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On the Statistical Mechanics of the Traveling Salesman Problem

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We consider the statistical mechanics of the traveling salesman problem (TSP) and develop some representations to study it. In one representation the mean field theory has a simple form and brings out some of the essential features of the problem. It shows that the system has spontaneous symmetry breaking at any nonzero temperature. In general the phase progressively changes as one decreases the temperature. At low temperatures the mean field theory solution is very sensitive to any small perturbations, due to the divergence of some local susceptibilities. This critical region extends down to zero temperature. We perform the quenched average for a nonmetric TSP in the second representation and the resulting problem is more complicated than the infinite-range spin-glass problem, suggesting that the free energy landscape may be more complex. The role played by "frustration" in this problem appears explicitly through the localization property of a random matrix, which resembles the tight binding matrix of an electron in a random lattice.

KEY WORDS: spin glass, N-P complete optimization problems.

1. INTRODUCTION

It has been realized recently that several complex optimization problems[1–7] can be studied with the aid of concepts and tools developed in the statistical mechanics of disordered systems (see, e.g., Refs. 3 and 8). One such problem is the minimization of the tour distance of a traveling salesman[9] who wants to visit N arbitrarily located cities. Problems of similar nature[10] occur in the design of very large-scale integrated circuits

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and in many other applications. The TSP is known to be an NP-complete problem[3]—it might take an exponentially long time to find the optimal tour with any algorithm. If we imagine a space of all possible tours and draw the "tour distance" surface, we will obtain a surface with complicated maxima–minima structures. This surface is similar to the free energy surface in a spin-glass problem. As we go down in this surface to regions corresponding to smaller and smaller tour distance, there will in general be many local minima separated by huge barriers. It is this similarity between the optimization problem and the problem of the spin-glass that has prompted the development of heuristic algorithms such as the simulated annealing technique.[(1)] Recently it has also been suggested that the spin-glass theory may play an important role in general theoretical studies of optimization problems.[(2,7)]

In this paper first we discuss qualitatively the form of the equilibrium free energy at various temperature regions. Then we provide two representations which are useful in the statistical mechanical study of the TSP.[(4)] Each one has its own advantage. One of the representations is amenable to a simple mean field theory treatment without performing any quenched average. It gives us a picture similar to Anderson's localization theory of spin-glasses.[(11)] However, as we shall see, there are important differences. The system has a spontaneous symmetry breaking at any finite temperature. There is a progressive change in the nature of the phase or the mean field as one decreases the temperature. Below a particular temperature, the system enters into a "critical region." In this temperature region the form of the mean field theory solution is very sensitive to small perturbations, due to the divergence of some "local susceptibilities." Consequently there is a successive and discontinuous change in the nature of the optimal tours in this temperature region as a function of temperature. At every temperature, the optimal tours are unstable to local modification of the tours. The role played by "frustration" in this optimization problem appears in a natural way through a specific property of the eigenvalue spectrum of a tight binding-like random matrix. The second representation, which is discussed in detail in the Appendix, involves the permutation group and brings out the complexities of the present problem in comparison with the spin-glass problem. These discussions are useful, both for a good understanding of the nature of the TSP and for a general study of the application of statistical mechanics to optimization problems, from which both fields will imensely benefit.

[3] For a general discussion of the relevance of the statistical mechanical study of NP-complete problems see, e.g., Ref. 1.

1.1. The Traveling Salesman Problem

The (generalized) TSP is defined in the following way. Suppose there are N points (cities) located at points R_i, $i = 1, 2,..., N$, in a d-dimensional space. A traveling salesman has to visit all of them and return to the starting point at the end of the tour. Taking into account the two traversals (in opposite directions) of each tour and the arbitrariness of the starting city, there are $(N-1)!/2$ distinct tours. We label the tours by t. One is asked to find the shortest tour(s) (the optimal one) among them. Let L_t be the length of a tour t. We define a partition function

$$Z = \sum_t \exp(-\beta L_t) \tag{1.1}$$

where β is a parameter to be called the inverse temperature. Formally, in the limit $\beta \to \infty$, the partition function should project out the optimal tours and $-\ln Z/\beta$ gives its length. This, however, is not of any practical significance. It is not feasible to compute Z for a general set of cities, and the formalism does not help one in solving specific problems. Instead, we are here interested in using (1.1) as a tool to study the general properties of the solution of the TSP. Below, we enumerate some of the questions that are of interest in thi problem. While we do not attempt to answer all these questions in thi paper, the simple mean field equation that we derive and its solutions are very helpful in identifying the qualitative features of the problem and finding approximate answers to the following questions:

1. Are there many solutions to a generic TSP? Numerical experience,[1,2] the spin-glass analogy,[3] and model calculations[4] strongly suggest an affirmative answer.
2. What is the distribution of L_t? What are the properties of the sub-optimal solutions?
3. What are the relations between different solutions? If one can find one solution, how would one go on to find another? How many modifications are needed? Do the common features of two solutions suggest a good characteristic for the further search for optimal solutions?
4. In the language of simulated annealing,[1] when temperature decreases, how does the system evolve? How is a good solution selected?

In general we will be interested in finite-temperature as well as zero-temperature properties of Z. In fact, the finite-temperature behavior is more interesting in that it displays most clearly the evolution and selection process of the tours.

There are various ways to represent the partition function Eq. (1.1), which is a formal sum over all tours. We would like to introduce auxiliary variables S_i associated either with the cities or with the links connecting two cities. We will call them "spin" variables. The various possible spin configurations should generate various allowed tours. The length of a tour t, $L_t \equiv E\{S_i\}$, is a function of the spin variables, which will be called the cost function or energy function. The partition function is

$$Z = \sum_t \exp(-\beta L_t) = \mathrm{Tr}\, \exp(-\beta E\{S_i\}) \tag{1.2}$$

If we can obtain a set of variables S_i that achieves the above, we have obtained a representation. We provide two representations for the TSP, in terms of (1) continuous field variables defined on cities, and (2) permutation group elements. Various questions raised above can be answered in principle by calculating various "spin correlation" functions and a proper understanding of the spin problem.

1.2. Free Energy at Various Temperatures

In this section we suggest the form of the equilibrium free energy at various temperatures by some qualitative arguments. This to some extent clarifies the problem of the anomalously large entropy in TSP. We discuss for simplicity the case of metric TSP (TSP in a d-dimensional Euclidean space). By definition, the distances between cities in a metric TSP are the Euclidean distances obeying triangular inequivalities. In a nonmetric TSP the distances between cities are independent random variables.

