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Fluctuations in the site-disordered traveling salesman problem

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Abstract
We extend a previous statistical mechanical treatment of the traveling salesman problem by defining a discrete 'site-disordered' problem in which fluctuations about saddle points can be computed. The results clarify the basis of our original treatment, and illuminate but do not resolve the difficulties of taking the zero-temperature limit to obtain minimal path lengths.

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1. Introduction

Theories describing disordered materials are based either on disorder arising from randomness in the strength of bonds or from randomness in site location. Although most theoretical progress has been made in the bond-disordered case, site disorder is probably closer to the picture of real materials. A similar situation exists in the best-known problem of combinatorial optimization, the traveling salesman problem (TSP), here taken to be the stochastic version. The Euclidean problem is defined in terms of randomly assigned city locations, but analytic progress is most developed for the random-link model [1, 2] in which inter-city distances are chosen independently from some probability distribution. Recently, we have presented a functional statistical mechanical technique to compute the average length of the TSP path at finite temperature for the site-disordered model [3, 4]. In this paper, we define a discrete model that provides a more rigorous foundation for our functional approach in the continuum and allows us to compute fluctuation terms that illuminate the difficulties of taking the zero-temperature limit to obtain minimal path lengths.

The site-disordered TSP populates a graph consisting of M nodes or sites with N cities and is a straightforward generalization of the ordinary TSP that has $N = M$. The graph can be an abstract or for geometric applications we could take it to be a regular lattice. Site disorder arises since the number of cities on each site, which may be 0, 1 or greater than 1, is part of the specification of the problem, and we will have in mind a quenched random distribution. This problem is defined in section 2 and various regimes depending on the average density of cities,

N/M, are identified. Section 3 shows how the results of our previous functional formalism can be obtained from the $N \gg M$ high density or 'coarse' regime of the discrete site-disordered TSP for a fixed rather than random distribution of cities. These results correspond to the leading-order saddle point approach, and we show how they can be extended by analyzing fluctuations in the discrete model.

Our interest in the fluctuations arises from the possibility that they may be used to probe minimal TSP path lengths. This was not possible in our previous work since the leading saddle point term always gives path lengths that grow proportional to N and correspond to strictly finite temperature. In certain cases, the fluctuation terms have the correct scaling and may be expected to dominate in the low-temperature regime where the minimal path lengths can be accessed. Unfortunately this program is not realized. The fluctuations can be computed explicitly for some graphs with simple structure, and we discover that in the limits needed to find minimal path lengths the saddle point approximation breaks down in a complicated manner. The manner of this breakdown is most clearly exposed for the case $M = 2$ that is analyzed in detail in the appendix.

The remaining sections of the paper discuss the site-disordered problem in two other regimes. First, the case $N = M$, precisely the ordinary TSP, where it is interesting to see that the saddle point approximation breaks down in a completely different way from in the $N \gg M$ coarse regime. Second, the case $N \ll M$, which for a regular, dilutely occupied lattice can also correspond to the ordinary geometric TSP, and we discuss the significant interest of this regime, and point out the additional techniques that may be needed to resolve the problem in this regime.

2. Formalism

Consider a graph consisting of M sites with a matrix J_{ij} specifying the distance between any pair of sites $i, j = 0, 1, 2, \ldots, M-1$. For simplicity, the diagonal terms $J_{ii} = J_D$ are taken all equal but the matrix need neither be symmetric nor positive though we shall generally take it to be so. Imagine that there are n_j cities ($n_j \geqslant 0$) at site j. We will call these quantities the 'occupation numbers' and for a total of N cities they obey $\sum_{j=0}^{M-1} n_j = N$. A path through the N cities is specified by the sequence of site indices $j_0, j_1, \ldots, j_{N-1}$, so depending on the occupation numbers (n_j's), some sites might never be visited, or visited more than once. A particular path, $j_0, j_1, j_2, \ldots, j_{N-1}$, can also be characterized by an element of the permutation group, $\sigma \in \Sigma_N$, consisting of permutations of M site indices, each repeated n_j times, so as to have a total of N indices. In this notation, the path is written $\sigma_0, \sigma_1, \ldots, \sigma_{N-1}$, and the cost or total length for this path is

$$D(\sigma) = \sum_{m=0}^{N-1} J_{\sigma_m, \sigma_{m+1}} = \sum_{m=0}^{N-1} J_{j_m j_{m+1}}, \tag{1}$$

where we identify j_N with j_0. As is often the case in this kind of problem, the cost is independent of cyclic changes and also (if J_{ij} is symmetric) reversals of the permutation.

A full statement of the problem involves a specification of the occupation numbers as well as the cost matrix between all sites. Because we take a site-disordered approach we shall generally assume that the cost matrix is a fixed known quantity and will often have a geometric basis in mind for which the cost matrix follows from a regular lattice graph. Disorder can appear through the occupation numbers on each site.

By varying N/M, the average number of cities per site, we see that this model describes various regimes. If we take $N = M$ and set all the $n_k = 1$, then we immediately return to

the TSP as usually formulated with an arbitrary cost matrix J_{ij} that may, or may not, have a geometric basis. When we consider geometric problems such as the Euclidean TSP it is numerically advantageous to imagine the sites as being on a regular lattice, thus allowing the use of integer arithmetic to compute J_{ij} [5], and by considering sufficiently dilute occupation $N \ll M$ the continuum result is recovered. In this Euclidean lattice case, the $N = M$ situation is trivial as it corresponds to a fully occupied lattice where the optimum TSP paths only involve nearest-neighbor links. The approach to the continuum and standard TSP as lattice occupation is made progressively more dilute, $N \ll M$, has been considered numerically in [6]. Analytically, the most tractable regime is when $N \gg M$ and this may be regarded as a coarse, in the renormalization group sense, approximation to the TSP in which groups of close cities are bunched together at the same site ignoring the detailed distances between them. Even in this coarse regime, information about the standard TSP can be obtained by arranging for the diagonal distances J_{ii} to be small.

The statistical mechanical partition function for this problem at temperature $1/\beta$ is defined by the following sum over permutations that visit sites the correct number of times:

$$Z_N(\beta, \{n_j\}) = \sum_{\sigma \in \Sigma_N} \exp(-\beta D(\sigma)). \tag{2}$$

This partition function $Z_N(\beta, \{n_j\})$ depends both on occupation numbers and J_{ij}'s and therefore encompasses both bond and site disorder. The sum over permutations may be written as an unconstrained sum over all possible paths of N links with a Kronecker delta constraint to ensure that site j is visited precisely n_j times:

$$Z_N(\beta, \{n_j\}) = \sum_{j_0, j_1, \ldots, j_{N-1}=0}^{M-1} \prod_{k=0}^{M-1} n_k! \delta_{n_k, \sum_{m=0}^{N-1} \delta_{k, j_m}} \exp\left(-\beta \sum_{m=0}^{N-1} J_{j_m j_{m+1}}\right). \tag{3}$$

The constraints appearing here should not be confused with the constraints that forbid disconnected paths in the linear programming approach to the TSP; here the path is always connected, but must be forced to visit sites the correct number of times. The combinatorial factors of $n_k!$ arise from the different possible orderings of visiting multiple cities at the same site, and are necessary to ensure that with no weights, $\beta = 0$, we recover $Z_N = N!$, corresponding to the total number of possible orderings of N cities. It is implicit in the formalism that $\sum n_k = N$ since this constraint is enforced by one of the Kronecker deltas.

