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Statistical mechanics of the travelling salesman on the Sierpinski gasket

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Résumé. — Nous étudions la mécanique statistique du problème du voyageur de commerce sur un tamis de Sierpinski dans lequel les longueurs des liaisons $\{ \lambda_i \}$ sont des variables aléatoires et gelées. Le problème de trouver le plus court chemin fermé qui visite tous les N sites est traitable si tous les $| \lambda_i - 1 |$ sont inférieurs à $(2 N + 1)^{-1}$. Pour un choix particulier d'une distribution de probabilité pour les longueurs des liaisons et aux basses températures, le système se comporte comme des spins d'Ising sans interactions dans un champ magnétique aléatoire. La pertinence d'un de nos résultats aux chaînes polymériques compactes en milieux aléatoires est aussi discutée.

Abstract. — We study the statistical mechanics of the travelling salesman on a Sierpinski gasket in which the bond lengths $\{ \lambda_i \}$ are quenched random variables. The problem of finding the shortest closed path which visits all N sites is tractable if all the $| \lambda_i - 1 |$ are less than $(2 N + 1)^{-1}$. For a particular choice of the bond-length probability distribution and at low temperatures, the system behaves like a set of non-interacting Ising spins in a quenched random magnetic field. The relevance of one of our results to collapsed polymer chains in random media is also discussed.

1. Introduction.

The travelling salesman problem (TSP) is of central importance in the field of combinatorial optimization [1] and its applications are manifold. In this problem the distances $d_{i,j}$ between N points are given. The object of the problem is to find the shortest closed path that visits all of the points at least once. Almost all TSP's belong to the class of nondeterministic polynomial (NP) complete problems (see [2] for details). Although it has not yet been proven, the problems in this class are apparently all « intractable », i.e., it seems that the computing time necessary for their solution grows faster than any power of N. The TSP in which N points are randomly placed on the sites of a square lattice and in which the salesman can only move along the bonds is an important example of an NP-complete TSP.

Recently a Monte Carlo method known as « simulated annealing » [3, 4] has been advanced as a way to rapidly find near-optimal solutions to TSP's. In this technique the configuration space is the set of all closed paths which visit all N points. The length of such a path, L_{path}, is considered to be its energy, and a « temperature » T is introduced into the problem. The « partition function » is then

$$Z = \sum_{\text{paths}} e^{-\beta L_{\text{path}}},$$

where $\beta \equiv T^{-1}$. The Metropolis algorithm [5] is used to slowly cool the system from a high initial temperature down to $T = 0$. If the annealing is sufficiently gradual, the length of the path obtained at zero temperature should be close to the minimum. Slow cooling helps to prevent the system from getting stuck in metastable states, so this technique represents an important improvement on algorithms in which only changes that reduce the path length are considered. Numerical studies [3, 4, 6, 7] have shown that simulated annealing is quite efficient, and it promises to become of increasing practical importance.

The method of simulated annealing has led naturally to the study of the statistical mechanics of TSP's. One of the primary objectives of these studies is to obtain new results on TSP's using the techniques of statistical mechanics [8]. Kirkpatrick and his collaborators [3, 7] and Vannimenus and Mézard [9] have pointed out that finite temperature TSP's resemble spin glasses [10] in many respects. In particular, it is believed that the configuration space for a

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NP-complete TSP has many near-optimal states that are separated by very large energy barriers. So far the correspondence between TSP's and spin glasses has been essentially qualitative, although Barahona *et al.* [11] have shown that the problem of finding the ground state of a two dimensional spin glass is equivalent to solving a relative of the TSP, a particular Chinese postman problem. If the correspondence between the two classes of problems could be made more precise, then the large body of knowledge on spin glasses could lead to new insights into TSP's.