The cities are distributed according to some probability distribution inside a box of volume L^d. Let ρ and N be the mean density and total number of cities, respectively. The mean distance a_m between two neighboring cities is $\sim \rho^{-1/d}$. Depending on the form of the distribution, there could be large fluctuation in the neighboring distance. The total number of allowed tours is

$$(N-1)!/2 \sim e^{N \ln N} \tag{1.3}$$

Thus, the high-temperature entropy of TSP is $\sim N \ln N$. We argue below that this anomalously large entropy is in fact suppressed at any finite temperature by the anomalously large length of the majority of allowed tours.

A randomly chosen tour from the total number of available tour is likely to have a length

$$\sim NL = a_m N^{1+1/d} \tag{1.4}$$

Thus the free energy at very high temperature is

$$F \sim a_m N^{1+1/d} - TN \ln N \tag{1.5}$$

Because of the large length (internal energy) associated with the most probable tours among all the tours, the system will choose the above form of free energy only for temperatures above

$$T_1 \sim a_m N^{1/d}/\ln N \tag{1.6}$$

This temperature tends to infinity in the thermodynamic limit.

Now we argue that at any finite temperature the entropy of the system scales as N. At very low temperatures, the most probable tours are the tours close to the optimal ones. These tours have a length $\sim a_m$. The entropy associated with them is $\sim N \ln z$, where z is the mean coordination number of the cities. This form of the entropy is suggested by the similarity of the tours to self-avoiding walks and Hamilton circuits on a lattice. Hence the free energy is

$$F \sim a_m N - TN \ln z$$

Thus, the low-temperature free energy is dominated by energy. The glassy behavior is expected at low temperatures because of the availability of a large number of optimal tours and the huge barriers separating them.

At very low temperatures the jump distance scale is set by the mean neighboring distance between the cities. At high temperatures, $T > \rho^{-1/d}$, the jump distance is set by T rather than the mean neighboring distance. Thus, we expect that at high temperatures [but far below T_1; Eq. (1.6)] the free energy has the form

$$F \sim NT - TN \ln(a_m T)^d \tag{1.7}$$

We get the above form of the enetropy since the jump can be to any of the cities in a radius of T. The above free energy is dominated by entropy.

Thus, the system is dominated by internal energy at low temperatures and entropy at high temperatures. The temperature separating the above two regions is given by

$$NT = NT \ln(a_m T)^d$$

$$T_c = a_m e^{1/d} \tag{1.8}$$

The system is likely to enter into a glassy phase below this temperature. Our analysis in the following sections shows that this need not happen as a sharp phase transition. The glassiness starts appearing at temperatures larger than T_c if there is large fluctuation in the nearest neighbor distances between the cities. In fact, glassiness may start appearing at temperatures below $T \sim \xi$, where ξ is the length scale at which inhomogeneities start appearing in the distribution of cities.

2. A FIELD THEORY REPRESENTATION

This representation was motivated by work in polymer physics[12] as well as by the recent interesting work of Orlando, Itzykson, and de Dominicis[13] (OID), who were interested in the number of Hamilton paths on a regular lattice. We found that a similar representation can be introduced for the partition function of TSP. Consider the following generating function:

$$\begin{aligned} Z_1 &= (2i)^{-N}\left(\prod_i \frac{\partial^2}{\partial\chi_i^2}\right)\prod_{i<j}(1+ie^{-\beta R_{ij}}\chi_i\chi_j)\Big|_{\{\chi_i=0\}} \\ &= (2i)^{-N}\left(\prod_i \frac{\partial^2}{\partial\chi_i^2}\right)\exp\left(i\sum_{i<j}V_{ij}\chi_i\chi_j\right)\Bigg|_{\{\chi_i=0\}} \end{aligned} \tag{2.1}$$

where χ_i is a real, continuous auxiliary variable ("spin variable") attached to every city, R_{ij} is the distances between two cities i and j, and

$$\begin{aligned} V_{ij} &\equiv e^{-\beta R_{ij}} \qquad \text{for} \quad i \neq j \\ &= 0 \qquad\qquad\quad\;\; i = j \end{aligned} \tag{2.2}$$

Each nonvanishing term in the above equation is a Boltzmann factor for a particular tour involving every city. However, some of the tours are disjoint. In fact, the above partition function corresponds to a modified problem, namely, the Many Traveling Salesmen Problem (MTSP): it is a TSP with no restriction on the number of salesmen. This is also a nontrivial problem.[2] To avoid any disjoint tours and to get the correct partition function for TSP, we use a well-known trick[12,13] to get

$$Z = (2i)^{-N}\lim_{n\to 0}\frac{1}{n}\left(\prod_i \frac{\partial^2}{\partial\boldsymbol{\chi}_i^2}\right)\exp\left(i\sum_{i<j}V_{ij}\boldsymbol{\chi}_i\cdot\boldsymbol{\chi}_j\right)\Bigg|_{\{\boldsymbol{\chi}_i=0\}} \tag{2.3}$$

where $\boldsymbol{\chi}_i = (\chi_i^1, {}_i^2, \ldots, \chi_i^n)$ is an n-component field. The imaginary unit i is introduced in the above equations in order to make some of the forthcoming Gaussian integrals well defined. We use the identity

$$\exp\left(\frac{i}{2}\sum V_{ij}\boldsymbol{\chi}_i\cdot\boldsymbol{\chi}_j\right) = \frac{\int \exp(-\frac{1}{2}i\sum V_{ij}^{-1}\boldsymbol{\phi}_i\cdot\boldsymbol{\phi}_j + i\sum\boldsymbol{\phi}_i\cdot\boldsymbol{\chi}_i)\prod d\boldsymbol{\phi}_i}{\int \exp(-\frac{1}{2}i\sum V_{ij}^{-1}\boldsymbol{\phi}_i\cdot\boldsymbol{\phi}_j)\prod d\boldsymbol{\phi}_i}$$

to rewritte the above partition function

$$Z = \lim_{n \to 0} \frac{1}{n} \frac{\int \exp(-\frac{1}{2} i \sum G_{ij} \boldsymbol{\phi}_i \cdot \boldsymbol{\phi}_j \prod \frac{1}{2} \boldsymbol{\phi}_i^2 \, d\boldsymbol{\phi}_i}{\int \exp(-\frac{1}{2} i \sum G_{ij} \boldsymbol{\phi}_i \cdot \boldsymbol{\phi}_j) \prod d\boldsymbol{\phi}_i} \tag{2.4}$$

that is,

$$Z \equiv \lim_{n \to 0} \frac{1}{n} \frac{\int \exp(-\beta F[\boldsymbol{\phi}]) \prod d\boldsymbol{\phi}_i}{\int \exp(-\frac{1}{2} i \sum G_{ij} \boldsymbol{\phi}_i \cdot \boldsymbol{\phi}_j) \prod d\boldsymbol{\phi}_i} \tag{2.5}$$

where $G_{ij} \equiv (V^{-1})_{ij}$ and the "free energy" F is defined as

$$-\beta F[\boldsymbol{\phi}] = -\frac{1}{2} i \sum G_{ij} \boldsymbol{\phi}_i \cdot \boldsymbol{\phi}_j + \sum \ln \boldsymbol{\phi}_i^2 \tag{2.6}$$

Notice that the temperature appears in an unusual way, via V_{ij}, in the partition function.