Writing each Kronecker delta in terms of an integral representation, we find

$$Z_N(\beta, \{n_j\}) = \sum_{j_0, j_1, \ldots, j_{N-1}=0}^{M-1} \oint \prod_{k=0}^{M-1} \frac{\mathrm{d}z_k z_k^{n_k - 1} n_k!}{2\pi \mathrm{i}} \prod_{m=0}^{N-1} \frac{1}{z_{j_m}} \exp\left(-\beta \sum_{m=0}^{N-1} J_{j_m j_{m+1}}\right) \tag{4}$$

$$= \sum_{j_0, j_1, \ldots, j_{N-1}=0}^{M-1} \int_{-\pi}^{\pi} \prod_{k=0}^{M-1} \frac{\mathrm{d}\mu_k n_k!}{2\pi} \exp\left(\mathrm{i} \sum_{k'=0}^{M-1} n_{k'} \mu_{k'} - \mathrm{i} \sum_{m=0}^{N-1} \mu_{j_m}\right)$$

$$\times \exp\left(-\beta \sum_{m=0}^{N-1} J_{j_m j_{m+1}}\right), \tag{5}$$

where the second form is obtained from the contour integral in the first line by setting $z_k = \mathrm{e}^{\mathrm{i}\mu_k}$. Although the integrals are finally evaluated using this second form, it is helpful to keep the first form in mind to check what deformations of the contour are possible in the presence of branch cuts or poles. Rearranging, the partition function can be written in terms of an integral over a subsidiary problem,

$$Z_N(\beta,\{n_j\}) = \int_{-\pi}^{\pi} \prod_{k=0}^{M-1} \frac{\mathrm{d}\mu_k n_k!}{2\pi} \exp\left(\mathrm{i}\sum_{k'=0}^{M-1} n_{k'}\mu_{k'}\right) \mathcal{Z}_N(\beta,\{\mu_j\}). \tag{6}$$

The subsidiary statistical mechanical problem does not depend on the occupation numbers, n_k, and is defined as

$$\mathcal{Z}_N(\beta,\{\mu_j\}) = \sum_{j_0,j_1,\ldots,j_{N-1}=0}^{M-1} \exp\left(-\mathrm{i}\sum_{m=0}^{N-1}\mu_{j_m} - \beta\sum_{m=0}^{N-1} J_{j_m j_{m+1}}\right) = \mathrm{Tr}\,\mathbf{T}^N, \tag{7}$$

where the $M \times M$ transfer matrix, $\mathbf{T}$, is of the symmetrized form:

$$\mathbf{T} = \mathbf{RBR}. \tag{8}$$

Here, $\mathbf{R}$ is the diagonal matrix with diagonal elements $R_k = z_k^{-1/2} = \exp(-\mathrm{i}\mu_k/2)$, and $\mathbf{B} = \exp(-\beta\mathbf{J})$ is defined in terms of the distance matrix. In this paper, we shall only consider symmetric distance functions, so the transfer matrix is symmetric, though generally complex and therefore not Hermitian.

Distance matrices that have some kind of regular geometric basis yield additional structure for $\mathbf{B}$. In one dimension this is most obvious, for example a regular one-dimensional lattice with $J_{ij} \propto |i-j|$ makes $\mathbf{B}$ Toeplitz, and if the lattice has periodic boundary conditions $\mathbf{B}$ is also circulant. For regular lattices in two dimensions $\mathbf{B}$ is block circulant with each of the blocks Toeplitz, or themselves circulant in the case of periodic boundary conditions. In higher dimensions, there is a hierarchical structure of $\mathbf{B}$ block circulant with blocks that are themselves block circulant. For all these regular lattices, the eigenvectors are related to discrete Fourier transforms [7]. We also consider fully connected M-dimensional graphs with $J_{ij} = J_N + (J_D - J_N)\delta_{ij}$, which are particularly tractable. We often allow a diagonal term in the cost matrix, as this can be used to probe certain aspects of the theory. We will not consider asymmetric cases in this paper, but examples such as the wallpaper problem [8] with $J_{ij} = \theta(i-j)$ can be treated.

The solution of the subsidiary problem can be written in terms of the eigenvalues λ_a of $\mathbf{T}$,

$$\mathcal{Z}_N(\beta,\{\mu_j\}) = \mathrm{Tr}\,\mathbf{T}^N = \sum_{p=0}^{M-1} \lambda_p^N. \tag{9}$$

For general values of the integration variables z_k or μ_k, the eigenvalues will be complex. Under the scaling $z_k \to az_k$, eigenvalues transform as $\lambda \to \lambda/a$, and below we shall find that this scaling symmetry is related to the Lagrange multiplier mode enforcing the constraint $\sum n_k = N$.

To close this section on the formalism, let us interpret it in the case of the $N = M$ regime with all occupation numbers $n_k = 1$, corresponding to the usual TSP. The partition function then becomes

$$Z_N(\beta) = \oint \prod_{k=0}^{N-1} \frac{\mathrm{d}z_k}{2\pi\mathrm{i}} \mathrm{Tr}(\mathbf{T}^N), \tag{10}$$

with $\mathbf{T} = \mathbf{RBR}$ and $\mathbf{R}^2 = \mathrm{diag}\left(z_0^{-1}, z_1^{-1}, \ldots, z_{N-1}^{-1}\right)$, the trace is a polynomial in the variables z_j^{-1} that acts as a generating function for paths that visit site j a number of times given by the power of z_j^{-1}. The weight associated with a particular path is the exponential of the length of the path. Since all paths visit N sites, every term in the generating function polynomial has equal degree N. Depending on the symmetry of the distance matrix, the generating function often has some symmetry in the variables z_j. The integration defining the partition function for the TSP picks out the pole corresponding to the term $\prod z_j^{-1}$ in the generating function,

thereby requiring each site to be visited exactly once. From this point of view, the approach is similar to other combinatorial problems where the generating function is known, and in many graph theoretic problems a similar integration can be used to select the desired term. For example, in the mathematical literature, the saddle point technique has been used to obtain asymptotic formulae for the number of Eulerian oriented graphs [9]. For $\beta = 0$, distances are irrelevant and vertices are either connected or not, so the system becomes purely topological and the problem is to count Hamiltonian paths for a graph with incidence matrix **B**. The formalism also resembles the field theory for studying random Euclidean matrices [10].

3. Coarse TSP regime: $N \gg M$

Consider the limit of many cities, $N \to \infty$, with M fixed. In this limit the occupancies, n_k, scale with N, and it is convenient to rewrite them in terms of a 'density of cities', ρ_k, where

$$n_k = \frac{N}{M}\rho_k. \tag{11}$$

The normalization of ρ_k is $\sum_{k=0}^{M-1} \rho_k = M$.

