(3)             | 1.37085(3)             |
| 160  | 0.13411(1)             | 0.28858(2)             | 0.44582(2)             | 0.62133(2)             | 0.79628(2)             | 0.98220(2)             | 1.16812(3)             | 1.36075(3)             |
| 200  | 0.13064(1)             | 0.28450(1)             | 0.44037(2)             | 0.61553(2)             | 0.78920(2)             | 0.97498(2)             | 1.15965(3)             | 1.35227(3)             |
| 256  | 0.12753(1)             | 0.28087(1)             | 0.43545(1)             | 0.61037(2)             | 0.78281(2)             | 0.96852(2)             | 1.15195(2)             | 1.34449(2)             |
| 320  | 0.12526(1)             | 0.27818(1)             | 0.43185(2)             | 0.60652(2)             | 0.77813(2)             | 0.96370(2)             | 1.14630(2)             | 1.33874(3)             |
| 512  | 0.12170(1)             | 0.27395(1)             | 0.42607(1)             | 0.60054(2)             | 0.77073(2)             | 0.95665(2)             | 1.13734(2)             | 1.32968(2)             |
| 1024 | 0.11852(1)             | 0.26993(1)             | 0.42075(1)             | 0.59497(2)             | 0.76407(4)             | 0.94948(4)             | 1.12965(5)             | 1.32211(6)             |
| 2048 | 0.11670(4)             |                      |                      |                      |                      |                      |                      |                      |
Table 2. Fit of the data in table 1 to equation (3) for the cost $c$. Only data for $64 < N < 2048$ has been utilized.

| $r$ | $\langle c_r \rangle_\infty$ | $A$ | $\omega$ | ndf | $\chi^2/ndf$ | $Q$ |
|-----|------------------|-----|--------|-----|-------------|-----|
| 3   | 0.114765         | 1.71| 0.88   | 6   | 0.178       | 0.98|
| 4   | 0.265240         | 1.77| 0.85   | 6   | 2.124       | 0.047|
| 5   | 0.414254         | 2.35| 0.85   | 6   | 0.410       | 0.87 |
| 6   | 0.587974         | 2.37| 0.84   | 6   | 0.622       | 0.71 |
| 7   | 0.755752         | 3.11| 0.86   | 6   | 0.138       | 0.99 |
| 8   | 0.940334         | 2.93| 0.84   | 6   | 2.124       | 0.047|
| 9   | 1.119390         | 3.74| 0.86   | 6   | 0.599       | 0.73 |
| 10  | 1.310780         | 3.37| 0.83   | 6   | 1.836       | 0.088|

Table 3. Fit of the data in table 1 to equation (5) with fixed $\omega = \frac{2}{3}$. Only data for $64 < N < 2048$ has been utilized.

| $r$ | $\langle c_r \rangle_\infty$ | $A$ | $B$   | ndf | $\chi^2/ndf$ | $Q$ |
|-----|------------------|-----|------|-----|-------------|-----|
| 3   | 0.116574         | −0.69| −1.29| 6   | 6.347       | 1.1 $\times 10^{-6}$ |
| 4   | 0.266936         | −0.56| −1.28| 6   | 11.886      | 2.2 $\times 10^{-13}$ |
| 5   | 0.416543         | −0.75| −1.73| 6   | 6.770       | 3.4 $\times 10^{-7}$  |
| 6   | 0.590277         | −0.71| −1.75| 6   | 2.311       | 0.031|
| 7   | 0.759679         | −1.21| −2.45| 6   | 2.585       | 0.017|
| 8   | 0.944030         | −1.02| −2.29| 6   | 0.645       | 0.69 |
| 9   | 1.124500         | −1.52| −3.01| 6   | 1.747       | 0.11 |
| 10  | 1.310780         | −1.14| −2.66| 6   | 0.600       | 0.73 |

that this exponent was most consistent with $\omega = \frac{2}{3}$, which has also been predicted for SK, see section 4.1. While it was argued in [35] that bimodal spin glass and GBP on Bethe lattices should be equivalent in the ground state energy, this equivalence apparently does not extend even to first-order corrections, as the values for $\omega$ in these fits are significantly higher. To analyze whether even higher-order corrections could rectify this discrepancy in scaling, we attempt a fit of the form in equation (4) with $\omega = \frac{2}{3}$ fixed but variable $B$ and $\omega_1$. Such a fit fails to converge, as in each iteration $\omega_1$ moves closer to $\omega$. Alternatively, we prescribe the form of a plausible logarithmic higher-order correction in equation (5). The results of this fit are listed in table 3. The quality of the fit is very poor for small degree $r$ but gets progressively better for increasing $r$, suggesting a possible approach to the SK result for $\omega$ for $r \to \infty$. Yet, the results for $\langle c_r \rangle_\infty$ are somewhat less in agreement with the conjectured equivalence in [35]. Generally, if the next-order correction contains a (possibly polynomial) logarithmic dependence of this sort, any attempt to predict $\omega$ may be futile.

Another alternative form to fit is provided by a series expansion in powers of $N^{-\omega}$. Thus, fitting to equation (4) with $\omega_1 = 2\omega$ we obtain the results listed in table 4. Now, the results for $\langle c_r \rangle_\infty$ are again in good agreement with the conjecture but the quality of the fit is not improved over the mere first-order fit in table 2. Interestingly, this form is now a better fit with even values for $r$ but terrible for odd ones, reversing the trend from the previous fits. Correction terms may differ between even and odd $r$ not only in their constants but in their very form.

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3.2. Ground state fluctuations

In figure 1, we plot the probability density functions (PDF) of ground state costs over the ensembles of Bethe lattices. Unlike for the spin glass problems below, transients due to finite-size effects diminish quickly. This leads to a solid collapse of the data when properly rescaled by their deviations $\sigma(c_r)_N$ in equation (2), apparently with little difference in the scaling function even for varying degrees $r$.

In table 5, we list the deviations $\sigma(c_r)_N$, as defined in equation (2), for each degree $r$ and system size $N$. A closer look at these deviations indeed provides a robust extrapolation for the exponent $\rho$. Equation (6) should yield a linear extrapolation for the exponent $\rho$ when plotted versus $1/\log N$, assuming negligible corrections (i.e. $N^{-\alpha} \ll N^{-\rho}$). In figure 2, we show these plots for all values of $r$. It is apparent that transient behavior decays very quickly and a smooth linear extrapolation is obtained. Also reassuring is the fact that this data shows a small even/odd effect, just as for the costs above in section 3.1. As figure 3 shows, the sequence of extrapolants for $\rho$ appear to converge towards the same value of $\rho = 0.77(2)$, at least for $r \to \infty$. It is surprising to find such an apparently non-trivial result in such a simple mean-field model. Comparing with theory, it comes closest to the value of $\rho = \frac{3}{4}$ previously proposed in [9] and seems far from that proposed for the SK model, $\rho = \frac{5}{6}$ [22]–[25]. There is, of course, no reason for it to be equal to that of SK. But the in-between value found here for GBP is arguably close to the corresponding extrapolations for the spin glasses below, which by themselves remain inconclusive due to strong transients up to large system sizes.