The above expression is for a given configuration of the cities. The possibility of a quenched average of this expression will be discussed later. We can regard the partition function either as a generating functional of a nonpolynomial ($\log \phi$) field theory or a statistical mechanical system with complex free energy. This nonlinearity is more difficult to handle than ϕ^4 nonlinearity. First, we attempt a simple mean field theory on this model. To do this, we need to understand the nature of the eigenvalue spectrum of the random matrix V_{ij}.

The matrix V_{ij} is a real, symmetric matrix with zero diagonal elements and positive off-diagonal elements. It resembles the tight-binding matrix of an electron in a random lattice with zero orbital energy for all sites and positive hopping matrix elements between any two sites. The matrix element is short-ranged at low temperatures and has a range β^{-1} at any temperature. Since the diagonal elements are zero, the density $\rho(\varepsilon)$ of eigenvalues satisfies the following equation:

$$\int_{-\infty}^{\infty} \rho(\varepsilon) \varepsilon \, d\varepsilon = 0 \tag{2.7}$$

Matrices of this type have been studied by many authors.[15] To begin, let us consider a regular lattice of cities.† The density of states is shown schematically in Fig. 1. The density of states is asymmetric in general. This is due to the presence of "frustration," which is defined in the following way. A tigh binding matrix of a simple cubic lattice with only constant positive nearest neighbor hoppings has an antibonding eigenfunction at the negative end of the tail. That is, the eigenfunction has opposite signs on the

† The finite temperature statistical mechanics of TSP on a regular lattice is nontrivial. The zero temperature version of this corresponds to the Hamilton circuit problem.

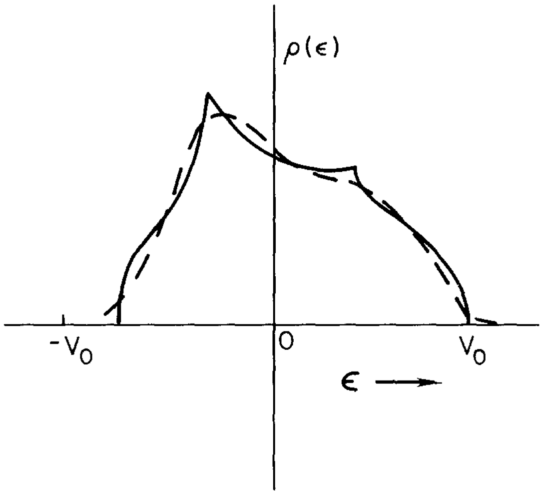

Fig. 1. (——) The density of states of a tight binding matrix with $V_{ij} = e^{-\beta R_{ij}}$ for a periodic array of cities; (- - - -) when the positions of the cities are made slightly random.

two sublattices. This is not possible in a lattice such as fcc or a random lattice which cannot be separated into two identical sublalttices. The inability to form perfect antibonding eigenstates is called frustration in this content. This is analogous to the absence of a simple antiferromagnetic ground states in an fcc lattice with nearest neighbor Ising antiferromagnetic interaction. Notice that even a hypercubic lattice which can be separated into two sublattices (bipartite lattice) can have frustration when the hopping matrix elements are not limited to nearest neighbors. This in turn is analogous to the absence of simple antiferromagntic ground states in a simple cubic lattice with a certain type of non-nearest neighbor Ising antiferromagnetic interaction. The positive band edge occurs at $V_0 = \sum_j V_{ij}$. The negative band edge is displaced from $-V_0$ to $-V$ due to the frustration. The quantity $(1 - V/V_0)$ is a measure of the frustration.

Now let us imagine making a simple random configuration of cities by displacing the above regular lattice of cities randomly by a finite amount. The matrix V_{ij} gets disordered. The density of states develops tails. The positive band edge moves beyond V_0. The negative band edge moves toward $-V_0$ as we increase the bond disorder (dashed curve in Fig. 1).

Al high temperatures, the spectrum has a simple form. Let R_0 be the typical largest distance between any two neighboring cities. Then for $\beta^{-1} > R_0$, the zero-momentum state is a good approximation to the real eigenstate and the density of states has the form shown in Fig. 2. As the temperature increases, the width of the states at the center decreases and collapses to the origin from both sides as $T \to \infty$. However, there are only

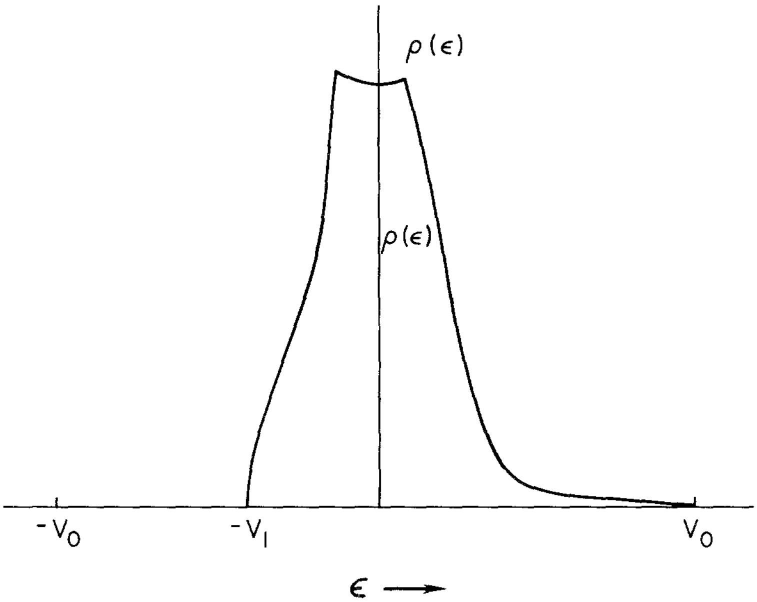

Fig. 2. The density of states at very low temperature.

$N-1$ states at the center. The zero-momentum state becomes an eigenstate and its eigenvalue alone remains at a finite value $N-1$.

At very low temperatures, the bandwidth decreases with decreasing temperature. The relative variation of the hopping matrix elements becomes very large. A typical ratio of the hopping matrix elements between pairs of cities ij and k is

$$V_{ij}/V_{ik} = \exp[-\beta(R_{ij} - R_{ik})] \tag{2.8}$$

This ratio becomes exponentially large or small depending on whether R_{ij} is greater or less than R_{ik}. Thus, the randomness increases as we go to low temperatures and we expct all the eigenstates to be localized.