In a geometric context, the formalism is now based on densities of cities rather than their explicit locations and this limit might be regarded as viewing the system at coarse resolution, smearing out the precise city locations. Such coarsening techniques are indeed used in heuristics for solving TSP instances, although in a different way, for example the Held–Karp heuristic [11] patches together paths from different cells.

In this regime, a diagonal term $J_{ii} = J_D$ in the cost matrix can have a special significance. If this self connection corresponds to a distance larger than typical neighbor distances, then it will have little effect at low temperature and the optimum path for uniformly distributed cities may correspond to the optimum of the standard TSP, repeated N/M times. If on the other hand, J_D is short in comparison with other distances, then the favored paths at low temperature will satisfy the requirement to visit cities n_k times by simply looping that many times before proceeding to a neighbor. In this case, the true TSP path is found simply by ignoring the contribution from the loops. For various simple models with small M, we have considered this small J_D situation explicitly. At low temperature, by regarding the neighbor couplings as corrections to the diagonal part of **B**, then a perturbative approach can be used to compute the eigenvalues of **T** and hence the contribution to the partition function which correctly predicts the true TSP path. The hope of being able to compute such terms for arbitrary M is a motive for studying the fluctuations about the saddle point. Unfortunately, it appears that the saddle point method, which is our main tool, generally fails to give the correct subleading term in this limit for technical reasons that are discussed in the appendix and sections where particular models are considered.

By inserting the solution of the subsidiary problem into the expression for the full partition function, we find

$$Z_N(\beta, \{n_j\}) = \exp\left(\sum_{k=0}^{M-1} \log n_k!\right) \sum_{p=0}^{M-1} Z_N^p(\beta, \{\rho_j\}), \tag{12}$$

$$\begin{aligned} Z_N^p(\beta, \{\rho_j\}) &= \oint \prod_{k=0}^{M-1} \frac{\mathrm{d}z_k}{2\pi \mathrm{i} z_k} \left(\lambda_p \prod_{k=0}^{M-1} z_k^{\rho_k/M}\right)^N \\ &= \int_{-\pi}^{\pi} \prod_{k=0}^{M-1} \frac{\mathrm{d}\mu_k}{2\pi} \exp N\left(\frac{\mathrm{i}}{M} \sum_{k'=0}^{M-1} \rho_{k'}\mu_{k'} + \log \lambda_p\right), \end{aligned} \tag{13}$$

where the contributions from each eigenvalue are now distinguished, at least by a label $p = 0, 1, 2, \ldots, M-1$. In practice, globally labeling the eigenvalues of $\mathbf{T}$ as the z_k vary is not straightforward.

By writing in terms of ρ_k, the N scaling in the exponent is exposed that allows the integrals for each Z^p to be evaluated using a saddle point approximation [12]. For the simplest application of this technique to be valid, the eigenvalue must have no N dependence so we are forbidden to scale the temperature with N [13]. The saddle point equations for each Z^p are

$$-\frac{1}{\lambda_p}\frac{\partial \lambda_p}{\partial \mu_k} = \mathrm{i}\frac{\rho_k}{M}. \tag{14}$$

Now, by taking derivatives of the eigenequation, $\mathbf{T}\mathbf{v}^p = \lambda_p \mathbf{v}^p$, noting that $\partial T_{ij}/\partial \mu_k = -\mathrm{i}(\delta_{ki} + \delta_{kj})T_{ij}/2$, recognizing that the left and right eigenvectors are the same due to the symmetry of the distance matrix and using normalization, $\mathbf{v}^p \cdot \mathbf{v}^p = \sum_k v_k^p v_k^p = 1$, we find the general relation

$$\frac{1}{\lambda_p}\frac{\partial \lambda_p}{\partial \mu_k} = -\mathrm{i}\left(v_k^p\right)^2. \tag{15}$$

So the saddle point equation may be rewritten as

$$\left(v_k^p\right)^2 = \frac{\rho_k}{M}. \tag{16}$$

The right-hand side of this saddle point equation does not depend on the eigenvalue index p. Ostensibly we may choose signs independently for each component of the eigenvector to generate distinct solutions for each Z^p, but we shall discover that the role of the signs is not transparent. The eigenvector is written $v_k^p = \zeta_k^p \sqrt{\rho_k/M}$, where the signs $\zeta_k^p = \pm 1$. Now decomposing the transfer matrix and writing $s_k^p = \zeta_k^p \, \mathrm{e}^{\mathrm{i}\mu_k/2}\sqrt{\rho_k \lambda/M}$, the signs disappear and the eigenequations become

$$s_k^p = \frac{1}{M}\sum_{k'} \mathrm{e}^{-\beta J_{kk'}} \frac{\rho_{k'}}{s_{k'}^p}. \tag{17}$$

For all reasonable choices of the distance matrix, this equation has a solution with real positive s_k (to denote this solution we omit the index p) that can be found by a numerically stable iteration procedure. In many of the explicit models we consider, this solution is in fact independent of the index k; for example, in the case of circulant $\mathbf{J}$ and $\rho_k = 1$, this positive solution is $s_k = s$; $s^2 = (1/M)\sum_j B_{ij}$. For certain particular choices of the distance matrix, additional solutions to (17) may be found. For all cases considered, these additional solutions, while not spurious, are less important in the large N limit than the real positive solution noted above. These solutions are discussed in the sections below that deal with particular models.

In the remainder of this section, we shall only be concerned with the real positive solution s_k. The location of the saddle points for this solution in terms of integration variables z_k is given by

$$\lambda z_k = M\frac{s_k^2}{\rho_k}. \tag{18}$$

Note that all reference to the signs ζ_k^p has disappeared. Evidently, since the right-hand side is real and positive, there is a saddle point on the real z_k-axis with $\mathrm{Re}\,\mu_k = 0$. At this saddle point, the transfer matrix is real and symmetric and has real eigenvalues. Moreover (provided that the cost matrix is positive), the Perron–Frobenius theorem assures us that the eigenvector $v_k = +\sqrt{\rho_k/M}$, where $\zeta_k^p = +1$, corresponds to the maximal eigenvalue.

Note that under the scaling symmetry $z_k \to a z_k$, eigenvalues transform as $\lambda \to \lambda/a$, so the combination λz_k appearing in (18) is invariant. As mentioned above, this scaling corresponds to the Lagrange multiplier mode involving a simultaneous shift of all μ_k, that enforces the constraint $\sum n_k = N$. Since this constraint is implicitly satisfied by the ρ_k that we specify, there is no need to integrate over it, and we may choose to set $\sum \mu_k = 0$ or $\prod z_k = 1$. As we shall see explicitly in section 4, the stationarity condition associated with this mode is not necessary to solve the saddle point equations since the normalization condition for ρ_k can replace this information. For the real solution, s_k, the requirement $\prod z_k = 1$ forces λ^M to be real. We can therefore identify a total of M saddle points simply related to the real one by overall phases. These saddle points, arising from the positive real solution to (17) will be termed dominant:

$$z_k^{(p)} = \mathrm{e}^{2\pi p \mathrm{i}/M} z_k^{(0)}, \qquad p = 0, 1, \ldots, M-1, \tag{19}$$

$$z_k^{(0)} = \frac{\frac{s_k^2}{\rho_k}}{\left(\prod_{k=0}^{M-1} \frac{s_k^2}{\rho_k}\right)^{1/M}}, \tag{20}$$

$$\lambda^{(p)} = \lambda^{(0)} \mathrm{e}^{-2\pi p \mathrm{i}/M}, \tag{21}$$

$$\lambda^{(0)} = M \left(\prod_{k=0}^{M-1} \frac{s_k^2}{\rho_k} \right)^{1/M}. \tag{22}$$

Note that for the case in which $\rho_k = 1$ and the solution s_k is independent of k, these equations simplify dramatically: $\lambda^{(0)} = M s^2$ and the saddle points are equally spaced around the unit circle.