4. Sherrington–Kirkpatrick model

We reconsider finite-size corrections in the SK model by expanding on the simulations in [11] with substantially more instances at many more system sizes, see table 6. It is found that the corrections to the average energies permit fits of reasonable quality with systematic improvements when higher-order corrections are incorporated, but the discussion of the energy fluctuations remains largely inconclusive. Interestingly, this scenario is the converse of that found in section 3 for GBP.
Figure 1. Plot of the PDFs for the ensemble fluctuations of the optimal costs per spin for GBP on Bethe lattices of degree $r = 3, 4, \ldots, 10$. When rescaled by their deviation $\sigma = \sigma(c_r)N$, the data collapses virtually for all system sizes onto a highly skewed master curve. There appears to be little change in skewness between degrees $r$. 

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Table 5. Standard deviation of the ground state costs in GBP. Statistical errors are estimated as 
\( \sigma/\sqrt{n_I} \), where \( n_I \) refers to the number of instances considered. Appropriately rescaled, this data is also plotted in figure 2. (Some of the data, in particular, for larger \( N \) and \( r \), shows an obvious systematic bias due to two likely sources: a bad approximation for some ground states and an undercount of rare instances with costs extremely far from the average. These data points have been left out of figure 2.)

| \( N \) | \( \sigma(c_3)_N \) | \( \sigma(c_4)_N \) | \( \sigma(c_5)_N \) | \( \sigma(c_6)_N \) | \( \sigma(c_7)_N \) | \( \sigma(c_8)_N \) | \( \sigma(c_9)_N \) | \( \sigma(c_{10})_N \) |
|-------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|----------------|
| 32    | 0.032 06(3)   | 0.041 08(4)   | 0.045 61(5)   | 0.052 22(5)   | 0.055 98(6)   | 0.061 18(6)   | 0.064 70(6)   | 0.069 10(7)   |
| 40    | 0.026 64(3)   | 0.034 28(3)   | 0.038 14(4)   | 0.043 70(4)   | 0.046 80(5)   | 0.051 29(5)   | 0.054 19(5)   | 0.057 90(6)   |
| 50    | 0.022 52(2)   | 0.028 60(3)   | 0.032 15(3)   | 0.036 53(4)   | 0.039 53(4)   | 0.043 01(4)   | 0.045 64(5)   | 0.048 69(5)   |
| 64    | 0.017 84(2)   | 0.023 33(2)   | 0.026 15(3)   | 0.029 98(3)   | 0.032 28(3)   | 0.035 39(4)   | 0.037 47(4)   | 0.040 09(4)   |
| 80    | 0.014 82(1)   | 0.019 45(2)   | 0.021 92(2)   | 0.025 11(3)   | 0.027 10(3)   | 0.029 67(3)   | 0.031 46(3)   | 0.033 67(3)   |
| 100   | 0.012 53(2)   | 0.016 22(2)   | 0.018 37(3)   | 0.020 96(3)   | 0.022 50(3)   | 0.024 90(4)   | 0.026 39(4)   | 0.028 25(4)   |
| 128   | 0.010 12(2)   | 0.013 29(1)   | 0.015 17(2)   | 0.017 25(2)   | 0.018 77(3)   | 0.020 51(3)   | 0.021 79(3)   | 0.023 29(3)   |
| 160   | 0.008 47(1)   | 0.011 13(2)   | 0.012 69(2)   | 0.014 45(2)   | 0.015 73(2)   | 0.017 16(2)   | 0.018 29(3)   | 0.019 48(3)   |
| 200   | 0.007 12(1)   | 0.009 35(1)   | 0.010 66(2)   | 0.012 09(2)   | 0.013 23(2)   | 0.014 42(2)   | 0.015 36(2)   | 0.016 41(3)   |
| 256   | 0.005 82(1)   | 0.007 69(1)   | 0.008 78(1)   | 0.009 96(2)   | 0.010 92(2)   | 0.011 83(2)   | 0.012 71(2)   | 0.013 51(2)   |
| 320   | 0.004 90(1)   | 0.006 43(1)   | 0.007 34(2)   | 0.008 35(2)   | 0.009 19(2)   | 0.009 95(2)   | 0.010 69(2)   | 0.011 40(3)   |
| 512   | 0.003 36(1)   | 0.004 41(1)   | 0.005 09(1)   | 0.005 80(2)   | 0.006 38(2)   | 0.006 97(2)   | 0.007 46(2)   | 0.007 98(2)   |
| 1024  | 0.001 95(1)   | 0.002 53(1)   | 0.002 95(1)   | 0.003 39(2)   | 0.003 86(4)   | 0.004 28(4)   | 0.004 63(5)   | 0.005 06(6)   |
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Figure 2. Extrapolation in the limit $N \to \infty$ for the exponent $\rho$, defined in equation (2), from the deviations $\sigma(c_r)N$ in table 5 obtained from the distribution of the GBP ground state. Appropriately rescaled via equation (6), the data for each degree $r$ extrapolates linearly to the thermodynamic limit, with rapidly diminishing transients. Note that for each $r$ the fitted region spans at least one decade in system size $N$. The goodness-of-fit is $Q = 1$ for all $r$ except for $r = 3$, where $Q \approx 0.73$.

Figure 3. Extrapolated values of $\rho$ for each degree $r$, obtained from figure 2, plotted as a function of inverse degree. For even and odd values of $r$ separately, each sequence extrapolates to the value of $\rho_{\infty} = 0.77(2)$ for $r \to \infty$. The error bars result from the fits in figure 2; systematic errors, e.g. due to higher-order corrections ignored in those fits, are potentially larger.

4.1. Average ground state energy

First, we want to consider the average energies, which provide an assessment of the quality of our simulations in reference to exactly known results about SK; a necessary step preliminary to a more demanding analysis of the data. In figure 5, we plot the data...
for the average ground state energy density $\langle e_0 \rangle_N$ from table 6 for the different $N$. It has been argued on the basis of theoretical studies [54, 55] at or near $T_c$ and on previous numerical investigations [11, 12, 21, 30, 56] that finite-size corrections to the energy behave for all $T \leq T_c$ according to equation (3) with $\omega = \frac{2}{3}$. We find this expectation confirmed within numerical accuracy, see figure 4 (left). Figure 4 also shows that a higher-order correction according to equation (4) even improves substantially on this leading behavior, which is plotted as a fit to the data in figure 5.