3. A MEAN FIELD THEORY

Here we discuss a mean field theory in which we obtain a simple picture of what could happen as one changes the temperature or increases the disorder in the configuration of cities. We are able to infer a good picture without doing any detailed calculations. The analysis is in spirit similar to the theory of Anderson and co-workers[11] for the spin-glass problem.

In a mean field theory with complex free energy we look for the saddle point of the multidimensional integral Eq. (2.5). Minimizing the free energy in Eq. (2.6), we obtain the following simple mean field equation:

$$i\sum_j G_{ij}\phi_j^\nu = \frac{2\phi_i^\nu}{\phi_i^2} \tag{3.1}$$

We will assume that the mean field is pointing in a specific direction at every city. In other words,

$$\phi_{i,\mathrm{mf}}^\nu = (\phi_{i,\mathrm{mf}}^1, 0, 0,..., 0) \tag{3.2}$$

Therefore,

$$i\sum_j G_{ij}\phi_j = 2/\phi_i \tag{3.3}$$

For convenience we suppress the indices 1 and mf hereafter. We make the mean field equation real by defining

$$\eta_i \equiv (i/2)^{1/2}\phi_i \tag{3.4}$$

Multiplying both sides of Eq. (3.3) by the matrix **V**, we get

$$\eta_i = \sum_j \frac{V_{ij}}{\eta_j} \tag{3.5}$$

We do not attempt to solve this mean field equation; the very from of this equation suggests several interesting features of TSP. First, the mean field has to be nonzero at every site. If there is a decrease in the mean field on the site i due to some perturbation, it results in a increase in the man field on the neighboring sites. This is analogous to an antiferromagnetic system in which the increase of spin on one site tends to increase the spins on neighboring sites in the opposite direction.

We will analyze how the mean field changes, starting from a known mean field, as we change either the temperature or the disorder. We will characterize the mean field by a parameter Δ. Let η_i be a known mean field at a given temperature β and given disorder Δ. Let there be a change in β or Δ so that the matrix V_{ij} changes by a small amount

$$V_{ij} \to V_{ij} + \delta V_{ij}$$

Let the mean field change from η_i to $\eta_i + \zeta_i$. We will linearize the mean field equation and obtain a linear equation satisfied by ζ_i,

$$\sum_j \left(\delta_{ij} + \frac{V_{ij}}{\eta_j^2}\right)\zeta_j = \sum_j \frac{\delta V_{ij}}{\eta_j} \tag{3.6}$$

Define $\xi_i \equiv \zeta_i/\eta_i^2$ and $f_i = \sum_j \delta V_{ij}/\eta_j$. Then we obtain

$$\xi_i = \sum_j \left(\frac{1}{\mathbf{I}\eta^2 + \mathbf{V}} \right)_{ij} f_j \tag{3.7}$$

where $\mathbf{I}\eta^2 = \delta_{ij}\eta_j^2$. We can go to the eigenvasis of the matrix $(\mathbf{I}\eta^2 + \mathbf{V})$ to get

$$\xi_\alpha = \frac{1}{\varepsilon_\alpha} f_\alpha \tag{3.8}$$

where ε_α are the eigenvalues of $(\mathbf{I}\eta^2 + \mathbf{V})$. The above equation is a linear response equation. It represents the change in the mean field due to a change in V_{ij}. Hence $(\varepsilon_\alpha)^{-1}$ can be interpreted as the susceptibility of the eigenmode α. Thus, when ε_α goes to zero, the susceptibility of the corresponding eigenmode becomes infinity.

Let us first consider the case in which we have a periodic lattice of cities with one city per unit cell. The mean field solution is

$$\eta_i^2 = \sum_j V_{ij} \equiv V_0 \tag{3.9}$$

and is independent of site. In this case we can diagonalize the mean field equation by Fourier transform to obtain

$$\xi_k = \frac{1}{\varepsilon_k} f_k \tag{3.10}$$

where $\varepsilon_k = V_0 + V(k)$ and $V(k) = \sum_j V_{ij} \exp(i\mathbf{k} \cdot \mathbf{R}_j)$. In the periodic case, as long as there is frustration, the denominator of the equation can never be zero, and all the susceptibilities $1/\varepsilon_k$ remain finite. Thus, the mean field changes by a small amount with disorder. We can linearize about the new mean field and add more disorder. The new mean field becomes space dependent. The spectrum of the matrix $(\mathbf{I}\eta^2 + \mathbf{V})$ develops a tail. By continuity this situation continues untill the tail grows and touches the origin (Fig. 3). When the tail just touches the origin, the susceptibility of the corresponding local model diverges.

This calls for a self-consistant local modification of the tour beyond the linear analysis. Once this is done, it is likely to continue as one increases the disorder, since in this case both the diagonal and off-diagonal elements become disordered. Even though we have not done a detailed analysis of the mean field equation, it seems difficult to escape this simple possibility. We will call this region a critical region or a region of marginal stability of the mean field. The proliferation of mean field solutions is

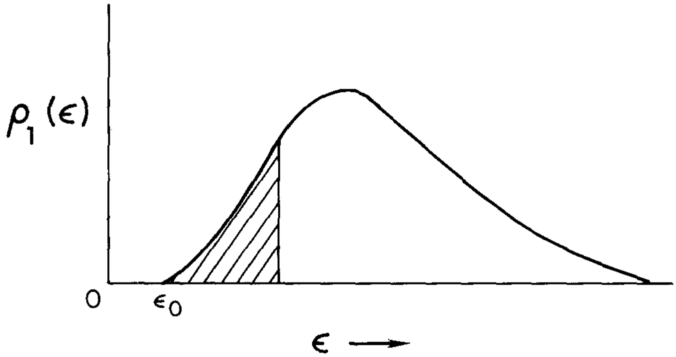

Fig. 3. The density of states $\rho_1(\varepsilon)$ of the matrix $(\mathbf{I}\eta^2 - \mathbf{V})$. The largest susceptibility is ε_0^{-1}.

related to the divergence of the localized susceptibility and the finite value of the density of states of $\mathbf{I}\eta^2 + \mathbf{V}$ close to the origin.

This behavior is to be contrasted with the Ising spin-glass. Above the spin-glass transition, some of the localized mode susceptibilities diverge. This does not alter the mean field. In fact, the mean field remains zero until we reach T_c. In the TSP the mean field changes because the symmetry is always spontaneously broken.

Another instance where we know the exact mean field is at infinite temperature. The mean field solution is a constant independent of the city. Decreasing the temperature amounts to increasing the disorder. By the same argument as above, there is a small modification of the mean field until a critical temperature, at which some of the local susceptibilities start to diverge. A schematic phase diagram is given in Fig. 4.