It is tempting to identify each of these M saddle point solutions with a single dominant saddle point for each of the M integrals Z^p in equation (13). In that case, the phase factors cancel in the leading contribution and each Z^p contributes equally to the total partition function, resulting in an overall factor of M that can be interpreted as arising from the redundancy of cyclic permutations or equivalently the choice of origin of the paths. However, the above derivation does not provide an unambiguous identification of the saddle points with the Z^p since the eigenvalues are not globally labeled. A suitable approach would be to label eigenvalues according to their order at some reference point, say $z_k = 1$ where they are real, and then to smoothly deform z_k. This procedure is subject to difficulties since the constraint $\prod z_k = 1$ should be maintained while deforming, and incorrect conclusions arise if one takes all $z_k = \mathrm{e}^{\mathrm{i}\theta}$ and varies $\theta = 0$ to $\theta = 2\pi p/M$. Some intuition can be gained from explicitly considering small M examples and in the appendix the TSP on two points is treated. In that case, although the picture is complicated by the existence of another solution to (17), the identification is correct, with the dominant contribution (from the positive real solution) yielding a single saddle point for each of the two eigenvalues.

Henceforth, we shall assume that the picture of saddle points given above is correct. In the following subsection, we consider the order $1/N$ fluctuations about the saddle point, but first we deal with the leading contribution from the dominant saddle points. The free energy is

$$-\beta F(\beta, \{\rho_k\}) = \log Z_N = \frac{N}{M} \sum_k \rho_k \log \lambda z_k + N \log N, \tag{23}$$

where we have used the Stirling's approximation for $n_k!$.

The expected path length, $\langle E \rangle$, and other quantities such as correlations along the path can be computed from the partition function by appropriate derivatives. The expression for

the path length can be rewritten in terms of s_k itself, but higher moments explicitly involve derivatives. The final equations determining the leading contribution in this coarse regime are

$$s_k = \frac{1}{M}\sum_{k'} \mathrm{e}^{-\beta J_{kk'}} \frac{\rho_{k'}}{s_{k'}}, \tag{24}$$

$$\beta F = -\log Z_N = -2N\frac{1}{M}\sum_k \rho_k \log s_k - N\log N, \tag{25}$$

$$\langle E\rangle = \frac{N}{M^2}\sum_{kk'} \frac{\rho_k \rho_{k'} J_{kk'}}{s_k s_{k'}} \mathrm{e}^{-\beta J_{kk'}}. \tag{26}$$

Note that the expected path length is always of order N in the limit we have considered. This is indeed expected at finite temperatures where the number of relevant contributing paths grows as a factorial of N. To see this, we may compute the entropy as

$$S(\beta, \{\rho_k\}) = \beta(E - F) = \left(1 - \beta\frac{\partial}{\partial\beta}\right)\left[\frac{2N}{M}\sum_k \rho_k \log s_k\right] + N\log N = NS_E + N\log N, \tag{27}$$

where in the final form we have isolated the extensive, S_E, from the non-extensive contributions to the entropy. Then, by inverting the expression for the path length obtained from equation (26), the entropy can be re-expressed as a function of path length. The significance of the entropy in this problem is that the number of paths of given length is

$$\mathcal{N}(E) \sim \mathrm{e}^{S(E)} = N!\,\mathrm{e}^{NS_E}. \tag{28}$$

The factorial growth in the number of paths with the number of cities characterizes this $N \gg M$ regime and indicates that this is not the regime where the optimum path can be found. To approach that regime, where cities are linked to one of their nearest neighbors thus making the number of paths grow exponentially, some scaling is necessary. Either the distances J_{ij} can be scaled so as to preserve constant density of cities as $N \to \infty$, or equivalently the temperature can be scaled with N [13]. This kind of scaling would invalidate the simple use of the saddle point to solve for the partition function as the large parameter N would not appear as a simple factor in the exponent. Therefore, the leading order of this coarse model cannot access the optimal paths of interest in the TSP. However, as we recall below, the approach can be used at finite temperature and in studying the maximal TSP problem [14] where no scaling is needed to find the regime of maximal optima.

3.1. Continuum geometric models

In order to relate the leading-order site-disordered TSP results above to the results of our previous functional approach, we take a continuum limit with indices j corresponding to points $\mathbf{r}_j$ in some d-dimensional domain. The distance matrix is defined by the Euclidean distances between the points, $J_{ij} = |\mathbf{r}_i - \mathbf{r}_j|$. Assuming a domain with unit volume, the appropriate lattice spacing scale is $M^{-1/d}$ and the translations necessary to obtain the continuum limit are

$$\sum_k \to M\int \mathrm{d}^d r, \tag{29}$$

$$n_k \to \frac{N}{M}\rho(r_k), \tag{30}$$

where $\rho(r)$ is the continuum density of cities.

In the simplest procedure, the points are laid down on a regular lattice and the continuum limit is straightforward. In this case, there is no randomness whatsoever. We could also imagine M points laid down at random on the domain, then some weight factor is needed as we take the continuum version of the discrete sum. This weight factor appears in exactly the same places that the density of cities ρ does and in the end they are the same. Irrespective of the way the continuum limit is taken, the formalism only depends on the density of cities and all information about the precise location of the sites disappears.

The equations now become

$$s(\mathbf{r}) = \int \mathrm{d}^d r\, \mathrm{e}^{-\beta|\mathbf{r}-\mathbf{r}'|} \frac{\rho(\mathbf{r}')}{s(\mathbf{r}')}, \tag{31}$$

$$\beta F = -2N \int \mathrm{d}^d r\, \rho(\mathbf{r}) \log s(\mathbf{r}) - N \log N, \tag{32}$$

$$\langle E \rangle = N \int \mathrm{d}^d r\, \mathrm{d}^d r' \frac{\rho(\mathbf{r})\rho(\mathbf{r}')}{s(\mathbf{r})s(\mathbf{r}')} |\mathbf{r} - \mathbf{r}'|\, \mathrm{e}^{-\beta|\mathbf{r}-\mathbf{r}'|}. \tag{33}$$

These are the same equations written down in [3] using a functional formalism in the continuum. We now briefly summarize some of the results for low-dimensional models based on these equations. The most interesting predictions of this theory are for the MAX TSP [14] corresponding to negative β.