As a first step toward this goal, in this paper I shall introduce an especially simple TSP which is equivalent at low temperatures to a set of non-interacting Ising spins in a quenched random magnetic field. This is the first example of a TSP which can be mapped onto a spin system with quenched disorder for temperatures $T > 0$. This problem also represents a new addition to the short list of TSP's which are « tractable », i.e., the time necessary to find the shortest path grows like a power of N [12]. Moreover, it is believed that NP-completeness and low-temperature glassy behaviour are in some way related [7, 13]. Since our problem is tractable and has no glassy phase, it provides corroborating evidence in favour of this belief.

The TSP considered in this paper is on a Sierpinski gasket [14]. TSP's on regular fractals have not previously been considered, although it is now common to study problems in statistical mechanics on these lattices. The motivation in statistical mechanics is twofold : to gain greater insight into the dependence on dimensionality, and also to model the behaviour of statistical systems on random fractals such as an infinite percolating cluster at threshold [15, 16]. Similarly, it is interesting to inquire into the behaviour of the TSP in dimensions between one (in which it is trivial) and two (in which it is NP-complete). One can also foresee applications in which a salesman is confined to a random fractal. For example, suppose that each site in a square lattice is occupied by « land » with probability p and by « water » with probability $1 - p$. We require the salesman to visit every site on his island. For p slightly less than p_c, the salesman on the incipient infinite cluster must visit all sites on a fractal with the correlation length ξ as its upper cutoff length [16]. Following Gefen *et al.* [15], we model the incipient infinite cluster by a Sierpinski gasket.

As a byproduct of this work, we will obtain the number of closed self-avoiding walks that visit all points on a Sierpinski gasket. This quantity is of interest in the theory of collapsed polymer chains in random media, and we shall compare our exact result with the predictions of the existing approximate theories.

2. The model and its ground state.

Consider the TSP on a Sierpinski gasket of order l with quenched, randomly distributed bond lengths

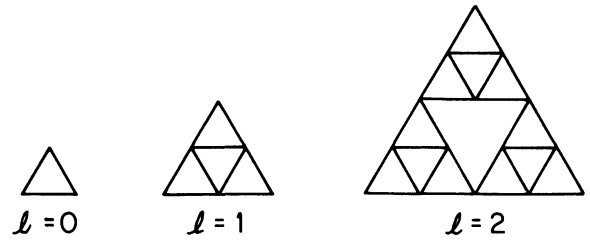

Fig. 1. — Sierpinski gaskets of order $l = 0$, 1 and 2 with all bond lengths equal.

$\lambda_1, \lambda_2, \ldots \lambda_{3^{l+1}}$ (see Fig. 1). The problem is simplest when the disorder is weak, so we shall require that each λ_i lie within ε of unity. In other words, we assume that

$$P(\{\lambda\}) = 0 \quad \text{if} \quad |\lambda_i - 1| \geqslant \varepsilon \quad \text{for any } i, \qquad (1)$$

and otherwise the probability distribution P can be arbitary [17]. The travelling salesman is to visit every site in the gasket at least once, and is to return to his starting point at the end of his journey. In so doing, he may only traverse bonds which belong to the gasket. Such a closed path will be called a circuit. The object of the problem is to find the shortest circuit (or circuits).

For $\varepsilon = 0$, there is no bond randomness and any self-avoiding circuit (SAC) will be optimal. As we shall see, the number of SAC's grows exponentially with the number of sites. This enormous ground state degeneracy is at least partially lifted for $\varepsilon > 0$. The shortest circuit must still be self-avoiding for sufficiently small ε, however. To see this, note that the length of any SAC must be less than $(1 + \varepsilon)N_l$, where $N_l \equiv \frac{3}{2}(3^l + 1)$ is the number of sites. The minimum length of a non-self-avoiding circuit, on the other hand, is $(1 - \varepsilon)(N_l + 1)$. Therefore, for $\varepsilon \leqslant (2N_l + 1)^{-1}$, the non-self-avoiding circuits are all longer than the self-avoiding circuits. We shall take $\varepsilon = (2N_l + 1)^{-1}$, so only SAC's need be considered as candidates for the optimal circuit. For this type of weak disorder, the fractal dimension [14] of the gasket is ln 3/ln 2, just as it is when $\varepsilon = 0$.

