Replica Symmetry and Replica Symmetry Breaking for the Traveling Salesperson Problem

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We study the energy landscape of the Traveling Salesperson problem (TSP) using exact ground states and a novel linear programming approach to generate excited states. We look at some different ensembles, notably the classic finite dimensional Euclidean TSP and the mean-field $(1,2)$-TSP, which has its origin directly in the mapping of the Hamiltonian circuit problem on the TSP. Our data supports previous conjectures that the Euclidean TSP does not show signatures of replica symmetry breaking neither in two nor in higher dimension. On the other hand the (1,2)-TSP exhibits a signature of broken replica symmetry.

Introduction The concept of *replica symmetry breaking* (RSB) was introduced in the context of spin glasses [1, 2], where it has a long history of debate to which models it applies [3]. RSB is an assumption about the structure of the phase space (or "energy landscape"), which leads to the correct results for the Sherrington-Kirkpatrick (SK) spin glass [4]. RSB basically means that the phase space is hierarchically structured such that two configurations of very similar energy may be far away from each other in the configuration space. The phase space becomes *complex*.

The physics-inspired analysis of the phase-space structure has also been applied to combinatorial optimization problems, namely problems belonging to the class of nondeterministic polymonial (NP)-hard [5–7] problems (or the corresponding decision problems belonging to the class of NP-complete problems). For NP-hard problems currently only algorithms are known which exhibit a worst-case running time which grows exponentially with system size. Examples of NP-hard problems are satisfiability [8] and vertex cover [9]. Here, ensembles are known where replica symmetry (RS) breaks at some value of a control parameter [10–12]. This appears not to be surprising to many researchers because intuitively a hard optimization problem may correspond to a non-trivial energy landscape. This prompted many attempts to distinguish easy from hard instances or explore the energy landscape of such problems [13–19].

One of the best-known NP-hard combinatorial optimization problems is the Traveling Salesperson Problem (TSP) [20]. Somewhat surprisingly, in contrast to the aforementioned problems, only indications for RS have been found within studies of some TSP ensembles so far [21–24]. Nevertheless, for these analytical and numerical studies various approximations had to be used, somehow questioning the previous claims for RS.

In this work, by calculating numerically exact ground states and excitations, we confirm the previous results for theses specific ensembles. But on the other hand we show that there are indeed ensembles also for the TSP where RSB seems to be present, namely the $(1,2)$-TSP ensemble [25]. In particular, in contrast to previous numerical studies, which used heuristics to generate tours near the optimum [23, 24], we use an exact algorithm to find the true optimum and very specific excitations. This approach is facilitated by the combination of flexibility and high performance (compared to other exact algorithms for the TSP) of linear programming (LP) with branch and cut. Combined with the general increase in computing power and the improvement of algorithms for TSP optimization, it enables us to simulate comparatively large instances.

Model The Traveling Salesperson problem [26, 27] is defined on a complete weighted graph, where the vertices are usually called *cities* and the symmetric edge weights $c_{ij} = c_{ji}$ *distances* or *costs*. On this graph one searches for the shortest cyclic path through all N cities, which is called *tour* and can be represented by a set of edges T. An equivalent representation is through an symmetric adjacency matrix $\{x_{ij}\}$ where $x_{ij} = 1$ if city i is followed by city j on the tour and $x_{ij} = 0$ else. The *length* of the tour, which we will also call *energy*, is thus

$$L = \sum_{\{i,j\}\in T} c_{ij} = \sum_i \sum_{j<i} c_{ij} x_{ij}.$$

Note that an instance of the problem is completely encoded in the distance matrix c_{ij}.

To compare two tours T_1 and T_2, their *distance* or *difference* d is defined as the number of edges, which are in T_1 but not in T_2 [13]

$$d = \sum_{\{i,j\}\in T_1} 1 - x_{ij}^{(2)},$$

where $x_{ij}^{(2)}$ is the adjacency matrix corresponding to T_2. Like the link overlap for spin glasses is robust against the flipping of *compact* clusters with a low domain-wall energy, this observable is robust against partial reversals of the tour. If one considered instead the order of the cities in the tour, roughly equivalent to the spin overlap used for spin glasses, this could introduce a difference in the order of N by just changing two links.