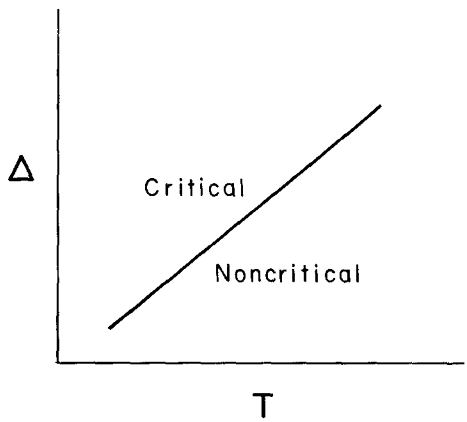

Fig. 4. Schematic phase diagram in the disorder–temperature plane.

From the form of the stability Eq. [(3.7) and (3.8)] it is obvious that there are two more possible types of behavior of the mean field. The first is that the susceptibilities remain finite at all temperatures and the mean field is stable. This is unlikely to be the case in a highly frustrated systems like ours. A second possibility is that the susceptibility of one of the extended modes diverges at low temperatures. This will be like a conventional "spin-glass" type of phase transition. In order for this to happen, the diagonal randomness in $\mathbf{l}\eta^2$ and the off-diagonal randomness in the matrix V_{ij} must conspire in such a way that all the localized states in the left end of the spectrum in Fig. 3 are depleted. This is possible in a spin-glass because the interaction matrix is temperature independent and the Hartree correction could screen the randomness at low temperatures. In our problem the matrix V_{ij} has a strong temperature dependence and the randomness effectively increases with decreasing temperature. Thus, this possibility looks remote.

Using the above arguments and the known properties of random tight binding matrices in two dimensions, we can make the following statements. In a two-dimensional TSP the phase progressively changes and enters into a critical region where some local mode susceptibilities diverge. At any finite temperature no extended mode susceptibility diverges. Absence of divergence of an extended mode susceptibility implies the absence of a critical point. The recent numerical results of Kirkpatrick and Toulouse[2] also seem to point to a progressive change in the behavior of properties of tours rather than an abrupt change. This point needs further detailed study.

Having found the mean field, one can find the man field free energy and the leading correction to it following OID. The mean field can point in any direction in the internal n-dimensional space. Thus, we have to integrate over these angular variables (global rotation) to get a factor

$$S_n = 2\pi^{n/2}/\Gamma(n/2) \tag{3.11}$$

which is the area of the unit sphere in n dimensions. This becomes $\sim n$ in the limit $n \to 0$ and cancels the $1/n$ factor in the partition function.

We can calculate the leading correction to the mean field free energy by looking at the Gaussian fluctuation about the mean field.[13] To do this, we expand the free energy Eq. (2.6) about the mean field $\phi_{\rm mf} = (2/i)^{1/2}\eta_i$ and keep terms quadratic in the fluctuation ζ_i to get

$$\begin{aligned} -\beta F = & -N + \sum_i \ln \eta_i^2 - \frac{i}{2}\sum_{ij}\left(G_{ij} + \frac{\delta_{ij}}{\eta_j^2}\right)\zeta_i^1\zeta_j^1 \\ & - \frac{i}{2}\sum_{\substack{ij \\ \nu = 2,\dots,n}}\left(G_{ij} - \frac{\delta_{ij}}{\eta_j^2}\right)\zeta_i^\nu\zeta_j^\nu + \cdots \end{aligned} \tag{3.12}$$

The first two terms are the mean field free energy. The third term is the longitudinal fluctuation term. The last term represents the $n-1$ transverse fluctuation modes. The inverse propagator matrix of the transverse fluctuation has a zero eigenvalue by virtue of the mean field Eq. (3.3). This represents the $n-1$ Goldstone modes in the system.

The longitudinal propagator matrix in the expression is related to the matrix that appears in the linearized mean field equation. Thus, when we enter the critical region, the inverse of the longitudinal propagator matrix starts getting zero eigenvalues, indicating the marginal stability of the mean field solution.

The Gaussian integration can now be performed to obtain the mean field free energy with Gaussian correction,

$$-\beta F_{\mathrm{mf}} = -N + \sum_i \ln \eta_i^2 + \ln \left| \det\left(G_{ij} + \frac{\delta_{ij}}{\eta_j^2} \right) \right|^{1/2} + \ln \left| \det\left(G_{ij} - \frac{\delta_{ij}}{\eta_j^2} \right) \right|^{(n-1)/2} \tag{3.13}$$

The zero-mode problem arising from the Goldstone modes can be taken care of by the Fadeev–Popov method. In the limit $n \to 0$ we get

$$-\beta F_{\mathrm{mf}} = -N + \sum_i \ln \eta_i^2 + \ln \left| \frac{\det(G_{ij} + \delta_{ij}/\eta_j^2)}{\det(G_{ij} - \delta_{ij}/\eta_j^2)} \right|^{1/2} \tag{3.14}$$

Multiplying the numerator and denominator inside the determinant by V_{ij}, we get

$$-\beta F_{\mathrm{mf}} = -N + \sum_i \ln \eta_i^2 + \frac{1}{2} \ln \left| \frac{\det(\delta_{ij} + V_{ij}/\eta_j^2)}{\det(\delta_{ij} - V_{ij}/\eta_i^2)} \right| \tag{3.15}$$

The second term in the above equation contains the effect of frustration and randomness. In the Hamilton circuit problem considered by OID there was no frustration and no randomness. The density of states of the matrix V_{ij}/η_j^2 was symmetric. This led to the cancellation of the two determinants. Thus, the absence of frustration seems to be the basic reason for the remarkable accuracy of the mean field result in lower dimensions in the Hamilton circuit problem. It will be interesting to study the Hamilton circuit problem in regular frustrated lattices in this light. In our problem, since there is frustration and randomness, the two determinants do not cancel each other.

The mean field at every city has a simple interpretation. Let the frustration and randomness be small. Then the mean field free energy is large compared to the Gaussian correction. At low temperatures, this free energy is approximately equal to the mean energy of the system. This is nothing but the sum of the distances between consecutive cities in an optimal tour. This means that in an optimal tour, with very high probability a city at a distance $(1/\beta)(-1+\ln \eta_i^2)$ from the ith city will be chosen in the next step.