We now proceed to classify and enumerate the SAC's on the lth Sierpinski gasket [18]. Before doing so, it will be convenient to introduce some terminology. A self-avoiding path which starts at one corner of the gasket and ends at another, and which visits all other sites will be called a *tour*. A self-avoiding path which starts at one corner and ends at another, and which visits all other sites *except* the third corner will be called an *n-tour*. Clearly, any SAC on the lth lattice can be decomposed into three tours on gaskets of order $l - 1$. It is therefore sufficient to consider tours on the $(l - 1)$th Sierpinski gasket.

For $l \geqslant 3$, any tour on the $(l - 1)$th Sierpinski gasket can be subdivided into tours and n-tours on the three sublattices of order $l - 2$. To see this, consider a tour that starts at A and ends at B in figure 2. The

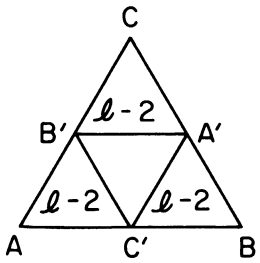

Fig. 2. — Decomposition of the $(l-1)$th Sierpinski gasket into three sublattices of order $l-2$.

tour must exist from the triangle AB'C' through the point B', since a path that leaves *via* C' and that visits all sites must ultimately visit A' or C' twice. Moreover, the tour must exit from the triangle B'CA' through A'. Once the tour has entered the triangle C'A'B, it cannot leave by C' because this would entail visiting either C' or A' twice. The tour terminates at B once all the sites within C'A'B have been visited. It is important to note that the point C' can be visited either in the course of visiting the sites within the triangle AB'C' or while visiting the points inside C'A'B. We conclude that any tour on the $(l-1)$th lattice can be decomposed into two tours and an n-tour on lattices of order $l-2$, as shown schematically in figures 3 and 4. In a completely analogous fashion, we can separate an n-tour on the $(l-1)$th lattice into two n-tours and one tour on the sublattices.

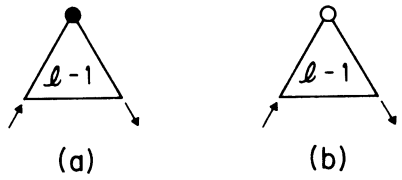

Fig. 3. — Schematic representation of a tour (a) and an n-tour (b) on the lattice of order $l-1$. A solid circle at the third corner indicates that this site is visited during this portion of the walk; an open circle indicates that it is not. The arrows indicate the corners where the self-avoiding walks enter and exit.

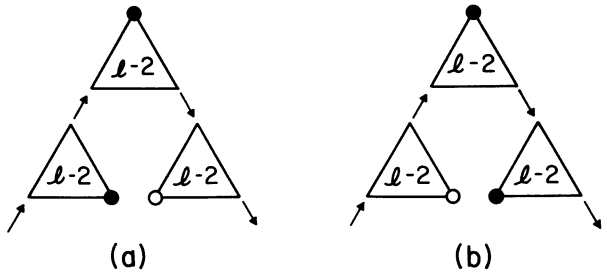

Fig. 4. — Figure showing how a tour on the $(l-1)$th Sierpinski gasket (Fig. 3a) can be decomposed into two tours and one n-tour on the three sublattices of order $l-2$. The two possible decompositions are shown in (a) and (b). For clarity, the order l sublattices have been separated slightly.