The formalism presented above yields the correct high-temperature expansion as a series in β, and has also been tested by comparison with the Monte Carlo simulation of the TSP at finite temperature [4]. Except for the case of closed symmetric domains to be discussed below, we have not found any non-trivial analytic solutions of the nonlinear equations (33). For the special closed domains, such as a disc and torus in two dimensions, a constant solution exists. The significance of this observation is that the annealed approximation, in which the average over cities is taken at the level of the partition function equation (2), is exact for these domains.

For the sphere, the annealed/quenched equations have a constant solution with

$$s^2 = \frac{1}{4\pi} \int_{S_2} \mathrm{d}^2 r\, \mathrm{e}^{-\beta\theta} = \frac{2\pi}{(\beta^2 + 4\pi)} (1 + \mathrm{e}^{-\sqrt{\pi}\beta/2}), \tag{34}$$

leading to an expression for the average path length

$$E/N = \frac{2\beta}{\beta^2 + 4\pi} + \frac{\sqrt{\pi}}{2(\mathrm{e}^{\sqrt{\pi}\beta/2} + 1)}. \tag{35}$$

Note that in the limit $\beta \to -\infty$, the path length per link becomes the half circumference corresponding, as is the case for all the closed domains, to the maximum distance two points can be apart.

For a torus we find that the equations yield

$$s^2 = \frac{8}{\beta^2} \int_0^{\pi/4} \left(1 - \mathrm{e}^{-\beta/2\cos\theta} - \frac{\beta\, \mathrm{e}^{-\beta/2\cos\theta}}{2\cos\theta} \right) \mathrm{d}\theta. \tag{36}$$

As $\beta \to -\infty$, the integral can be approximated and again the path length per link becomes the maximum distance two points can be apart, $E/N \to 1/\sqrt{2}$.

For most domains, including the traditional square box domain, the quenched result is different from the annealed approximation and there is little hope of a general analytic solution. In this case, our primary tool is the iterative numerical solution of equation (33) which is stable and can be solved to any required accuracy.

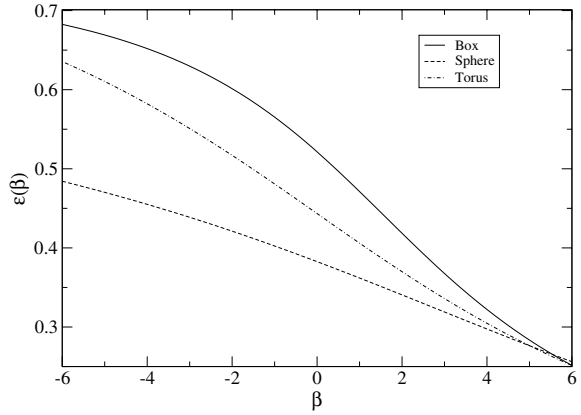

Figure 1. Theoretical prediction for the average path length E for two-dimensional continuum TSP on a box, sphere and torus as a function of β. Negative β corresponds to the MAX TSP.

Figure 1 shows the average path length for each of the three two-dimensional domains we have considered. For the sphere this is given by (35), for the torus it is based on numerical integration of (36) and for the box we resort to an iterative solution of the original quenched equations. The accuracy of this iterative technique is confirmed by reproducing the results for the other domains. In all these cases, we have also performed the Monte Carlo simulations and obtain excellent agreement with the theory. At large positive β, the topology starts to become unimportant and each domain has an average path length $\sim 2N/\beta$. In dimension d we expect $E \sim dN/\beta$, so this leading term vanishes at low temperature.

3.2. Fluctuations

Despite the inability of the leading term of this approach to access minimal length paths, it is interesting to consider the fluctuations which can contain terms with the correct scaling form. Gaussian fluctuations about the saddle point yield subleading corrections in N, containing a factor $\det^{-1/2}\mathbf{H}$, where $\mathbf{H}$ is the matrix,

$$\mathbf{H}_{kk'} = -\frac{\partial^2 \lambda}{\partial \mu_k \partial \mu'_k} = \left.\frac{\partial v_k^2}{\partial \mu_{k'}}\right|_{SP}. \tag{37}$$

In this coarse regime, the order of the corrections from these fluctuations will be $1/N$ with respect to the leading $O(N)$ term in the free energy and will thus correspond to an N-independent term. In one dimension, such an N-independent term corresponds to the scaling of the true TSP optimum. To proceed explicitly requires additional knowledge of the distance matrix. We shall consider the special case of $\rho_k = 1$ and a circulant $\mathbf{B}$ where a constant solution s exists and the eigenvectors are well known to be related to Fourier transforms [7]. This restricted choice of circulant matrix still covers various interesting geometrically based possibilities and the slightly different case of block circulant matrix is a simple generalization. Rather than to use the general determinant formula above, we proceed by explicitly expanding about the saddle points. We assume the picture of M dominant saddles and find that besides the phase cancellation at leading order, all saddle points contribute equally at the level of fluctuations, and we only need to consider fluctuations about the real saddle point, which in

this case is at $z_k = 1$. To expand about this saddle point write $z_k = \mathrm{e}^{\mathrm{i}\mu_k}$, where μ_k is small but may in general be complex. Then the transfer matrix is given by

$$\mathbf{T} = \left(\mathbf{I} - \frac{\mathrm{i}}{2}\mathbf{R}_1 - \frac{1}{8}\mathbf{R}_1^2 + \cdots\right)\mathbf{B}\left(\mathbf{I} - \frac{\mathrm{i}}{2}\mathbf{R}_1 - \frac{1}{8}\mathbf{R}_1^2 + \cdots\right) = \mathbf{T}^{(0)} + \mathbf{T}^{(1)} + \mathbf{T}^{(2)}\cdots, \tag{38}$$

where the matrix $\mathbf{R}_1$ is diagonal and given by

$$\mathbf{R}_1 = \mathrm{diag}(\ldots \mu_k \ldots) \tag{39}$$

and

$$\mathbf{T}^{(0)} = \mathbf{B}, \tag{40}$$

$$\mathbf{T}^{(1)} = -\frac{\mathrm{i}}{2}(\mathbf{R}_1\mathbf{B} + \mathbf{B}\mathbf{R}_1), \tag{41}$$

$$\mathbf{T}^{(2)} = -\frac{1}{8}\left(\mathbf{R}_1^2\mathbf{B} + 2\mathbf{R}_1\mathbf{B}\mathbf{R}_1 + \mathbf{B}\mathbf{R}_1^2\right). \tag{42}$$

The eigenvalue is written in a similar manner as $\lambda^{(0)} + \lambda^{(1)} + \lambda^{(2)} + \cdots$ (not to be confused with the labeling of the different eigenvalues of $\mathbf{T}$), and we shall usually drop the superscript on the unperturbed $\lambda^{(0)} = \lambda_0 = Ms^2$. The first- and second-order corrections can now be found using the standard techniques of quantum mechanical perturbation theory (though note that the matrix $\mathbf{R}_1$ is not generally Hermitian). It is convenient to use Dirac bracket notation for the eigenvectors of the unperturbed $\mathbf{T}^{(0)} = \mathbf{B}$:

$$\mathbf{B}|k\rangle = \lambda_k|k\rangle. \tag{43}$$

According to the analysis above, the maximal eigenvector $|0\rangle$ has constant components $v_j = 1/\sqrt{M}$ for constant density. The choice of a circulant $\mathbf{B}$ also fixes the other eigenvectors, $|k\rangle$ to have components $v_j = \mathrm{e}^{-2\pi\mathrm{i}jk}/\sqrt{M}$.