We can obtain a revealing insight into the quality of the EO data by extracting the leading behavior to explore the correction term in more detail. Because the energy in the thermodynamic limit is well known [53], $\langle e_0 \rangle_\infty = -0.763\,166\,7265(6)$, we can rewrite equation (3) as

$$A \sim [\langle e_0 \rangle_N - \langle e_0 \rangle_\infty]N^{2/3} + \cdots \quad (N \to \infty),$$

(8)

and plot the EO data in this form in the inset of figure 5. Since the form of higher-order corrections is unknown, we plot the data again as a function of $1/N^{2/3}$, which provides a near-linear collapse of the data and an extrapolated value for the amplitude $A \approx 0.695(5)$, which is consistent with the value obtained by the fit in figure 5. But the most important aspect of the inset resides in the sharp crossover in the behavior of the data at around $N \approx 1000$. The consistent behavior of the data for $N \lesssim 1000$ suggests sufficient numerical accuracy in the obtained ground state energies to this level of analysis, without any discernible systematic bias. The data points for $N = 799$ and 1024 both exhibit a systematic error of about $\Delta A/A \approx 2/70 \approx 3\%$ in the prediction of $A$, hence a relative systematic error of $\epsilon(e_\infty) = \Delta e_\infty/e_\infty \approx \Delta A/N^{2/3}/e_\infty \approx 0.03\%$ (see also figure 4) in the prediction of typical ground state energies overall. Unfortunately, the systematic error for the $N = 2047$ data point is about $\Delta A/A \approx 1/7 \approx 15\%$, leading to
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Figure 4. Various fits to the average ground state energies \( \langle e_0 \rangle_N \) of SK in table 6. Leftmost, we consider first-order corrections only for a fit involving the thermodynamic limit value \( e_\infty \) and the correction amplitude \( A \) for varying the correction exponent \( \omega \). The best-quality fit to this form, possessing minimal \( \chi^2/\text{ndf} \), occurs just above \( \frac{2}{3} \) at \( \omega \approx 0.68 \). Adding a higher-order correction (with coefficient \( B \), middle panel), a square of the first-order term, bottoms out at \( \omega \approx 0.66 \) with much lower \( \chi^2/\text{ndf} \) values overall. Instead, fixing the first-order exponent to \( \omega = \frac{2}{3} \) and varying the second-order exponent \( \omega_1 \) (right panel) implicates an optimal exponent much above \( 2\omega \), namely \( \omega_1 \approx 1.8 \). Remarkably, the optimal choice for \( \omega \) or \( \omega_1 \) about coincides in all three fits with the lowest relative error \( \epsilon(e_\infty) \) (lower panels) in the fitted value for \( e_\infty \).

a relative systematic error of 0.1% in the prediction of putative ground states, which is sufficiently noticeable in figure 5 to exclude that point from the extrapolation.

It is worthwhile to compare the inset of figure 5 with the corresponding plot, the inset of figure 1, in [12]. While the data there is also falling for increasing \( N \) (arguably to the same asymptotic value of \( A \approx 0.7 \), see equation (8)), the variation of the data there is far more rapid. Point for point, the data there represents a systematically higher value in the average ground state energy than is obtained here. This could potentially indicate a bias in the heuristic methods used, which may fail to find true ground states across the board. (Notably, the data there does not show drastic degradation in the quality of the results for increasing \( N \), as is found here.) Alternatively, such disagreement could be attributed to the difference in the bond distribution used: Gaussian there and bimodal here. Although the leading thermodynamic properties should be universal, higher-order corrections can be sensitive to microscopic details.

In figure 4, we present an alternative procedure to explore corrections that also allows a probe of higher-order terms. In this procedure, we select (the most important) one of
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Figure 5. Extrapolation plot of the average ground state energy densities $\langle e_0 \rangle_N$ from table 6 as a function of the presumed finite-size corrections, $1/N^{2/3}$. The statistical errors indicated are much smaller than symbol sizes. For $N \to \infty$, the EO data extrapolates to the Parisi energy [53], $\langle e_0 \rangle_\infty = -0.7631667265(6)$, at the intercept. The indicated fit (dashed line) predicts $e_\infty = -0.76323(5)$. The slope of the line is $A = 0.70(1)$, consistent with the inset, which shows the same data appropriately rescaled to extrapolate for $A$. It is $B \approx 0.48$, and $\omega_1 \approx 1.8$ suggests surprisingly weak higher-order corrections, see also figure 4.

the parameters to be fitted as fixed and evaluate the quality of the fit for the remaining parameters over a range of values for the selected one. As a measure of quality, we utilize $\chi^2$ per numbers of degrees of freedom (ndf), which should be minimized. The first panel displays this procedure for just the first-order correction, again confirming the expectation of equation (3). In the remaining two panels we test possible higher-order corrections. In the first of these, we test a fit to a regular Taylor series in powers of $N^{-\omega}$ to second order. Incorporation of such a second-order term improves the quality of the fit noticeably over the first-order term alone. Furthermore, the optimal choice for $\omega$ again proves consistent with $2/3$, despite the extra degree of freedom provided, which attests to its robustness. Then, taking $\omega = 2/3$ as a given, we explore an independent second-order correction with scaling exponent $\omega_1$. This yields the highest-quality fit thus far, also used in figure 5, but predicts that $\omega_1$ would be much larger than simply $2 \omega$, suggesting that such corrections would be even weaker.

We have also tried to fit higher-order corrections of the form $1/N$ or $\ln N/N$ in addition to $1/N^{2/3}$ corrections, which are plausible by analogy with the results obtained for finite-size corrections near the critical temperature [54, 55]. A fit to equation (5) does not produce acceptable results compared to those found in figure 4 for any value of $\omega$. Instead, a fit to equation (4) with $\omega_1 = 1$ fixed produces a very narrow window of reasonable results near $\omega = 2/3$ but, at best, of the quality of what is seen correspondingly at $\omega_1 = 1$ in the last panel of figure 4. Further higher-order corrections may improve on this alternative. But if the ratio between a previous and its next higher-order correction is a weakly falling function, i.e. $(1/N)/(1/N^{2/3}) = N^{-1/3} \approx 0.1$ at least for $N \approx 1000$ here, resolving the impact of such corrections with the available data becomes near impossible and they can never be fully excluded.

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Figure 6. Plot of the probability density functions (PDF) of obtained ground state energy densities $e_0$ for SK in units of the standard deviation $\sigma$. For reference, the exact probabilities for $N = 9$ are re-plotted from [57]. Unlike for the PDFs for GBP in figure 1, there is a significant finite-size effect noticeable, especially in the right tail of the distribution.

4.2. Ground state energy fluctuations

Next, we consider the distribution of ground state energies around their averages. In units of their standard deviation, the probability density function (PDF) for each value of $N$ exhibits clearly the asymmetric shape that is skewed towards a broader (exponential) tail of instances with lower-than-average ground state energy and a cutoff that is much sharper than exponential for those with higher energy. This shape is largely unchanged across the sizes and can be shown, by exhaustive enumeration [57] of the entire ensemble for $N \leq 9$, to arise already for very small $N$. In figure 6 we show the PDF for all system sizes, which demonstrates the skewness and the small variation of the shape with $N$. Yet, finite-size effects larger than for GBP in figure 1 emerge deep in the tails of these PDFs.