When we have large frustration, the Gaussian fluctuation term complicates the interpretation. Let the disorder be so large that all the eigenstates of the matrices $(\delta_{ij}+V_{ij}/\eta_j^2)$ and $(\delta_{ij}-V_{ij}/\eta_j^2)$ are well localized in space, so we can associate one localized state to every city, on which that localized state has a maximum overlap. Then the fluctuation term can be approximately written as

$$\frac{1}{2}\ln\left|\frac{\det(\delta_{ij}+V_{ij}/\eta_j^2)}{\det(\delta_{ij}-V_{ij}/\eta_j^2)}\right|=\frac{1}{2}\sum_{\alpha}\ln\frac{\lambda_\alpha^+}{\lambda_\alpha^-}\approx\frac{1}{2}\sum_{i}\ln\frac{\lambda_i^+}{\lambda_i^-} \tag{3.16}$$

where λ_α^+ and λ_α^- are the eigenvalues of the matrices $(\delta_{ij}+V_{ij}/\eta_j^2)$ and $(\delta_{ij}-V_{ij}/\eta_j^2)$, and $\lambda_{\alpha_i}^+$ and $\lambda_{\alpha_i}^-$ the eigenvalues of the state α_i that has maximum overlap with the city i. Thus,

$$\frac{1}{\beta}\left(-1+\ln\eta_i^2+\frac{1}{2}\ln\frac{\lambda_{\alpha_i}^+}{\lambda_{\alpha_i}^-}\right)$$

is the distance of the next city that is likely to be chosen in an optimal tour at very low temperatures.

In the above we have presented a possible scenario in a simple mean field theory without doing any explicit average. We have assumed that the mean field points in the same direction in all the cities. This assumption seems to work quite well in the Hamilton circuit problem studied by OID, which has no frustration. The validity of this approximation to the present problem with randomness and frustration has to be studied further.

The mean field that we have chosen is complex. Thus, one has to change the contour in the multidimensional integral into the complex plane. There may be saddle points that give complex free energies. Since the final free energy is real, they have to occur as complex conjugate pairs. Such saddle points give rise to very strong N dependence of the free energy, such as $\ln\cos(bN)$, where b is some constant. On physical grounds we do not expect such saddle points to exist.

The mean field theory solution has to have nonzero values at every site, as is obvious from the mean field equation. This suggests that a spatially varying mean field solution (having mean fields with different signs at different cities) cannot be continuously deformed into another one in which the mean fields at some cities have changed signs as the parameters of the problem are changed. This is possible only if we make the mean field orientation space dependent.

From the above analysis one expects the number of mean field solutions to proliferate once we enter the critical region. It should be pointed out that the number of mean field solutions is not directly related the number of optimal tours. For example, when we are at a very high temperature, where the ferromagnetic solution is a good mean field solution, and where the value of the mean field is approximately $\beta^{-d/2}$, any tour in which the nearest neighbor jumps are of the order of β^{-1} is an optimal tour. In general, each mean field solution describes a class of optimal tours.

It will be interesting to test numerically or analytically the multiplicity of the mean field solutions at low temperatures. Another useful analysis will be to perform detailed analysis of the mean field equation, including the Onsager type of reaction field correction to get a TAP-type equation.[16]

3.1. Spontaneous Symmetry Breaking at All Temperatures

We observed from Eq. (3.5) that the mean field value cannot be zero at any city. This means that there is spontaneous symmetry breaking at any finite temperature. This need not be a consequence of the man field approximation, if we use the following argument. Let us assume that there is a paramagnetic phase. Then the high-temperature Boltzmann factor is effectively (in the sense of renormalization group) a product of Gaussian factors corresponding to the independent normal modes. This integration can be performed to get

$$Z_n \sim \frac{1}{n} \frac{(\det A)^{n/2}}{1} b \tag{3.17}$$

and

$$Z_n \to \infty \qquad \text{as} \quad n \to 0 \tag{3.18}$$

where det A arises from the independent normal modes and b is a constant independent of n. The constant b arises from the integration over the short-wavelength fluctuations. It is unlikely that this term will be proportional to n to cancel the n in the denominator. Thus, even when corrections are made to the mean field theory, the spontaneous symmetry breaking is likely to survive.

3.2. Quenched Average

In the field theory representation there are some difficulties in performing the quenched average in a replica method. This is related to the fact that the random variables, namely the distances between pairs of cities, appear in a strange place in the partition function. Even if we assume that the cities are randomly distributed in a volume without any correlation, the averaging operation with respect to the position of the cities after introducing the replica is still more difficult than the classical statistical mechanics of particles interacting through repulsive exponential interaction.

We have attempted a quenched average based on the following argument. The matrix G_{ij} is the lattice propagator at zero energy. In a random system the average of this is known to decay exponentially and also exhibits rapid spatial oscillations. Thus, we may model G_{ij} by a Gaussian random variable. A detailed analysis shows that this leads to serious divergences. This arises due to the fact that with the above probability distribution, some of the G_{ij} become arbitrarily small with finite probability, leading to violent fluctuations in ϕ's. This leads to divergence, because our partition function, Eq. (2.4), is a complicated higher order moment of a Gaussian distribution.

In the Appendix we will see that the quenched averaging can be explicitly performed in a replica treatment of the problem if one makes certain assumptions about the distribution of the intercity distances.

4. DISCUSSIONS

In this paper we have provided a simple analytical treatment of the statistical mechanics of the TSP. We have provided two representations of the problem, following recent work of Orlando *et al.*[13] and Hopfield and Tank.[17]

The first representation has several interesting features. First, we have obtained a very simple and nontrivial mean field equation. A stability analysis of the mean field equation suggests that at low temperatures the mean field may undergo drastic changes as we decrease the temperature. This is due to the divergence of some localized mode susceptibilities. This also points to the possibility of the proliferation of the mean field solutions. We have also given a simple interpretation to the man field solution. Since the man field equation is for a given random configuration of the cities, it may prove useful to specific optimization problems. It will be interesting to see how close the tours constructed from the solutions of our mean field equation are to the best optimal solutions obtained by other means (say, by simulated annealing).

It is interesting to note that, as in the spin-glass problem, the localization property of tigh binding random matrices enters our mean field theory. This brings out the role played by frustration. The role played by dimensionality is also brought out in our mean field theory through the random matrices. The appearance of random matrices and their localization properties may be generic to a class of optimization problems.

Dimensionality plays a crucial role in phase transition problems in general. The TSP conventionally defined is on a two-dimensional place. Thus, the statistical mechanical problem is two dimensional. A one-dimensional TSP has a trivial solution. Our mean field analysis shows that there is no possibility of extended mode susceptibility divergence in the two-dimensional TSP. This may imply the absence of any conventional phase transition. It is, however, possible to have a phase transition with proliferation of mean field solutions at low temperatures, with nontrivial overlap properties between the mean field solutions. Since the range of the matrix V_{ij} becomes shorter and shorter as we go to low temperatures, the detailed low-temperature properties of the problem may strongly depend on dimensionality. The nonmetric model discussed by Vannimenus and Mézard[4] and also by us in Section 4 can be thought of as an infinite-dimensional model.