Here, we study various enembles. First, the most intuitive and probably the most scrutinized [15, 20, 28–31] ensemble is the Euclidean TSP (ETSP). Here a Poisson point process in a square determines the locations of the cities and the distance matrix is filled with their Euclidean distances. We use periodic boundary conditions. An example for an optimal tour in such a configuration is shown in Fig. 1(a). It is straight forward to generalize this in higher dimensions using a Poisson point process in a hypercube and the corresponding Euclidean distances. The *random link model* (RLTSP) [13, 32] is an approximation, which disregards any correlations of the distance and therefore does not obey the triangular inequality. For this approximation in the statistical physics literature solutions were obtained under the premise that replica symmetry holds based on the replica method [21] and cavity method [24, 32, 33]. For our work, we studied the original ETSP ensemble, in which the density of the cities is constant, such that the average optimal tour length $L^o \sim N$ [28], i.e., the energy is extensive.

The $(1,2)$-TSP is the result of the classical mapping of the Hamilton circuit problem (HCP) onto the TSP [6]. The HCP is whether a cycle visiting every vertex exactly once exists on a given graph. The mapping from HCP to TSP is simply assigning the distance matrix as

$$c_{ij} = \begin{cases} 1, & \text{if } i \text{ and } j \text{ are adjacent,} \\ 2, & \text{otherwise.} \end{cases}$$

A Hamiltonian cycle exists, iff the length of the optimal tour is equal N. For simplicity sake, the ensemble we are looking at, is derived from an Erdős-Rényi graph where edges occur with probability $p = 1/N$, which results in an average degree of 1. Note that both limiting cases $p = 0$ and $p = 1$ are trivial since every tour will be optimal with length $2N$, respectively N. $p = 1/N$ was chosen since it is the percolation threshold, i.e., the graph is a forest like structure and to form a cycle almost surely non existent edges, i.e., distance 2, need to be used.

Like other studies on the solution space structure of different optimization problems, we look at excitations [34–36]. To detect signatures of RSB, we use a criterion introduced in the context of TSP by Mézard and Parisi in Ref. [22]. A configuration is called *quasi-optimal* if the relative difference of its energy L^* to the optimal energy L^o behaves as

$$\frac{L^* - L^o}{L^o} = \mathcal{O}\left(\frac{1}{N}\right). \tag{1}$$

According to Ref. [22], replica symmetry is broken, if there exists a quasi-optimal configuration, whose difference to the optimum goes as

$$\frac{d(T^o, T^*)}{N} = \mathcal{O}(1). \tag{2}$$

Intuitively this means, that a finite, i.e., $\mathcal{O}(1)$, energy is sufficient to change a finite fraction, i.e., $\mathcal{O}(N)$, of the system [34]. Furthermore, we have to ensure that some kind of order exists in the ground state, since an unordered system, where every edge has equal length and the solution space structure is trivial since every tour is identical, also fulfills the criterion. While a random tour and the optimal tour in this degenerate ensemble behave the same in every aspect, this is not true for the (1,2)-TSP, where a random tour has $\mathcal{O}(1)$ edges of length *one* but a optimal tour has $\mathcal{O}(N)$ edges of length *one*. Our measurements show the number of length *one* edges to be $0.4218(3)N$, corresponding to an ordered ground state. The ETSP shows a very similar behavior [37].

Note that degeneracy alone does not mean that a solution space structure is trivial, since a the degenerate solutions may be contained in one big cluster, at least in the thermodynamic limit. Famous examples, where this is the case include the two-dimensional Ising spin glass with ± 1 couplings [38] and the satisfiability problem in the range of few constraints [39].