Unlike the overall shape of the PDF for energy fluctuations, their actual width, measured in terms of the standard deviation $\sigma_N(e_0)$ in equation (2), varies in a characteristic way with $N$. A plot of the data for $\sigma_N(e_0)$ in table 6 on a double-logarithmic scale in figure 7 suggests a power-law decay with $N$, but the data does not exhibit purely linear behavior on this scale, as a simple fit reveals. Only when we restrict to $N > 100$, a fit of the data according to equation (2) with just the leading ($\rho$-dependent) term provides satisfactory results, with a value of $\rho$ just above $5/6$. A more consistent fit of all the data is provided when higher-order corrections are considered. This can only succeed for a reasonable, fixed value of $\rho$. We indeed accomplish almost identical fits of this sort for either $\rho = 2/3$ or $5/6$ (and probably any nearby value), see figure 7. In this regard, the fit for fixed $\rho = 5/6$ has the added benefit that the higher-order term appears to scale with $a \approx 1$, a likely candidate for a next-order correction. But if leading and next-order correction are that close, for instance $N^{-5/6}/N^{-1} \sim N^{1/6}$, to obtain the asymptotic scaling of $\rho$ separated by a decade from any transient behavior would require results for $N \gtrsim 10^6$. Thus, with the present data, a conspiracy between such terms leading to the observed behavior could not be excluded.

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Figure 7. Double-logarithmic plot of the data from table 6 for $\sigma_N(e_0)$ as a function of $N$. The data is fitted by a first-order fit with $a + bN^{-\rho}$ restricted to $100 < N < 800$ (dotted line), giving $\rho \approx 0.76$ with $\chi^2/\text{ndf} \approx 0.24$ for $\text{ndf} = 13$. Second-order fits with $a + bN^{-\rho} + cN^{-\alpha}$ allowing all $N < 800$ and fixed $\rho = 3/4$ (dashed–dotted line) or $\rho = 5/6$ (dashed line) both give essentially indistinguishable results with $\chi^2/\text{ndf} \approx 0.7$ for $\text{ndf} = 25$ in either case. For $\rho = 3/4$ we find $a \approx 1.3$, and for $\rho = 5/6$ it is quite consistent with unity, $a \approx 1$.

To illustrate the difficulty more clearly, we follow the procedure for GBP in section 2 and extrapolate for $\rho$ according to equation (6). The variables $y = -\log \sigma/\log N$ plotted versus $x = 1/\log N \rightarrow 0$ should provide an asymptotically linear extrapolation (with exponentially small corrections $\sim xe^{-(a-\rho)/x}$, if $a > \rho$) towards the exponent $\rho$ at the $y$ intercept for $N \rightarrow \infty$. Plotting the SK data up to $N \approx 1000$ in this fashion in figure 8 again indicates a value just above $\rho = 3/4$ and apparently far below $\rho = 5/6$. But unlike the GBP data in figure 2, the data for SK still has transient features even for such large values of $N$. Only a nonlinear fit according to all three terms in equation (6), but taking an already fixed $\rho = 5/6$ as given, makes such a high value for $\rho$ plausible. Further support for such a higher value of $\rho$ is provided by the following study of spin glasses on Bethe lattices. On the other hand, the GBP example above and the likely result for the $m$-vector model of $\rho = 4/5$ [27, 28] would suggest that an altogether different value of $\rho$ between these two rational values is conceivable. In fact, a purely linear extrapolation in figure 8 and the fit in figure 7 for $N \gtrsim 100$ would lead to an asymptotic value for $\rho$ very close to that of GBP in section 3 above.

4.3. Extreme fluctuations

Considering the large amount of data we have obtained for SK, we can inspect further details of the energy fluctuations. In particular, we can look deeper into the tails of the PDFs displayed in figure 6, where they are rescaled by their respective $\sigma_N$. Here, we treat these PDFs unscaled, according to the form proposed in [25]. There, it was shown that, for ground state energies lower than the average, the corresponding branch far in the negative tail of each PDF falls exponentially with an argument proportional in $N$,
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Figure 8. Extrapolation plot according to equation (6) towards a prediction of $\rho$ at the ordinate intercept for SK (black circles) and spin glasses on Bethe lattices (blue squares). The abscissa denotes the system sizes $N$ on a scale of $1/\log N$. A linear fit (red dashed line) of the SK data in the apparent scaling regime for $N \geq 80$ predicts a value of $\rho \approx 0.76$. The inclusion of the alternative value $\rho = \frac{5}{6}$ (dotted line) here shows the dramatic change required for the data to attain such a value. Yet, a fit (black dashed line) according to equation (6) involving nonlinear corrections down to the smallest $N$ is possible, if $\rho = \frac{5}{6}$ is assumed. The corresponding situation for Bethe lattices makes such an extrapolation further plausible.

while configurations with larger energies are particularly rare for larger system sizes such that the positive tail is suppressed by a factor $N^2$. This system-size dependence is largely lost when each PDF is rescaled by its width $\sigma_N$ in figure 6.

In figures 9 and 10, we extract the argument of the exponential tails and plot the data for each tail reduced by the indicated power of $N$. In the process, the PDF data $P(e)$ for each system size has to be gauged by an arbitrary reference point $P_{\text{max}}$, typically near $P(\langle e \rangle_N)$. To assess scaling, transient behavior too close to the average or statistically deficient data too deep in the tails have to be discarded. The resulting collapse of all the intermediate data onto a power-law function is presented in the upper panel of each figure on a logarithmic scale. According to [25], the power-law exponent can be interpreted as $\rho^{-1}$ for $e \ll \langle e \rangle$ and as $\rho^{-2}$ for $e \gg \langle e \rangle$. There, it was calculated that $\rho = \frac{5}{6}$, exact at least for the negative tail. To provide a reference, we have include also the analysis for $\rho = \frac{3}{4}$ in these plots. While the differences are again slim (and it could be argued that true asymptotic behavior has not been reached), the consistent scaling collapse of this vast amount of data, in fact, would have favored a value closer to $\rho = \frac{3}{4}$ instead of the predicted $\rho = \frac{5}{6}$. Either way, both tails independently exhibit similar scaling behavior.