The first-order correction to the eigenvalue vanishes as expected,

$$\lambda^{(1)} = \langle 0|\mathbf{T}^{(1)}|0\rangle = -\frac{\mathrm{i}\lambda_0}{M}\sum_{k=0}^{M-1}\mu_k = 0. \tag{44}$$

At second order, there are two contributions:

$$\lambda^{(2)} = \langle 0|\mathbf{T}^{(2)}|0\rangle + \sum_{k\neq 0}\frac{\langle 0|\mathbf{T}^{(1)}|k\rangle\langle k|\mathbf{T}^{(1)}|0\rangle}{\lambda_0 - \lambda_k}. \tag{45}$$

The expression for the partition function (13) involves the following integral over the Gaussian fluctuations:

$$Z_N = M\left[\left(\frac{N}{M}\right)!\right]^M \lambda_0^N \int \prod_{k=0}^{M-1}\frac{\mathrm{d}\mu_k}{2\pi}\exp\left(\frac{N\lambda^{(2)}}{\lambda_0}\right), \tag{46}$$

where the terms in the exponent arise from expanding the logarithm and the prefactor M just counts the contribution from all the equivalent saddle points. To perform the integrals, it is convenient to change from the μ_k's to Fourier transform variables a_j in which the exponent will be diagonal:

$$\mu_k = \frac{1}{\sqrt{M}}\sum_{j=0}^{M-1} a_j\,\mathrm{e}^{2\pi\mathrm{i}jk/M}, \tag{47}$$

$$a_j = \frac{1}{\sqrt{M}} \sum_{k=0}^{M-1} \mu_k \, \mathrm{e}^{-2\pi \mathrm{i} jk/M}. \tag{48}$$

The constant part of μ_k corresponding to the Fourier mode a_0 imposes the constraint which we have implicitly assumed so the integration is omitted, and indeed no a_0 terms arise in the integrand. Using these variables, we find

$$\langle 0|\mathbf{T}^{(2)}|0\rangle = \frac{-1}{4M} \sum_{j=1}^{M-1} (\lambda_0 + \lambda_j) a_j a_{M-j}, \tag{49}$$

$$\sum_{k\neq 0} \frac{\langle 0|\mathbf{T}^{(1)}|k\rangle\langle k|\mathbf{T}^{(1)}|0\rangle}{\lambda_0 - \lambda_k} = \frac{-1}{4M} \sum_{j=1}^{M-1} \frac{(\lambda_0 + \lambda_j)^2}{(\lambda_0 - \lambda_j)} a_j a_{M-j}, \tag{50}$$

$$\lambda^{(2)} = \frac{-\lambda_0}{2M} \sum_{j=1}^{M-1} \frac{(\lambda_0 + \lambda_j)}{(\lambda_0 - \lambda_j)} a_j a_{M-j}. \tag{51}$$

It is now straightforward to evaluate the integral over the Gaussian fluctuations since we can take a contour in the direction where μ_k is real and therefore $a_j^* = a_{M-j}$. This corresponds to the imaginary direction in the z_k plane and for other dominant saddles the integration should be along the tangent to the unit circle. In this representation, the fluctuations are already diagonal and it is clear that all the eigenvalues of the fluctuation matrix are negative.

$$\beta F = -2N \log s + \frac{1}{2} \sum_{j\neq 0} \log\left(\frac{\lambda_0 + \lambda_j}{\lambda_0 - \lambda_j}\right) - N \log N. \tag{52}$$

The final fluctuation part is a simple expression in terms of the eigenvalues of the coupling matrix $\mathbf{B}$. Below we consider some particular examples with circulant $\mathbf{B}$ in this $N \gg M$ regime, the fully connected and geometrically motivated problems where expressions for the eigenvalues are available and the computation of the fluctuations can be taken further.

3.3. Fully connected graph

Consider the regular fully connected graph $J_{ij} = J_N(1 - \delta_{ij}) + J_D\delta_{ij}$ where all sites are connected by equal length links and we have allowed a diagonal term. We write $\mathrm{e}^{-\beta J_D} = d$ and $\mathrm{e}^{-\beta J_N} = n$ to obtain the circulant form:

$$\mathbf{B} = \begin{pmatrix} d & n & n & \cdots & n \\ n & d & n & \cdots & n \\ n & n & d & \cdots & n \\ \vdots & \vdots & \vdots & & \vdots \\ n & n & n & \cdots & d \end{pmatrix}. \tag{53}$$

For a uniform distribution of cities $\rho_k = 1$, equations (17) have a uniform solution $s_k = s$, where

$$s^2 = \frac{1}{M}(d + (M-1)n). \tag{54}$$

Saddle points are equally spaced about the unit circle and the eigenvalue $\lambda^{(0)} = Ms^2$.

Based on the dominant saddle points associated with this solution, the leading contribution to the expected path length is

$$\frac{\langle E\rangle}{N} = \frac{dJ_D + (M-1)nJ_N}{d + (M-1)n}. \tag{55}$$

At low temperature, depending on the relative size of the diagonal and neighbor distances, we obtain $\langle E\rangle = NJ_D$ or $\langle E\rangle = NJ_N$. These results correspond to two regimes in which paths either prefer to revisit the same site or move to a neighboring site.

As explained in the beginning of this section, we hope that the fluctuation term may yield interesting information in the limit $J_N > J_D$ when $\beta \to \infty$, i.e. $n/d \to 0$. Fluctuations around the dominant saddle points can be evaluated as described above since this problem has a circulant cost matrix. The eigenvalues are very degenerate and besides the maximal eigenvalue given above all others take the value $d - n$. Using the expression (52), we find

$$\begin{aligned}\beta F = {} & -N\log(d + (M-1)n) + \frac{M-1}{2}\log(2d/n + (M-2)) \\ & + \left(N - \frac{M-1}{2}\right)\log M - N\log N.\end{aligned} \tag{56}$$

So, in the limit $n/d \to 0$, the path length is

$$\langle E\rangle = \left[N - \frac{M-1}{2}\right]J_D + \frac{M-1}{2}J_N. \tag{57}$$

In this limit, the fluctuations about the saddle point fail to give the expected optimum: $(N - M)J_D + MJ_N$. The reasons for the failure concern branch points approaching the saddle points and possibly other (non-dominant) solutions becoming important. Indeed, other solutions for s_k besides the symmetric solution exist. The details of the failure are most clearly exposed in the simplest $M = 2$ example given in the appendix.