Algorithms To solve an instance of the TSP, the following integer program, i.e., an LP with additional integer constraints Eq. (6), can be used [40]

$$\text{minimize} \quad \sum_i \sum_{j<i} c_{ij} x_{ij} \tag{3}$$

$$\text{subject to} \quad \sum_j x_{ij} = 2 \qquad i = 1, 2, ..., N \tag{4}$$

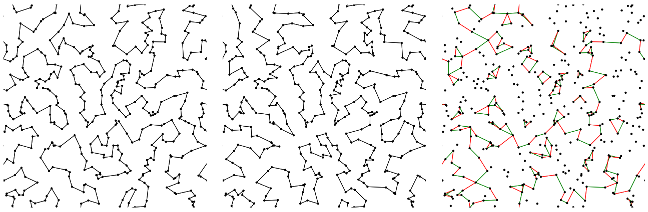
$$\sum_{i \in S, j \notin S} x_{ij} \geq 2 \qquad \forall S \subset V, \tag{5}$$

$$x_{ij} \in \{0, 1\} \tag{6}$$

where x_{ij} is the searched for adjacency matrix defining the tour. Eq. (3) minimizes the tour length, Eq. (4) ensures that the number of incident edges into every city is two, such that the salesperson enters every city once and leaves it again. Eq. (5) are the *subtour elimination constraints* (SEC), which prevent the tour to fragment into multiple not-connected subtours.

To construct the excitations T^*, we modify the linear program formulation using the obtained optimal tour T^o. This allows us to construct excitations with very specific properties. Since we want to check the criterions Eq. (1) and (2), we construct a very specific integer program which fixes Eq. (1) to be fulfilled and maximizes Eq. (2). If the replica symmetry of the problem is broken, the result should show the criterion to be fulfilled.

So we fix the allowed energy difference $L^* - L^o = \epsilon$ to a constant, which will lead to the desired relative energy difference Eq. (1) if the energy is extensive. For this reason our definitions of the ensembles are formulated in a way that leads to extensive energy, i.e., $\langle L^o \rangle \sim N$. Within this excitation energy window ϵ, the number of



(a) ETSP, optimal (b) ETSP, MaxDiff (c) ETSP, difference

FIG. 1: (color online) (a) and (b) show a configuration with $N = 400$ of the ETSP. Left is the optimal tour, right the MaxDiff excitation with $d = 129$ difference to the optimum. (c) shows the difference of the optimum and the excitation, red edges are removed, green are added for the excitation.

common edges with the optimal tour needs to be minimized to maximize the distance of the configurations. Thus replacing the objective with

$$\text{minimize} \sum_{\{i,j\}\in T^o} x_{ij} \tag{7}$$

and adding the additional constraint

$$\sum_i \sum_{j<i} c_{ij} x_{ij} \leq L^o + \epsilon \tag{8}$$

results in a suitable LP. We will call this LP *MaxDiff*. An exemplary solution of this LP is visualized in Fig. 1 in comparison to the optimal tour.

Results All values which are shown in this section are usually averaged over 10^2 to 10^3 exact solutions of realizations of the ensembles. Also note that due to the nature of the TSP and our solution approach, some realizations take far more computational resources than most and could not be solved in reasonable time respectively memory. The shown data is only for runs where more than 80% of instances were solved. We had to discard these few instances only for the largest system sizes anyway. For example, of the (1, 2)-TSP instances every single one with $N \leq 256$ was solved exactly. To test whether this still has a slight influence on the results, we created a biased sample by artificially discarding that half of the sample which consumed the most running time, respectively which needed the most memory, for the system sizes where every instance was solved exactly within the limits of the computational resources. For all tests the resulting distances d of the exact sample and the biased sample coincide within statistical errors, with no obvious trend. Also comparison with literature values for known values of the Beardwood-Halton-Hammersley constant β [28] match within 2 standard errors. Thus we are confident that the obtained statistics are robust against this sampling bias. As a technical detail, we use distances rounded to integers. To avoid effects of this discretization, we choose the range of values large. Hence this should not introduce notable effects. We use Concorde [41] to generate optimal tours, which implements this procedure at its core but also extends it with heuristics to speed up the process. For the excitations we use a custom implementation of the LP. Both programs use CPLEX [42] as the LP solver or for branch and cut.