When viewed on a linear scale, by taking the respective power, only a value closer to $\rho = \frac{3}{4}$ provides consistent linear behavior for the extant data (see the lower panels of figures 9 and 10). In [25], a similar linear plot was shown to scale consistently (up to $N = 150$) with their analytical prediction, $\rho = \frac{5}{6}$ and $\sim -1.5044(e - \langle e \rangle)$ (for the negative branch only). It is clear from our direct comparison here that, even with the vast amount of additional data, an ultimately conclusive decision on the true value of $\rho$ would be...
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Figure 9. Data collapse on logarithmic scale of all SK data for energies smaller than the average from figure 6. On top, rescaled by an appropriately chosen $P_{\text{max}}$, the data collapses onto a power-law curve, which exhibits scaling over more than a decade. (Transient data points with $P$ too close to $P_{\text{max}}$ have been removed for clarity.) The collapse is most consistent (see dashed–dotted line) with $\rho^{-1} = \frac{4}{3}$ and differs, although only slightly, from $\rho^{-1} = \frac{6}{5}$ (dashed line). On the bottom, the same data (for $N > 100$) is plotted on a linear scale. The collapse in either case compares favorably with the exact result from [25], $1.5044\Delta e$, marked by a straight line.

elusive. The comparison also shows that an analysis of these tails on a logarithmic scale is favorable over a linear scale which squashes the most asymptotic data points originating with larger system sizes. Even on a logarithmic scale, though, it is not easy to extract the relevant asymptotic information, as ever deeper in the tails only ever smaller-sized systems contribute. But overall, in this data, small-sized and large-sized systems seem to follow similar scaling and project a self-consistent picture.

5. Spin glasses on Bethe lattices

To provide a new perspective on the ground state energy fluctuations in SK, we revisit spin glasses with $\pm J$ bonds on Bethe lattices (SG), in particular on those of degree $r = 3$. A similar study has been undertaken in [30, 31], which concerned thermodynamic averages
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Figure 10. Data collapse on logarithmic scale of all SK data for energies larger than the average from figure 6. Rescaled by an appropriately chosen $P_{\text{max}}$, the data collapses onto a power-law curve, which exhibits scaling over more than a decade. (Transient data points with $P$ too close to $P_{\text{max}}$ have been removed for clarity.) The collapse is most consistent (see dashed–dotted line) with $\rho^{-2} = \frac{8}{3}$ and differs, again only slightly, from $\rho^{-2} = \frac{12}{5}$ (dashed line). On the right, the same data (for $N > 50$) is plotted on a linear scale. In this form, $\rho = \frac{3}{4}$ is clearly more consistent with linear scaling. Except for very small values, this case does not compare so well with the perturbative result from [25], $0.55(6)\Delta e$, marked by a straight line.

of ground state energies and entropies. Here, we extend the sampling of ground state energies to measure the PDF of ground state energy fluctuations and the scaling of their width. To that end, in table 7 we have added a large number of instances at each system size, up to $N = 4096$. Unlike for Bethe lattices of higher degree, at degree 3 we can utilize exact methods [41, 42, 58] to reduce the number of variables in the optimization problem by about 42%, hence, making larger system sizes accessible at sufficient statistics.

5.1. Average ground state energy

In figure 11, we present the average energy densities obtained with EO at the system sizes simulated. As in [30], the extrapolation of the data is virtually linear when plotted...
Table 7. List of all the data obtained with EO for Bethe lattices of degree $r = 3$ for various system sizes $N$. Given are the number of instances $n_I$ considered at each $N$, and the average ground state energy density $\langle e_0 \rangle_N$ and standard deviation $\sigma(e_0)$ over these instances.

| $N$  | $n_I$  | $\langle e_0 \rangle_N$  | $\sigma(e_0)$ |
|------|--------|--------------------------|---------------|
| 16   | 1000000| $-1.1467(1)$             | 0.10177       |
| 32   | 1000000| $-1.19375(6)$            | 0.06003       |
| 44   | 1680320| $-1.20895(4)$            | 0.04695       |
| 64   | 1000000| $-1.22314(4)$            | 0.03515       |
| 80   | 1486688| $-1.23005(2)$            | 0.02952       |
| 128  | 2000000| $-1.24153(1)$            | 0.02043       |
| 160  | 3273585| $-1.24583(1)$            | 0.01714       |
| 256  | 1498807| $-1.25296(1)$            | 0.01181       |
| 350  | 4015909| $-1.25660(1)$            | 0.00921       |
| 512  | 7638942| $-1.26007(1)$            | 0.00680       |
| 750  | 1718511| $-1.26274(1)$            | 0.00501       |
| 1024 | 743404 | $-1.26444(1)$            | 0.00390       |
| 2048 | 113389 | $-1.26710(1)$            | 0.00226       |
| 4096 | 4886  | $-1.26867(2)$            | 0.00135       |

as a function of $N^{-2/3}$. Such a linear extrapolation yields $\langle e_3 \rangle_\infty = -1.2715(1)$ for the thermodynamic energy density, consistent with the value determined in [30] and consistent with the one-step replica symmetry breaking result reported in [3, 59]. Remarkably, an attempt at adding a higher-order correction term contrasts with the same discussion for SK. Neither of the two types of higher-order fits presented in figure 4 provide reasonable results here. In turn, a fit to equation (5), which failed for SK, does converge on this data, see figure 12. Across the plotted regime, the thermodynamic value for $e_\infty$ remains quite robust. The optimum is rather close to $\omega = 2/3$; such a second-order fit including $\omega$ also shown in figure 11 converges to $\omega \approx 0.677$.

5.2. Ground state energy fluctuations

In figure 13, we show the probability density functions (PDF) of the energy densities around those averages. Overall, those PDFs are a bit more symmetrical than for SK in figure 6, but exhibit even more finite-size effects in both tails, especially in comparison with the corresponding PDFs of GBP in figure 1. Despite their more symmetrical appearance, the scaling with $N$ of the deviations $\sigma$ listed in table 7 seems to indicate an even higher value of $\rho$, as figure 8 suggests. There, those $\sigma$ for the Bethe lattice are displayed in an extrapolation plot together with that of SK, to highlight their similarity. This data is somewhat smoother than for SK, but just as much beset with transients. A family of extrapolants for each degree $r$ seems conceivable, reaching all the way to the SK limit at $r = \infty$. In parallel with the discussion for SK in section 4.2, we can at best argue that $\rho = 3/6$ is consistent with the trend of the extrapolation. In this plot, a value of $\rho = 3/4$ or even that from GBP seems to be ruled out by that trend.
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Figure 11. Extrapolation plot of the average ground state energy densities \( \langle e_0 \rangle_N \) for Bethe lattices of degree \( r = 3 \) as a function of the presumed finite-size corrections, \( 1/N^{2/3} \). As in figure 5, the statistical errors indicated are much smaller than symbol sizes. For \( N \to \infty \), irrespective of the order of the fit, the data extrapolates to \( \langle e_0 \rangle_\infty = -1.2715(1) \) at the intercept.

Figure 12. Second-order fit over a range of fixed \( \omega \), with logarithmic corrections, to the average ground state energies \( \langle e_0 \rangle_N \) for spin glasses on Bethe lattices of degree \( r = 3 \) in table 7.