By repeatedly applying these decompositions of tours and n-tours, we find that for $l \geqslant 2$ an arbitrary SAC on the lth Sierpinski gasket can be reduced to tours and n-tours on gaskets of order 1. The $l=1$ Sierpinski gaskets containing the corners of the original gasket of order l must be traversed by tours. The remaining $l=1$ gaskets are grouped into $P_l = \frac{3}{2}(3^{l-2}-1)$ « elementary pairs ». The two $l=1$ gaskets in an elementary pair share a vertex, and each of them has a fixed entry and a fixed exit point for SAC's. One of the two $l=1$ gaskets is traversed by a tour which visits the common point, and the other gasket is traversed by an n-tour (see Fig. 5). To complete our classification and enumeration of the SAC's on the lth gasket, we note that there are two tours and three n-tours on the $l=1$ gasket with fixed starting and finishing points. There are therefore 12 possible configurations for each elementary pair and a total of

$$C_l = 2^3 \times 12^{P_l} = \frac{8}{12^{5/3}} \exp\left[\left(\frac{1}{9}\ln 12\right) N_l\right] \quad (l \geqslant 2) \tag{2}$$

SAC's on the lth Sierpinski gasket.

It is now easy to see how to obtain the SAC of shortest length. Because the two entry and two exit points of each elementary pair are fixed, the process of selecting the path within any given pair is entirely independent of the bond lengths in the other pairs and in the three special $l=1$ gaskets at the corners. Therefore, we choose one of the 12 possible configurations within each pair sheerly on the basis of which is the shortest. Similarly, we select the shorter of the two allowed configurations for each $l=1$ gasket at a corner. The total number of decisions (or computational operations) made in determining the optimal circuit, D_l, is therefore

$$D_l = P_l + 3 = \frac{3}{2}(3^{l-2}+1) = \frac{1}{9}N_l + \frac{4}{3} \text{ for } l \geqslant 2. \tag{3}$$

We conclude that the computing time necessary to find the shortest circuit grows linearly with the number of sites to be visited. This is true in spite of the fact that the number of SAC's grows exponentially with N_l. Thus, this problem is a non-trivial tractable TSP.

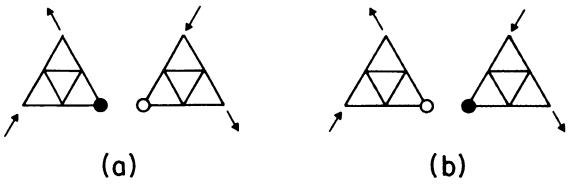

Fig. 5. — The two possible decompositions of the portion of a SAC on a elementary pair into a tour and an n-tour. For clarity, the $l=1$ gaskets in the pair have been separated slightly at their common point.

The purely local decision-making process found here is a special characteristic of the TSP on the weakly-disordered Sierpinski gasket. For NP-complete TSP's, the local structure of the optimal circuit is strongly dependent upon the distances between all N points to be visited, and the decision-making process is inherently nonlocal.

Kirkpatrick *et al.* [3] have observed that in the method of simulated annealing, the large distance structure of the optimal circuit is determined first. As the temperature is lowered, the structure of the path is found on progressively shorter and shorter length scales. It is interesting that the reason that the TSP on the Sierpinski gasket is tractable is that we can deduce much of the structure of the optimal circuit at successively smaller lengths. Once this process of deduction has been carried out, a relatively small number of computational steps remain to be done.

Before going on, let us briefly consider the implications of our result (2) for polymer theory. The conformations of collapsed polymer chains are often modelled as compactly packed self-avoiding walks [19]. It sometimes proves more convenient to study closed circuits rather than walks, and fortunately this is not expected to change the asymptotic properties [20, 21]. Therefore, an important quantity in this theory is the number of closed self-avoiding walks that visit all sites in a finite subsection of a given regular lattice (such walks are called Hamiltonian circuits in graph theory). On the other hand, there has been considerable interest recently in the behaviour of polymers in random media [22, 23]. This has led to the study of self-avoiding walks on percolation clusters [22] and hence on Sierpinski gaskets [23]. Our result (2) gives the number of SAC's or Hamiltonian circuits on the Sierpinski gasket of order l, and so is relevant to the theory of collapsed polymer chains in random media. We found that the number of conformations C_l grows like ω^{N_l}, where the « connective constant » $\omega = 12^{1/9} \cong 1.3180$.