There are certain difficulties associated with introducing the replica method and doing explicit quenched averaging in the first representation. Other types of difficulties arise in studying mean field solutions that change in direction from city to city in the internal space. Even if one can find such a solution for a finite n, it is not clear how to analytically continue such a solution to the $n \to 0$ limit.

In the permutation group representation discussed in the Appendix, we have performed the quenched average explicitly for a nonmetric model. The anomalously large low-temperature entropy is clearly brought out in this representation. If one succeeds in calculating various overlaps, it will probably be through this representation. The partition function of an optimization problem is in general an average over the appropriate permutation group. Hence, the permutation group representation may find use in several other combinatorial optimization problems.

As a general practice it may be useful to search for several representations in any combinatorial optimization problem. Each representation may bring out different special features of the problem. In polymer problems, which are closely related to TSP, a useful representation is available in terms of the Grassman variables. Fu and co-workers[20] have developed representations in terms of the Grassman variables of MTSP and TSP.

After this paper was written we came across an interesting paper by Orland.[21] He gives a representation of the TSP whose origin is identical to ours, but the details are different. However, the discussion is concentrated on another combinatoric optimization problem, the bipartite matching problem.

APPENDIX. A PERMUTATION GROUP REPRESENTATION

The introduction of permutation group elements as "spin" variables is similar to a representation introduced by Hopfield and Tank.[17] In this representation we are able to perform explicit quenched averages for a model distribution of distances between the cities. The resulting quenched partition function is quite complex. We introduce an Edwards–Anderson type of order parameter and make a simple Ansatz for the equilibrium value of the order parameter. The resulting free energy is not extensive at low temperatures. Our analysis points out that the Ansatz used is not correct and that the problem is more complicated than the finite-range spin-glass problem.

Hopfield and Tank studied the TSP using their neuron system, in which N^2 neurons are used. Each neuron can be in one of two states, which we will call up and down. These neurons are placed in an N by N array. A tour is uniquely coded by a set of N up-neurons with one and only one up-neuron per row and per column in such a way that the (ij)th neuron is up if and only if the ith stop along the tour is at city j. To ensure that no more than one city is visited at the same time and that every city is visited once, four penalty functions are used. This approach produced interesting result, but is hopelessly cumbersome for theoretical discussions. In fact, since there are about $N!$ different tours and

$$2^{N^2} \gg N! \gg 2^N \tag{A1}$$

it is obvious that Ising spin-like variables are not convenient for describing different tours; N^2 Ising spins will be far too many, while N spins will not be nearly enough.

Inspired by Hopfield and Tank, we use a matrix V to describe different tours. V is an N by N matrix, with one and only one 1 per each row and column; the rest of the matrix elements are zero. A given tour is uniquely specified by such a matrix in the following way:

$$V_{ij} = \begin{cases} 1 & \text{if the } i\text{th stop is at city } j \\ 0 & \text{otherwise} \end{cases} \tag{A2}$$

We define $V_{N+1,i} = V_{1,i}$ to have the trip end at its starting point. For example, if $N = 6$, the tour

$$1 \to 3 \to 4 \to 6 \to 5 \to 2 \to 1$$

is specified by

$$V = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \end{bmatrix}$$

The V's form a faithful representation of the permutation group S_N. Its $N!$ elements are in one-to-one correspondence with all possible tours. It is natural to use the elements of the permutation group as the dynamical variables for a *combinatoric* optimization problem.

One can verify that this representation of the permutation group is unitary. The unitarity follows from the way V is defined,

$$(V^{\dagger} V)_{jk} = \sum_{i=1}^{N} V_{ij} V_{ik} = \delta_{jk} \tag{A3}$$

The N cities are assumed to be distributed randomly. Here we shall choose the elements of the distance matrix d_{ij} to be Gaussian random variables centered at zero:

$$[d_{ij}]_{av} = 0, \qquad [d_{ij}^2]_{av} = D^2 \tag{A4}$$

Notice that there is nothing wrong in allowing a negative distance. The shortest tour (which typically will have a negative total length) is still well defined, and still hard to find. The problem has not been modified in any essential way. If one insists on having a positive distance, one can always add a constant $a \gg D$ to each d_{ij} so that the probability of having a negative distance is negligibly small. The total length of the tour is

$$L = Na + \sum d_{ij} \tag{A5}$$

The nontrivial part is still given by the distance matrix with zero mean. All these random variables are assumed to be independent, subject only to the conditions

$$d_j = d_{ji}, \qquad d_{ii} = 0 \tag{A6}$$

This implies that the space is no longer geometrical. In general the triangular inequality does not hold. We have tranformed a problem with site randomness into one of "bond randomness." This is similar to describing spin-glasses with randomly located magnetic impurities by the Edwards–Anderson model.

We can now formulate the TSP as a statistical mechanical problem. The cost function is

$$L = \sum_{i,j,k} V_{ij} d_{jk} V_{i+1,k} = \mathrm{tr}(V \cdot d \cdot V^{\dagger} \Delta) \tag{A7}$$

where

$$\Delta_{ij} = \delta_{i,j+1} \tag{A8}$$

Introducing replicas, we have

$$[Z^n]_{\mathrm{av}} = \mathrm{Tr}\exp \frac{\beta^2 D^2}{2} \sum_{a \neq b}^{n} \sum_{i,l=1}^{N} [(V_a V_b^{\dagger})_{il} (V_a V_b^{\dagger})_{i+1,l+1} + (V_a V_b^{\dagger})_{i,l+1} (V_a V_b^{\dagger} (_{i+1,l}] \tag{A9}$$

where we have used Eq. (A6). In Eq. (A9) Tr stands for the summation over the group elements of each of the n copies of the permutation group S_N. We will use tr for the trace of an ordinary matrix. Since V_a and $V_b^{\dagger} = V_b^{-1}$ are both elements of S_N, so is $T^{ab} = V_a V_b^{\dagger}$, and

$$\begin{aligned} [Z^n]_{\mathrm{av}} &= \mathrm{Tr}\exp\left[\beta^2 D^2 \sum_{a<b} \sum_{i,l} (T_{il}^{ab} T_{i+1,l+1}^{ab} + T_{i,l+1}^{ab} T_{i+1,l}^{ab})\right] \\ &= \mathrm{Tr}\exp\left[\frac{\beta^2 D^2}{2} \sum_{a<b} \sum_{i,j,k,l} T_{ij}^{ab} T_{kl}^{ab} M_{ijkl}\right] \end{aligned} \tag{A10}$$

In (A10)

$$M_{ijkl} = (\delta_{i,k+1} + \delta_{i,k-1})(\delta_{j,l+1} + \delta_{j,l-1}) = [m \otimes m]_{ij,kl} \tag{A11}$$

and m is a nearest neighbor hopping matrix

$$m_{ij} = \delta_{i,j+1} + \delta_{i,j-1} \tag{A12}$$

The T's are not independent matrices, since

$$T^{ab} T^{bc} = V_a V_b^{-1} V_b V_c^{-1} = T^{ac} \tag{A13}$$

This type of correlation is expected, since we have constructed $n(n-1)/2$ T's from n V's.