5.3. Extreme fluctuations

We have attempted a detailed analysis of the tails of the fluctuations for Bethe lattices with the identical approach as conducted in section 4.3 for SK. The results shown in figures 14 and 15 are indistinguishable from those for SK above, and would also suggest a value closer to \( \rho = \frac{3}{4} \) for the Bethe lattice, which seems to contradict the indication provided by the extrapolation of \( \sigma \) in figure 8.
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Figure 13. Plot of the probability density functions (PDF) of the ground state energy densities $e_0$ obtained for the spin glass on a Bethe lattice of degree $r = 3$ in units of the standard deviation $\sigma$. Here, in comparison with figures 1 and 6, significant finite-size effects are detectable in both tails.

6. Spin glasses on random graphs

As a useful reference point to the previous studies, we also include a comparison with a spin glass on sparse, ordinary random graphs of mean degree $C = 2$. It provides an example where fluctuations in the ground states, whether the energy or the cost, appear to converge to a normal distribution. As argued in section 2.2, it is essential for the case of a fluctuating geometry to focus on the actual cost, i.e. the total absolute weight of the violated bonds, of the ground state. Still, even the PDF for these ground state costs seems asymptotically Gaussian, as has been predicted recently in [24].

6.1. Average ground state costs

In table 8, we have listed the average ground state costs and their deviations for a number of system sizes up to $N = 4096$. A large number of instances have been averaged over, even at the largest sizes, since the exact graph reduction methods [41, 42, 58] used for the Bethe lattice above are even more effective here: even at the largest size, those reductions result in graphs of at most 15% of the original size that need to be optimized with the EO heuristic.

In figure 16, we plot the extrapolation of those average ground state costs to the thermodynamic limit. Again, the extrapolation proves most consistent with $N^{-2/3}$ corrections at finite size, although stronger transients are apparent here. In fact, figure 17 indicates that finite-size corrections may be a pure power series in $N^{-2/3}$, the first two orders of which are also shown as asymptotic fits in figure 16.

6.2. Ground state cost fluctuations

In figure 18, we have plotted the PDF for the ground state cost fluctuations. It shows no sign of asymmetry for any size $N$. Therefore, it is quite surprising that the finite-size
Figure 14. Data collapse on logarithmic scale of all Bethe lattice data for energies smaller than the average from figure 13. Top, rescaled by an appropriately chosen $P_{\text{max}}$, the data collapses onto a power-law curve, which exhibits scaling over more than a decade. The fit (straight line) gives an exponent of $\rho^{-1} \approx 1.36$. Bottom, the same data is plotted on a linear scale. In this form, $\rho = \frac{3}{4}$ is more consistent with linear scaling (dashed straight lines guide the eye).

Table 8. List of all the data obtained with EO for spin glasses on random graphs of average degree $C = 2$ at system sizes $N$. Given are the number of instances $n_I$ considered at each $N$, and the average ground state cost density $\langle c_0 \rangle_N$ and average standard deviation $\sigma_N(c_0)$ over these instances.

| $N$  | $n_I$    | $\langle c_0 \rangle_N$ | $\sigma_N(c_0)$ |
|------|----------|--------------------------|-----------------|
| 64   | 1050000  | 0.05504(2)               | 0.01693         |
| 128  | 1050000  | 0.04994(1)               | 0.01062         |
| 180  | 1050000  | 0.04808(1)               | 0.00846         |
| 256  | 1050000  | 0.04652(1)               | 0.00671         |
| 360  | 1050000  | 0.045296(5)              | 0.00537         |
| 512  | 1050000  | 0.044266(4)              | 0.00429         |
| 1024 | 395722   | 0.042808(4)              | 0.00278         |
| 2048 | 668638   | 0.041883(4)              | 0.00183         |
| 4096 | 319036   | 0.041304(4)              | 0.00123         |

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values obtained for the deviation $\sigma_N(c_0)$ plotted in figure 19 and extrapolated in figure 20 exhibit a rather slow convergence to a normal width. These results serve as a warning how, even for seemingly trivial fluctuations, the asymptotic behavior might be reached only quite slowly.

7. Three-spin interactions on Bethe lattices

To complement the discussion of glasses with two-spin interactions, and to compare with related work [32,33,60], we have also considered spin glasses on Bethe lattices with three-spin interactions, both with discrete ($\pm J$) and Gaussian bonds, as listed in tables 9 and 10. This study succeeds in confirming recent observations regarding finite-size corrections to the average ground state energy [33]. But our simulations can merely give a crude picture of deviations within the distribution of those energies. This inadequacy has two origins: first, it proves inherently challenging to determine ground states for instances of this problem with any accuracy already at moderately sized systems. The systems are
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Figure 16. Extrapolation plot of the average ground state cost densities \( \langle c_0 \rangle_N \) for ordinary random graphs of average degree \( C = 2 \) as a function of the presumed finite-size corrections, \( 1/N^{2/3} \). As in figure 5, the statistical errors indicated are much smaller than symbol sizes. Also shown are a first-order (blue dashed–dotted line) and a second-order fit (black dashed line) in powers of \( 1/N^{2/3} \). For \( N \to \infty \), the data extrapolates to \( \langle c_0 \rangle_\infty = 0.040\,30(5) \) at the intercept.

Figure 17. Second-order fit in powers of \( N^{-\omega} \) over a range of fixed \( \omega \), to the average ground state costs \( \langle c_0 \rangle_N \) for spin glasses on random graphs of degree 2 in table 8. The minimum in \( \chi^2/ndf \) in the upper plot strongly suggests a pure power series with \( \omega = \frac{2}{3} \); such a fit is included in figure 16. The lower panel shows the range of extrapolated values in the thermodynamic cost density.

large enough to predict average energies with reasonable errors, but insufficient for the asymptotic analysis for the deviations. Second, those deviations in their own right appear to be far narrower for this problem than for any of the two-spin models above. In fact, for discrete bonds the ground states seem to cover only a few states above and below the average, with almost an invariant width, such that the deviations in the density seem to fall with \( \sim 1/N \), similar to theoretical predictions for the corresponding SK model in [32].

A somewhat wider distribution is observed for Gaussian bonds, which provides for a smoother appearance for the PDF at all system sizes compared to the discrete case. Any
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Figure 18. Plot of the probability density functions (PDF) of the ground state cost densities \( c_0 \) obtained for the spin glass on an ordinary random graph of average degree 2 in units of the standard deviation \( \sigma \).

Figure 19. Double-logarithmic plot with system size \( N \) of the deviations in the ground state costs, here given as \( N^{1/2} \sigma N (c_0) \) to highlight any difference from Gaussian behavior, for a spin glass on an ordinary random graph of average degree \( C = 2 \). The plot is far from flat or linear, suggesting significant corrections to scaling. Expecting asymptotically normal scaling with \( \rho = \frac{1}{7} \), we fitted the data with an additional higher-order correction term with \( \sim N^{-a} \) (dashed line), as in equation (2). The fit determines \( a \approx 0.75 \).