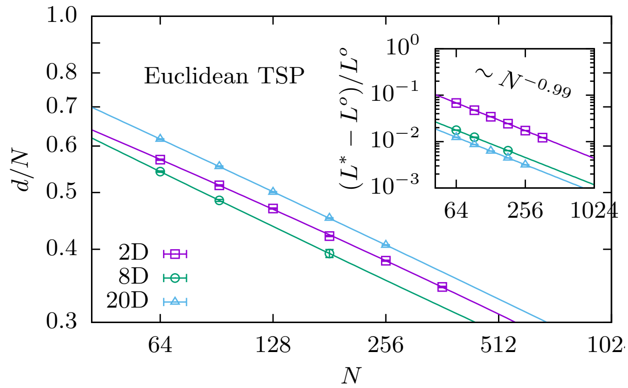


FIG. 2: (color online) The relative difference of the optimum and the MaxDiff excitation decreases as a power law with the system size N. For large N, the difference vanishes which is a hint for replica symmetry and a trivial solution space structure. The inset shows that the premise Eq. (1) is fulfilled. The higher dimensional cases have a 10 times larger ϵ.

The results for the MaxDiff excitation simulations for the two-dimensional ETSP are shown in Fig. 2. We found a $1/N$ behavior of the relative energy difference (inset) as required. Nevertheless the difference d of the tours also vanishes in the large N limit as a power law. So to change a finite fraction of an infinite system, a finite energy ϵ does not suffice. Thus, the results do not show the signature of replica symmetry breaking, hinting at a trivial solution space structure. This is consistent with previous studies expecting the ETSP to be replica symmetric. Results for the RLTSP lead to the same conclusion (not shown, but see Tab. I).

The same behavior indicating RS is present for the 8-dimensional and 20-dimensional ETPS, also shown in Fig. 2. Thus a simple increase in dimensionality does apparently not change the behavior regarding replica symmetry much. This is in strong contrast to spin glasses, where in high dimensions above the upper critical dimension the system is believed to behave [43–46] like the mean-field SK model [1, 2], corresponding to RSB.

Next, we will look at an ensemble which is closer to a direct mapping from the Hamilton circuit, which is usually used to prove the TSP NP-complete. The mapping creates an instance of the $(1, 2)$-TSP. For three tested values of the finite excitation energy $\epsilon \in \{20, 30, 60\}$, we calculated the difference between the optimal and excited tours d, shown in Fig. 3. First, see inset, the relative energy difference decreases as $1/N$ as required. The measured difference d does not follow a pure power law, but seems to converge to a non-zero offset. Extrapolating the difference for large N with $\frac{d}{N} = aN^b + D^\infty$ (cf. Ref. [34])

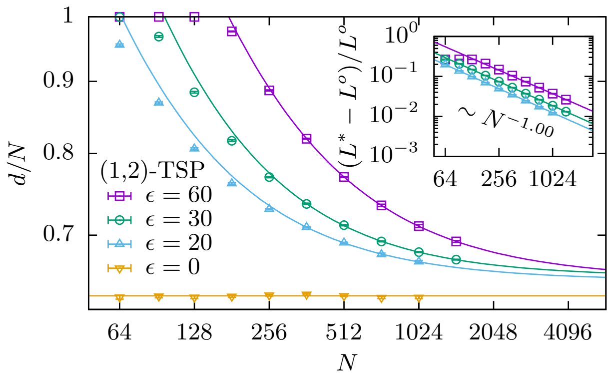


FIG. 3: (color online) Statistics of the $(1, 2)$-TSP for a connectivity of $Np = 1$. The MaxDiff constraints with the finite excitation energy $\epsilon \in \{20, 30, 60\}$ are used for the three curves respectively. The distance of the excitation to the optimal tour is extrapolated with an offsetted power law ansatz $\frac{d}{N} = aN^b + D^\infty$. The fit parameters are obtained for $N > 256$. All three result in a convergence to a finite D^∞ for large N, i.e., a finite fraction, indicating RSB. The inset shows the relative energy difference of the optimum and the excitation, showing a perfect $1/N$ form, as required by the RSB criterion.