3.4. 1D lattice

Several models corresponding to a one-dimensional lattice with nearest-neighbor couplings can be imagined depending on the boundary conditions and symmetry of the couplings. On a ring with uniform distribution of cities $\rho_k = 1$, we may simply allow nearest-neighbor connections, $J_{ij} = J_N\delta_{i,j+1} + J_N\delta_{i,j-1} + J_D\delta_{ij}$, or consider the possibility of longer links, $J_{ij} = J_N|i-j| + J_D\delta_{ij}$ or $J_{ij} = J_N(N - |i-j|) + J_D\delta_{ij}$, according to which is the closest way around the ring. In each case we have allowed a diagonal term, $J_{ii} = J_D$. The generalizations to problems on a line with fixed boundaries do not have a circulant form, but the difference is only a surface effect which corresponds to ignoring terms of order $e^{-M\beta/2}$.

In the nearest-neighbor case, we have the circulant form:

$$\mathbf{B} = \begin{pmatrix} d & n & 0 & \cdots & n \\ n & d & n & \cdots & 0 \\ 0 & n & d & \cdots & 0 \\ \vdots & \vdots & \vdots & & \vdots \\ n & 0 & 0 & \cdots & d \end{pmatrix}. \tag{58}$$

Equations (17) then have a uniform solution $s_k = s$, where

$$s^2 = \frac{1}{M}(d + 2n). \tag{59}$$

The leading term in the path length is then

$$\frac{\langle E\rangle}{N} = \frac{dJ_D + 2nJ_N}{d+2n}. \tag{60}$$

At low temperature, the picture is similar to the fully connected case. Depending on the relative size of the diagonal and neighbor distances, we obtain $\langle E\rangle = NJ_D$ or $\langle E\rangle = NJ_N$, corresponding to regimes in which paths either prefer to revisit the same site or move to a neighboring site.

The eigenvalues at the typical saddle point $z_k = 1$ are

$$\lambda_k = d + 2n\cos(2\pi k/M). \tag{61}$$

So, using (52), the free energy may be written as

$$\beta F = -N\log(d+2n) + \frac{1}{2}\sum_{k=1}^{M-1}\log\left(\frac{d+2n\cos^2\pi k/M}{n\sin^2\pi k/M}\right) + (N-1/2)\log M - \log N!. \tag{62}$$

For a large number of sites, M, the sum can be approximated as

$$\sum_{k=1}^{M-1}\log\left(\frac{d+2n\cos^2\pi k/M}{n\sin^2\pi k/M}\right) \to (M-1)\log 2 + \frac{M}{2\pi}\int_0^{2\pi} \mathrm{d}\omega \log\left(\frac{d/n+1+\cos\omega}{1-\cos\omega}\right) \tag{63}$$

$$= M\log 2 + M\log\left(\frac{d}{n} + 1 + \sqrt{\left(\frac{d}{n}\right)^2 + 2\frac{d}{n}}\right). \tag{64}$$

The corrections to the path length can then be read off, and in the limit $n/d \to 0$, we have

$$E = \left[N - \frac{M}{2}\right]J_D + \frac{M}{2}J_N. \tag{65}$$

The finite correction, were it not for the factor of 2, would be exactly what we expect for the ordinary TSP. The approach fails again for technical problems with the saddle point approach in this limit as is most clearly exposed in the appendix. An additional non-dominant solution for s_k is found in this case also.

These results can be generalized to one-dimensional models with long range interactions and regular periodic lattices in higher dimensions with block circulant **B**. However, in view of the difficulties at the simplest level, we do not pursue this route.

4. Fully occupied $N = M$ regime

With the occupation numbers set to $n_k = 1$ and $N = M$, we recover the usual formulation of the TSP with a given cost matrix J_{ij} that was discussed in section 2:

$$Z_N(\beta) = \oint\prod_{k=0}^{N-1}\frac{\mathrm{d}z_k}{2\pi\mathrm{i}}\exp(N\log\lambda) = \int_{-\pi}^{\pi}\prod_{k=0}^{N-1}\frac{\mathrm{d}\mu_k}{2\pi}\exp\left(\sum_{k'=1}^{N}\mathrm{i}\mu_{k'} + N\log\lambda_{\max}\right). \tag{66}$$

For a regular lattice, there is no randomness in this regime and the TSP optimum is a trivial problem. However, it is difficult to recover the trivial result from the approach based on the expression above. For example, the one-dimensional lattice can only be solved explicitly for small N. We investigate this case in some detail to illustrate that the saddle point approach in principle yields the scaling that would allow a low-temperature limit to access minimal path

lengths, but that other reasons invalidate the approach. Moreover, we hope that results on regular lattices might form the basis of an expansion towards more dilute lattices.

The saddle point method cannot be applied directly since the factor N does not multiply all terms in the exponent, but consider the following (unitary) change of variables:

$$\mu_k = \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} a_j \, \mathrm{e}^{2\pi \mathrm{i} jk/N}, \tag{67}$$

$$a_j = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \mu_k \, \mathrm{e}^{-2\pi \mathrm{i} jk/N}. \tag{68}$$

This is a one-dimensional discrete Fourier transform, but note that it is independent of any possible dimension underlying the J_{ij}'s and holds for arbitrary cost matrices. Unitary normalization has been chosen so the Jacobean is 1 and we obtain

$$Z_N(\beta) = \int \prod_{j=0}^{N-1} \frac{\mathrm{d}a_j}{2\pi} \exp(\mathrm{i}\sqrt{N} a_0 + N \log \lambda). \tag{69}$$

Now, by considering the structure of the general transfer matrix, we find that the a_0 dependence factors out so the eigenvalues are of the form $\lambda(a_0, a_1, \ldots, a_{N-1}) = \mathrm{e}^{-a_0/\sqrt{N}} \lambda'(a_1, \ldots, a_{N-1})$. Therefore, all a_0 dependence cancels in the action as we expect since this mode simply imposes the implicit constraint $\sum n_k = N$ that we have satisfied by setting $n_k = 1$. Integration over this mode should be omitted to obtain

$$Z_N(\beta) = \int \prod_{j=1}^{N-1} \frac{\mathrm{d}a_j}{2\pi} \exp(N \log \lambda'(a_1, a_2, \ldots, a_{N-1})). \tag{70}$$

A saddle point technique can again be attempted, but we must take care that the eigenvalue itself does not have any residual N dependence. In the case of the $N \gg M$ regime, this was straightforward as the matrix was $M \times M$, here it is $N \times N$, but for local J_{ij}, where the number of nearest neighbors does not grow with N, the eigenvalue can be N independent.

