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 polynomial (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, 11]. 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 [12–19].

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 these 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 ensembles. First, the most intuitive and probably the most scrutinized \[21, 22, 28, 31\] 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 straightforward to generalize this in higher dimensions using a Poisson point process in a hypercube and the corresponding Euclidean distances. The random link model (RLTSP) \[23, 32\] 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 \[21\].

According to Ref. \[22\], replica symmetry is broken, if quasi-optimal energy $L^\ast$ behaves as

$$L^\ast - L^o \sim o(1) N. \tag{1}$$

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

$$d(T^o, T^\ast) = O(1). \tag{2}$$

Intuitively this means, that a finite, i.e., $O(1)$, energy is sufficient to change a finite fraction, i.e., $O(N)$, of the system \[31\]. 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 $O(1)$ edges of length one but a optimal tour has $O(N)$ 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 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 $\pm 1$ 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 \[40\]

$$\text{minimize } \sum_{i=1} \sum_{j \in S} c_{ij} x_{ij} \tag{3}$$
$$\text{subject to } \sum_{j \in S} x_{ij} = 2, \quad i = 1, 2, \ldots, N \tag{4}$$
$$\sum_{i \in S, j \not\in S} x_{ij} \geq 2, \quad \forall S \subset V, \quad \forall x_{ij} \in \{0, 1\} \tag{5}$$

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 $T^\ast$, 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 $L^\ast - L^o = \epsilon$ 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 $\epsilon$, the number of
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 $\epsilon$ 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 ETSP, 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 \cite{43–46} like the mean-field SK model \cite{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
exceptionally well the (1,2)-TSP for a connectivity of \( N_p = 1 \). 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 \( d/N = aN^b + D^\infty \). The fit parameters are obtained for \( N > 256 \). All three result in a convergence to a finite \( D^\infty \) 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.

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 straightforward 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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