Skewness can only be observed when plotted for ground state cost fluctuations; energy fluctuations would always be normal, originating from the random fluctuations in the total bond weight themselves, as described in section 2.2. Surprisingly, these cost fluctuations skew exactly in the opposite direction from any previous studied PDF, such as those above. Although the deviations \( \sigma \) extracted from those PDFs indeed seem inconsistent with \( 1/N \) scaling, the system sizes attained in this study are rather small, \( N \leq 100 \), and asymptotic behavior may not have been reached in this study.

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Figure 20. Extrapolation plot of the data for the deviation $\sigma$ in table 8 according to equation (6). A fit is only possible for a fixed $\rho = \frac{1}{2}$.

Table 9. List of all the data obtained with EO for $p = 3$-spin glasses on Bethe lattices of degree $r = 4$ at system sizes $N$ for discrete bonds. Given are the number of instances $n_I$ considered at each $N$, and the average ground state energy density $\langle e_0 \rangle_N$ and standard deviation $\sigma$ over these instances. The largest system size has unacceptable systematic errors and is ignored in any fit.

| $N$  | $n_I$  | $\langle e_0 \rangle_N$ | $\sigma_N(e_0)$ | $N$  | $n_I$  | $\langle e_0 \rangle_N$ | $\sigma_N(e_0)$ |
|------|--------|--------------------------|-----------------|------|--------|--------------------------|-----------------|
| 15   | 10000  | $-1.104(1)$              | 0.0995          | 51   | 130000 | $-1.1760(1)$            | 0.0296          |
| 18   | 100000 | $-1.1171(3)$             | 0.0834          | 54   | 800000 | $-1.17843(3)$           | 0.0267          |
| 24   | 100000 | $-1.1406(2)$             | 0.0584          | 60   | 25000  | $-1.1829.2(2)$          | 0.0242          |
| 30   | 30000  | $-1.154(3)$              | 0.0500          | 75   | 40000  | $-1.18892(3)$           | 0.0189          |
| 33   | 100000 | $-1.1576(2)$             | 0.0460          | 90   | 35000  | $-1.1929(1)$            | 0.0157          |
| 36   | 100000 | $-1.1619(1)$             | 0.0411          | 120  | 11000  | $-1.1973(1)$            | 0.0121          |
| 39   | 100000 | $-1.1665(1)$             | 0.0365          | 150  | 20000  | $-1.20087(2)$           | 0.0103          |
| 45   | 30000  | $-1.173(2)$              | 0.0329          | 180  | 80000  | $-1.20264(3)$           | 0.0087          |
| 48   | 800000 | $-1.17435(3)$            | 0.0319          | 240  | 350    | $-1.1995(4)$            | 0.0067          |

Table 10. List of all the data obtained with EO for $p = 3$-spin glasses on Bethe lattices of degree $r = 4$ at system sizes $N$ for Gaussian bonds. Given are the number of instances $n_I$ considered at each $N$, and the average ground state cost density $\langle c_0 \rangle_N$ and standard deviation $\sigma$ over these instances. The largest system size has unacceptable systematic errors and is ignored in any fit.

| $N$  | $n_I$  | $\langle c_0 \rangle_N$ | $\sigma_N(c_0)$ |
|------|--------|--------------------------|-----------------|
| 33   | 100000 | 0.02366(3)               | 0.00916         |
| 39   | 120000 | 0.02261(2)               | 0.00783         |
| 51   | 120000 | 0.02122(2)               | 0.00616         |
| 66   | 80000  | 0.02016(3)               | 0.00495         |
| 99   | 25000  | 0.01901(2)               | 0.00356         |
| 144  | 3500   | 0.0193(1)                | 0.00274         |
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Figure 21. Extrapolation plot of the average ground state energy densities \( \langle e_0 \rangle_N \) for a spin glass with discrete bonds in which \( p = 3 \) spins mutually interact on a Bethe lattice of degree \( r = 4 \), as a function of the presumed finite-size corrections, \( 1/N \).

Figure 22. Extrapolation plot of the average ground state cost densities \( \langle e_0 \rangle_N \) for a Gaussian spin glass with three-spin interactions on a Bethe lattice of degree \( r = 4 \), as a function of the presumed finite-size corrections, \( 1/N \).

7.1. Ground state energy

In figures 21 and 22, we extrapolate the obtained average ground state energies (for discrete bonds) or costs (for Gaussian bonds) in tables 9 and 10. In both cases, finite-size corrections appear to decay with volume corrections, like \( 1/N \), stronger than in any of the \( p = 2 \)-spin models above. Hence, even though the system sizes are small, quite reasonable extrapolations are achieved. In the discrete case in figure 21 there appears to be significant structure in the transients. By reproducing the exact ground states for a sample of those instances up to size \( N = 51 \) with exact (branch-and-bound) algorithms, we have verified that these are not due to systematic errors in the optimization heuristic, as 100% agreement was achieved for each instance. Rather, we expect that those effects are due to the constraints in the formation of 4-regular hypergraphs at small \( N \) in combination...
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Figure 23. Log–log plot of the deviations $\sigma$ in the ground state energy fluctuations of a $p = 3$-spin glass on Bethe lattices of degree $r = 4$ as a function of system size $N$. The data is very difficult to fit, and we only provide the dashed line $\sim 1/N$ as a guide to the eye.

with the discrete set of bonds available. Correspondingly, the Gaussian data is free of any such structure, and thus extrapolates with comparable accuracy despite the overall smaller system sizes used.

For $N \to \infty$, the discrete data in figure 21 extrapolates to $\langle e_0 \rangle_\infty = -1.213(2)$ at the intercept, slightly above the one-step replica symmetry breaking (RSB) prediction [60], as would be expected for the true ground state at full RSB. With bonds drawn from a Gaussian distribution, we instead plot the actual cost of violated bonds. It is difficult to obtain good minima already at $N \approx 100$, such that we can only extrapolate data for smaller $N$. For $N \to \infty$, the extrapolation yields a cost of $\langle c_0 \rangle_\infty = 0.0167(4)$ at the intercept. Since average cost and energy density for Gaussian bonds are related via equation (7), we obtain with $\langle |J| \rangle = \sqrt{2/\pi}$, $r = 4$, and $p = 3$ that $\langle e_0 \rangle = -1.030(1)$.

7.2. Ground state fluctuations

In light of the limited ability to produce ground states at larger system sizes, any prediction for the fluctuation exponent $\rho$ is poor. Furthermore, extreme fluctuations are difficult to attain, since the width is rather narrow. Yet, for discrete bonds the data plotted for $\sigma$ in figure 23 is quite consistent with $1/N$ decay, i.e. $\rho = 1$. But there does not seem to be a clear trend towards asymptotic scaling in the case of Gaussian bonds shown in figure 24. If anything, the data appears to exhibit upward curvature, away from a $1/N$ scaling regime, indicating that $\rho$ in this case may be even lower than the fitted value of $\approx 0.87$. Such a discrepancy between discrete and Gaussian bonds on Bethe lattices was also noted for the $p = 2$-spin model [34].