leads to an offset for each ϵ, which are consistent with the most accurate value we obtained $D^\infty = 0.652(2)$ and exponents consistent with $b = -1$. All values are shown in Table I. Note that for small N finite size effects are visible, where ϵ is of the order of the optimal length and the excitation can differ in every single edge. Therefore, the difference is clamped at $d/N = 1$. For larger N this does not seem to play a role anymore. In particular, different values of ϵ lead to consistent results. According to the criterion Eq. (2) our results indicate that replica symmetry is actually *broken* for this ensemble.

To further test these results, we conducted simulations above the percolation threshold, for $p = 3/N$, and below the threshold for $p = 1/2N$. The results exhibit qualitatively the same behavior (not shown), but with different values of the asymptotic D^∞. Apart from the limits $p \to 0$ and $p \to 1$, where every tour is optimal, the precise structure of the graph does not seem to have a critical influence on this result. As another test, we can lift the degeneracy by adding a slight perturbation on each edge. Therefore we scale the edge weights and ϵ by $5 \cdot 10^5$ and add a random disturbance $U(-250, 250)$ to each edge. Except for a vanishing degeneracy $D_{\text{degeneracy}}$ at $\epsilon = 0$, this procedure also does not change the results beyond statistical errors (not shown).

Conclusion To summarize, we tested multiple ensembles of the TSP by applying sophisticated exact combinatorial optimization algorithms. As suspected before, we find evidence for the replica symmetry of the Euclidean TSP and the related random link model. Interestingly, we find this results also in very large space dimensions, in contrast to spin glasses where RSB is believed to appear above the upper critical dimension $d_u = 6$. Our results strengthen the conjecture that replica symmetry holds for the these ensembles, which is often used to tackle this problem from a statistical mechanics point of view.

TABLE I: Values of the fit parameters extrapolating the behavior of d/N. Interestingly all ensembles, converging to a finite value of D^∞, show an exponent consistent with $b = -1$.

	b	D^∞	RSB
ETSP, 2D	$-0.24(2)$	$-0.08(5)$	-
ETSP, 8D	$-0.267(/)$	$0.08(/)$	-
ETSP, 20D	$-0.27(5)$	$-0.05(10)$	-
RLTSP, pseudo 1D	$-0.350(4)$	$0.019(4)$	-
(1, 2)-TSP, $\epsilon = 20$	$-1.04(20)$	$0.650(8)$	✓
(1, 2)-TSP, $\epsilon = 30$	$-1.04(6)$	$0.652(2)$	✓
(1, 2)-TSP, $\epsilon = 60$	$-1.01(5)$	$0.652(5)$	✓
$c_{ij} = 1$	-	1	disordered

One the other hand, the (1,2)-TSP, inspired by the classical mapping of the Hamilton circuit to the TSP, shows signs of replica symmetry breaking. Thus, we provide the first evidence for a complex phase-space behavior of this classical NP-hard optimization problem.

For future work, especially for the degenerate case of the (1,2)-TSP it would be interesting to study the solution space structure with a focus on clustering. One could define a neighborhood relationship in the configuration space, e.g. k-opt moves [47], and search for clusters of configurations which can be reached from each other by paths traversing only neighboring instances [8, 48–50].

The linear programming approach we used is very general and can be applied to a large range of problems. Since for many problems mappings to integer programs are already known and it is quite straight forward to formulate additional constraints enforcing some specific excitations, this technique could be quite generally used to explore a very specific range of the energy landscape of many problems.

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