Exact values of the connective constant have been obtained only for a few special Euclidean lattices [24]. Accordingly, various « mean-field » theories of Hamiltonian circuits have been proposed [21, 25, 26]. These theories give estimates of ω that depend only on the coordination number z. For a lattice with $z = 4$, a Flory-Huggins type of theory [25] yields $\omega_{\mathrm{FH}} = 3/e \cong 1.1036$, Huggins [26] predicts $\omega_{\mathrm{H}} = 1.5$, and Orland *et al.* [21] give the value $\omega_{\mathrm{O}} = 4/e \cong 1.4715$. Although ω_{O} is close to numerical values of ω obtained for the square lattice [27], it is very different from the exact value of ω for the Sierpinski gasket. We conclude that ω must depend in general on other lattice characteristics besides the coordination number.

3. Low-temperature behaviour.

Now that we have seen how to determine the ground state of our TSP on the lth Sierpinski gasket, we move on to study its behaviour at low temperatures. It is instructive to first consider a particularly simple but rather artificial bond-length distribution P. We shall then generalize our conclusion. Thus, we assume that the nine bonds within each $l = 1$ gasket are equal in length, and that only two lengths, $1 + \varepsilon$ and $1 - \varepsilon$, are possible. These two lengths are to be equally probable. Each $l = 1$ gasket will be assigned an Ising spin s which is to be $+1$ if the bond lengths are $1 + \varepsilon$; otherwise, $s = -1$. We shall also assume that the bond-length distributions in different $l = 1$ gaskets are uncorrelated. With these assumptions, the six configurations shown schematically in figure 5(a) all have energy $5(1 + s_1\,\varepsilon) + 4(1 + s_2\,\varepsilon)$, where s_1 is the spin on the left $l = 1$ gasket in the elementary pair and s_2 is the spin on the right gasket. Similarly, the six configurations in figure 5(b) have energy $4(1 + s_1\,\varepsilon) + 5(1 + s_2\,\varepsilon)$. It will also be useful to assign an Ising spin σ to each elementary pair. We shall take σ to be $+1$ for the six configurations described by figure 5(a) and to be -1 for the six configurations shown in figure 5(b). The energy of an elementary pair is then

$$E_{\mathrm{pair}} = \left[4 + \tfrac{1}{2}(1 + \sigma)\right](1 + s_1\,\varepsilon) + \left[4 + \tfrac{1}{2}(1 - \sigma)\right](1 + s_2\,\varepsilon), \quad (4)$$

for $\sigma = \pm 1$. Finally, we put $\varepsilon = (1 - \Delta)(2N_l + 1)^{-1}$, where $0 < \Delta < 1$. This ensures that the non-self-avoiding circuits are separated from the SAC's by a nonzero gap Δ. For temperatures $T \ll \Delta$, then, only SAC's will contribute appreciably to the partition function. The average quenched free energy may now be written

$$\overline{F}_l \cong -\frac{1}{4} P_l\, T \sum_{s_1, s_2} \ln\left(6 \sum_{\sigma} \exp\left\{-\beta\left[4 + \tfrac{1}{2}(1 + \sigma)\right](1 + s_1\,\varepsilon) - \beta\left[4 + \tfrac{1}{2}(1 - \sigma)\right](1 + s_2\,\varepsilon)\right\}\right) - \frac{3}{2} T \sum_{s} \ln\{2 \exp[-5\beta(1 + s\varepsilon)]\} \quad \text{for} \quad T \ll \Delta, \quad (5)$$

where the bar denotes an average over the bond-length distribution. Equation (5) may be recast as