With the rapid decay of the width for discrete bonds, it is not surprising that the PDF for its energy fluctuations has a somewhat rugged appearance: only a few, discrete energy values can be taken on the left or right of the mean. As shown in figure 25, the PDF otherwise skews similarly to all previous cases. It comes as a surprise then that the corresponding PDF for Gaussian bonds in figure 26 skews exactly in the opposite
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Figure 24. Log–log plot of the deviations $\sigma$ in the ground state energy fluctuations for a $p = 3$-spin glass on Bethe lattices of degree $r = 4$ as a function of system size $N$, here for Gaussian bonds. As for the plot for discrete bonds in figure 23, this data is also difficult to fit, and there is a visible trend to even lower values in the exponent than 0.87 found by only fitting to sizes $N \leq 100$ (dashed line).

Figure 25. Plot of the probability density functions (PDF) of the ground state energy densities $e_0$ obtained in units of the standard deviation $\sigma$, for the $p = 3$-spin glass with discrete bonds on an $r = 4$-regular random graph. The rugged appearance of the data is due to the discreteness of the bonds and the fact that only a very narrow set of energy values around the mean is taken on.

direction. Although it is plotted for the cost fluctuations instead—the energy fluctuations in the inset are purely normal—this does not explain the difference in the skewness, since cost and energy are linearly related (as in equation (7)). Lower cost correlates with lower energy and vice versa. We speculate that the skewness here has a rather trivial origin: as indicated by the very low average ground state cost per spin, $\langle c_0 \rangle_\infty = 0.0167(4)$ (about 1/4 of that for discrete bonds), below-average-cost instances may be hard to find due to the proximity of entirely cost-free, ‘perfect’ solutions (although we have not actually generated
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Figure 26. Plot of the probability density functions (PDF) of the ground state cost densities $c_0$ obtained in units of the standard deviation $\sigma$, for the $p = 3$ spin glass with Gaussian bonds on an $r = 4$-regular random graph. The data is skewed with a sharp cutoff for costs less than the average and a long tail for larger cost, exactly opposite to any previous PDF for energy fluctuations. The inset shows the same data plotted as energy fluctuation PDFs, which are purely normal distributed.

We can address the puzzling skewness for the Gaussian case further by comparing with previous results with Gaussian bonds on $p = 2$-spin glasses on Bethe lattices. While we have experienced this case already for discrete bonds at $r = 3$ above in section 5 without any qualitative difference in behavior compared to the SK model, its Gaussian version presents a very odd pattern. In [34] we have already remarked on the unusual finite-size corrections to the thermodynamic average ground state cost or energy and the confusing trend that already beset the cost deviations $\sigma(c_0)$. We therefore missed the even more surprising evolution with $r$ and $N$ of the skewness in the corresponding PDFs. Aside from some finite-size effects, all PDFs for the energies are approximately normal distributions. But the PDFs for cost fluctuations shown in figure 27 range from those strongly skewed, comparable to figure 26, for small $r$ to those with only mild skewness at larger $r$. For all cases, but most drastically for larger $r$, increasing system size $N$ symmetrizes the PDFs towards an apparently normal shape. Note that, for the SK limit $r \rightarrow \infty$, these distributions should approach a normal form for the cost. While energy

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Figure 27. Plot of the PDFs for the fluctuations of the ground state costs per spin for a $p = 2$-spin glass with a Gaussian bond distribution on Bethe lattices of degree $r = 3, 4, \ldots, 10, 15$. For smaller $r$ and sizes $N$, the PDFs are right-skewed, just as in figure 26, but especially for larger $r$ those PDFs appear to approach a normal distribution for large sizes $N$.

fluctuations should become the non-trivial PDF in the SK limit, $r = 15$ is apparently not large enough for this effect to be discernible.

8. Conclusions

To elucidate the origin of the unusual ground state deviations observed in the SK model, we have parsed over a range of different spin glass and combinatorial models in an effort to provide context for any typical or atypical properties. The clearest picture emerges from graph bipartitioning (GBP) on Bethe lattices. The scaling exponent $\rho$ for each degree $r$ of the network possesses a convincing extrapolation, but to values unlike those proposed for SK [20–25], suggesting a very different origin for the fluctuations in GBP. At best, they come closest to the value of $\rho = \frac{4}{3}$ proposed for the $m$-vector spin glass [27, 28]. The situation for SK is less clear, apparently due to very strong higher-order corrections in the finite-size behavior. Although far from a scaling with the theoretically favored value, such a behavior for SK becomes plausible with very close $1/N$ corrections, a scenario further
Simulations of ground state fluctuations in mean-field Ising spin glasses supported by the Bethe lattice spin glass at degree $r = 3$ (with discrete bonds) exhibiting very similar behavior but inherently closer to $\rho = \frac{5}{6}$. As the example of the vector model demonstrates, entirely distinct values are conceivable for any of these models, but since in the limit $r \to \infty$ the Bethe lattices approach SK, such a distinction seems implausible. A look deep into the tails for SK and the Bethe lattices, for which extensive results have been generated, would suggest that the scaling of the deviations $\sigma$ with the exponent $\rho$, which is dominated by near-typical fluctuations, may be disconnected from the extremely atypical fluctuations deep in the tails, which is more consistent with $\frac{3}{4}$ scaling for both models. But, despite the massive amount of data obtained here, any true asymptotic scaling for the tails may still be elusive.

The situation might be simpler for models in which more than two spins interact. For instance, we find for a $p = 3$-spin glass model with discrete bonds on a $r = 4$-regular Bethe lattice that fluctuations scale about with $1/N$, i.e. $\rho = 1$. This result was found also for the REM ($p \to \infty$) in [23]. Indeed, for any $p \geq 3$, $1/N$ fluctuations were calculated for above-average energies in SK in one-step RSB, using an argument that should also hold for the sparse graphs [61] used here. On the other hand, the same model with Gaussian bonds demonstrates the fragility of the phenomenon: energy fluctuations get overwhelmed by trivial (normal) fluctuations in the continuous bond weights, while the more pertinent cost fluctuations are skewed exactly in the opposite direction from those from SK, or even those on the same graph with discrete bonds. A same effect is found for $p = 2$ on Bethe lattices at low $r$. In summary, the large variation in behaviors of fluctuations not only between models, but even within models for different bond distributions, hints at the strong dependence on minute details of the underlying graph geometry and variability in bond weights. Either can impact on whether and how frustrated plaquettes correlate to ease the cost when an instance possesses more or less of those than the average.

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