Introducing a set of auxiliary variables Q, we can write Eq. (A10) as

$$\int DQ^{ab} \exp\left[-\frac{1}{2\beta^2 D^2} \sum_{a<b} \sum_{i,j,k,l} Q_{ij}^{ab} Q_{kl}^{ab} M_{ijkl}^{-1}\right] \mathrm{Tr}\exp \sum_{a<b} \sum_{i,j} Q_{ij}^{ab} T_{ij}^{ab} \tag{A14}$$

where

$$DQ^{ab} = \prod_{a<b} \frac{dQ^{ab}}{\beta D(2\pi)^{1/2}} \tag{A15}$$

This expression is exact. As a first step toward solving the problem, we shall use the mean field approximation. It is clear that at high temperature the entropy term will be of the order of $N \ln N$. On the other hand, the expected tour length at high temperature as a sum of N random variables is

$$L \sim -\sqrt{N}\, D \tag{A16}$$

In order to have an energy term with an N dependence comparable to that of the entropy part, we need to scale D in such a way that

$$D = N^{1/2}\, D_0(N) \tag{A17}$$

with $D_0(N) \sim \ln N$. We will decide on a form for $D_0(N)$ from our final result for the free energy. Note that the estimate of (A16) is rough, and does not by itself imply that this problem is always dominated by the entropy term, with a possible transition at zero temperature ($T_c \sim 1/\ln N$) into a low-temperature phase dominated by the energy part. A more careful treatment is needed.

Now we can try to construct a mean field theory solution. We assume that the integral in (A14) is dominated by the contribution coming from a saddle point

$$Q_{ij}^{ab} = q_{ij}^{ab} \tag{A18}$$

Lacking further insight into the problem, we shall try various Ansätze. In the high-temperature phase we expect no replica symmetry breaking. We also assume the mean field theory order parameter to be homogeneous in real space and to have no variation from site to site. This restricts the choice to either

$$q_{ij}^{ab} = q \tag{A19}$$

or

$$q_{ij}^{ab} = q\delta_{ij} \tag{A20}$$

Equation (A19) does not lead to any sensible result. Since T^{ab} has the same form as V,

$$\sum_{ij} T_{ij}^{ab} = N \tag{A21}$$

independent of the group element. The trace part of (A14) can be calculated exactly. Using

$$\sum_{ijkl} M_{ijkl}^{-1} = \left(\sum_{ij} m_{ij}^{-1}\right)^2 = \left[\sum_i \left(\sum_j m_{ij}\right)^{-1}\right]^2 = (N/2)^2 \qquad \text{(A22)}$$

we have that the free energy F is given by

$$\frac{\beta F}{N} = -(\ln N - 1) - \frac{q^2}{16\beta^2 D_0^2(N)} + \frac{q}{2} \qquad \text{(A23)}$$

It can be easily shown that no simple N dependence in $D_0(N)$ can remove the $\ln N$ term in the above free energy.

The second Ansatz (A20), is more promising, since it couples to

$$\operatorname{tr} T^{ab} = \operatorname{tr}(V_a V_b^\dagger) \qquad \text{(A24)}$$

which is the overlap between two tours. Experience from the study of spin-glass models strongly suggests that this is the correct order parameter. Unfortunately, it does not work either. Using

$$\sum_{ijkl} \delta_{ij}\delta_{kl} M_{ijkl}^{-1} = \operatorname{tr}(m^{-2}) = N^2/\pi \qquad \text{(A25)}$$

we have

$$\frac{\beta F}{N} = -\frac{q^2}{4\pi\beta^2 D_0^2(N)} + \frac{1}{nN}\left[-1 + \operatorname{Tr}\exp\left(q \sum_{a<b} \operatorname{tr} T^{ab}\right)\right] \qquad \text{(A26)}$$

The second term within the square brackets is hard to calculate in general, but we can expand it for small q, a good approximation for high temperatures and the transition region. The result is disappointing. None of the terms containing q is extensive. Also, no simple temperature-independent choice of $D_0(N)$ removes the nonextensive terms. This is also true if we choose q_{ij} to be a cyclic matrix, or any other element of the representation of S_N, by a well-known theorem of group theory.

Major difficulties include:

1. The anomalously large entropy. In the mean field theory described above with two simple Ansätze for the order parameters, the large entropy survives at every temperature. The system is always in the high-temperature phase. For finite systems, this is not a serious problem. If we let the temperature go to zero, the partition function still projects out the low-lying states. But for finite systems an annealed average is not much different from a quenched average, and it is not clear how the replica method

can be used to study the overlap between states in that case. Either this is a peculiar feature of the nonmetrical model (recall that the large entropy problem is not there in the metric model, as we discussed at the beginning of this paper), or it may be an artifact of our aproximation and the choice of the order parameters.

2. The proper choice of order parameters. Gross[18] has made the following observation, which indicates very clearly why the TSP may be much harder to solve than the spin-glass problem, and why a naive treatment of the problem (such as the one we just gave) is unlikely to succeed. Unlike spin-glasses, for which the two-state overlap contains all the information, in TSP one may have to consider higher order overlaps. In the high-temperature phase of spin-glasses, the overlap between any two states is of the order of 1. This overlap becomes of order N below the transition temperature. On the other hand, in the low-temperature phase of the TSP, three-, four, and in general p-tour overlaps will all be of the order of N, where p is some finite number. This can be seen from the existence of many common links in different short tours generated on the computer. It seems that one needs more order parameters [say, p functions $q_1(x)$, $q_2(x)$,..., $q_p(x)$] to describe the transition (or transitions). It is not clear how to study such a problem.

There is a valid lesson that that one can learn from our discussion of the TSP in this paper. Using the representation of a permutation group to describe different configurations can make the problem free of uncontrollable penalty functions, and may thus be important for all combinatorial optimization problems. The partition function of an optimization problem is always an average over the appropriate permutation group. Future development of the relevant mathematical techniques will be welcome.

Kirkpatrick and Toulouse[2] have found evidence for ultrametricity and high-order overlaps. The Traveling Salesman Problem may well belong to a new category of complex systems, one different from that of spin-glasses, and needs as its order parameter not a function $q(x)$ or the probability law associated with that function, but a family (finite or infinite) of functions and their corresponding probability laws.

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