$$\overline{F}_l \cong -\frac{1}{4} P_l T \sum_{s_1,s_2} \ln\left\{\sum_\sigma \exp\left[-\frac{1}{2}\beta\varepsilon(s_1 - s_2)\,\sigma\right]\right\} + A_l T + B_l \quad \text{for} \quad T \ll \Delta\,, \quad (6)$$

where A_l and B_l are easily determined constants. Thus, up to terms that are linear in T, $\overline{F}_l$ is the average free energy of P_l uncoupled Ising spins in a quenched, random magnetic field, h. The probability distribution of this field is

$$p(h) = \frac{1}{2}\delta_{h,0} + \frac{1}{4}\delta_{h,\varepsilon} + \frac{1}{4}\delta_{h,-\varepsilon}\,. \quad (7)$$

Since the P_l Ising spins do not interact, the average over the field configurations is easily performed. We find

$$\overline{F}_l \cong -\frac{1}{2} P_l T \ln(\cosh \beta\varepsilon) + A_l' T + B_l' \quad \text{for} \quad T \ll \Delta\,, \quad (8)$$

where A_l' and B_l' are constants. All evidence of randomness has vanished, so there cannot be a low-temperature spin-glass phase in this problem. It is simple to show that the average energy at $T = 0$ is

$$\overline{E}_l(0) = 9 P_l + 15 - \frac{1}{2} P_l \varepsilon\,, \quad (9)$$

and this is the average length of the shortest path. The average zero-temperature entropy is

$$\overline{S}_l(0) = \frac{1}{2}(\ln 72) P_l + 3 \ln 2\,. \quad (10)$$

Our conclusion that there is no low-temperature spin-glass phase can be extended to arbitrary bond-length distributions P which are subject only to the constraint (1) with $\varepsilon = (1 - \Delta)(2 N_l + 1)^{-1}$. This can be done by a trivial generalization of the approach used in the previous paragraph. In the general case each elementary pair is described by a 12-state variable σ with a quenched random energy for each state, and these variables are non-interacting. Here I shall take an approach which is more heuristic but less precise : I shall consider the configuration space « landscape » directly. With our choice of ε, the SAC's on the lth Sierpinski gasket are separated from the remainder of the circuits by an « energy » gap Δ. A natural topology on the set of SAC's is obtained by letting the « distance » $d_{\tau,\tau'}$ between the SAC's τ and τ' be the fraction of bonds in τ that are not in τ'. (This distance is just one minus the overlap of Kirkpatrick and Toulouse [7].) Clearly, the maximum distance between two SAC's is 1. Any SAC τ can be obtained from a given SAC τ_0 by a special sequence of $P_l + 2$ intermediate SAC's $\tau_1, \tau_2, \ldots, \tau_{P_l+2}$. At each step in this sequence the configuration is changed in one of the elementary pairs or in one of the $l = 1$ gaskets at the corners. Any two successive circuits in this sequence are separated by a distance of at most $9/N_l$ and differ in energy by no more than $18\,\varepsilon = 18(1 - \Delta)(2 N_l + 1)^{-1}$. Therefore, the SAC's are closely spaced for large l and there is a path between any two on which the slope of the energy surface never exceeds $1 - \Delta$. Finally, all SAC's lie within an energy $1 - \Delta$ of the ground state. We conclude that although there are a large number of near-optimal states when l is large, these are not separated by large energy barriers. Moreover, any two points on the energy surface can be joined by a path over which the rate of change of the energy is bounded. The topography of the energy surface, then, suggests that there cannot be a spin-glass transition.

4. Conclusion.

In this paper I introduced a new tractable travelling salesman problem and studied its statistical mechanics. The tractability of the problem was shown to be intimately related to the absence of a low-temperature spin-glass phase and to the lack of high energy barriers between minima in the configuration space « landscape ». For a particular bond-length probability distribution, the low-temperature free energy reduced to that of a set of non-interacting Ising spins in a quenched random magnetic field.

Acknowledgments.

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