The stationary conditions from varying a_k, $k = 1, 2, \ldots, N-1$, are

$$\sum_{j=0}^{N-1} \mathrm{e}^{2\pi \mathrm{i} jk/N} v_j^2 = 0. \tag{71}$$

So, when complemented with the normalization condition on v_k, we have

$$v_k^2 = 1/N \tag{72}$$

resembling the saddle point condition obtained in the $N \gg M$ regime. As in the $N \gg M$ regime, there are spurious signed solutions of the saddle point equations that do not give a distinct saddle point from the solution with $v_k = +1/\sqrt{N}$. Proceeding through similar steps to that regime and writing $s_i = \sqrt{\lambda'} \exp(\mu_i/2 - \sqrt{N} a_0/2)$, we obtain the final equations:

$$s_k = \sum_{k'=0}^{N-1} \frac{\mathrm{e}^{-\beta J_{kk'}}}{s_{k'}}, \tag{73}$$

$$\beta F = -\log Z_N = -2 \sum_k \log s_k, \tag{74}$$

$$\langle E \rangle = \sum_{jj'} \frac{J_{jj'} \, \mathrm{e}^{-\beta J_{jj'}}}{s_j s_{j'}}. \tag{75}$$

Note that no $1/N$ factors appear in front of the sums, however, for local cost matrices at sufficiently low temperature only neighbors will contribute to the sums, and we find an N-independent expression for s_i. Such a solution suggests that the saddle point is valid as it has no untoward N dependence. Moreover, this constitutes a correct low-temperature scaling solution since the nearest-neighbor distance is fixed as N increases and the size of the domain increases keeping the density of cities constant. We therefore expect that this approach might access sufficiently low temperatures to provide information about the optima.

To investigate further, we take into account the fluctuations about the saddle point, and following the discussion for the coarse regime we consider $\mathbf{B}$ to be a symmetric circulant matrix. For these special distance matrices, the saddle point equations have a constant solution $z_k = z$, the transfer matrix becomes $\mathbf{T} = z^{-1}\mathbf{B}$ and all eigenvalues are directly related to those of $\mathbf{B}$. Using the scaling symmetry of the a_0 mode we can choose $z = 1$. In fact there are a set of N saddles, with z any Nth root of unity, but they all contribute equally to the integral and we only need to study the one at $z = 1$. Determining the Hessian matrix becomes an exercise in second-order perturbation theory that when aided by the structure of the matrix yields the following quadratic correction to the exponent:

$$\frac{1}{2}\sum_{k=1}^{N-1}\frac{\lambda_0+\lambda_k}{\lambda_0-\lambda_k}|a_k|^2, \tag{76}$$

where the eigenvalues λ_k are of the unperturbed transfer matrix, which at this constant saddle is simply $\mathbf{B}$ (λ_0 is the maximal eigenvalue corresponding to the eigenvector with all 1's). Note that the zero mode has dropped out as expected, and that in the a_k variables the Hessian is already diagonal. With some care about the direction of integration over the saddle, the quadratic correction to the free energy is

$$\beta F = -\log Z_N = -N\log\lambda_0 + \frac{1}{2}\sum_{k=1}^{N-1}\log\left(\frac{\lambda_0+\lambda_k}{\lambda_0-\lambda_k}\right). \tag{77}$$

Note that there are N terms in the eigenvalue sum and typically each term in the sum contributes. For example, for the nearest-neighbor one-dimensional ring, the eigenvalues are given by (61) and the sum is of order N. The fluctuation correction is of the same order as the leading term indicating a failure of the saddle point approach since we can anticipate similar magnitude corrections at cubic, quartic, etc, levels.

5. Dilute lattice regime: $N < M$

The dilute regime is the most interesting from the site disorder perspective. We consider a regular lattice with sites either occupied or not, $n_k = 0, 1$. As the system becomes very dilute, the discrete nature of the underlying lattice can be ignored and we recover the traditional TSP. Indeed, numerical TSP optimization codes use integer arithmetic following this principle. Here we would be content to investigate the leading correction to the path length for small dilution as the numerical simulations [6] seem to suggest a fairly linear dependence of energy against probability of site occupation.

For the first time in this work, it is necessary to explicitly average over the disorder, in this case the occupation numbers. This must be a quenched average and for this kind of site-disordered problem it is natural to use a formalism originally due to Morita [15] and recently championed by Kühn [16]. Essentially, the method consists of taking an annealed average, but inserting constraints to fix the distribution of the occupation numbers at its quenched value. In practice, this is achieved through an approximation in which only moments of the distribution

are fixed. As a first step, we would only consider the first two moments from the hierarchy corresponding to the constraints:

$$\sum_{k=0}^{M-1} n_k = N, \tag{78}$$

$$\sum_{\langle kk' \rangle} n_k n_{k'} = d\frac{N^2}{M}. \tag{79}$$

The first constraint is straightforward and is incorporated simply by including the integration over the a_0 mode that was dropped in earlier sections since the set of n_k's chosen already obeyed the constraint. The second constraint involves a sum over nearest neighbors and prevents the occupied sites from clustering together thus minimizing path lengths:

$$Z_N(\beta) \approx \sum_{n_k=0,1} \delta\left(\sum_{\langle kk' \rangle} n_k n_{k'} - d\frac{N^2}{M}\right) \int \prod_{k=0}^{M-1} \mathrm{d}\mu_k \, \mathrm{e}^{\mathrm{i}\sum n_k \mu_k} \sum_p \lambda_p^N. \tag{80}$$

This approach relies on a better understanding of the unperturbed, $N = M$, lattice and takes us away from the aim of this paper, so we defer further study for the future.

6. Conclusions

We have introduced a well-defined discrete problem: the site-disordered TSP with N cities on M sites, and have studied it using a saddle point approach.

- In the coarse, $N \gg M$ limit, we obtain a discrete version of the continuum theory we developed previously using a functional approach. The discrete approach shows that M saddle points contribute to the result rather than the single one identified in the functional work, but that (at least for constant density of cities) they are all equivalent. The effect of fluctuations can also be computed using the discrete approach. However, in the limit where there is a diagonal distance much shorter than neighbor distances and this correction might give information about the minimal path length in one-dimensional problems, the saddle point approach suffers technical difficulties and gives incorrect results. The nature of the difficulties were exposed in the $M = 2$ example as being associated with additional saddle points becoming relevant and saddle points approaching branch cuts.
- The saddle point approach to the ordinary $N = M$ TSP has the correct scaling to be able to access the interesting low-temperature regime even at the leading order. However, this fails to give correct results since the saddle is shallow and $O(N)$ modes all contribute to the fluctuations about the saddle generating a correction that is of the same order as the leading term thus invalidating the approach.
- We have discussed the dilute model and speculated on an approach based on an approximation originally due to Morita.
- We expect that it would be possible to use the saddle point method to analyze models that are intermediate between the $N \gg M$ regime and the $N = M$ case with city densities that vary as N^α for some power $0 < \alpha \leqslant 1$. The quadratic fluctuations in these models will be of order $N^{1-\alpha}$ and generally allow an expansion in $N^{-\alpha}$, but we anticipate the same problems with the low-temperature limit.

Of course a saddle point approach is not the only way to proceed and one interesting aspect of the formalism we have presented is that it describes the path weights in terms of particular terms in a generating function thus resembling approaches to other combinatorial optimization problems. This approach can certainly be used to enumerate for small N.

Figure A1. TSP on two sites.

Acknowledgment

DL would like to acknowledge a Discipline Hopping Award from the EPSRC during which much of this work was done.

Appendix. Explicit calculation for $M = 2$

The general derivation of the coarse regime given in the text did not label the eigenvalues globally and concentrated on the real positive solution of the saddle point equation. Explicit computations for particular small values of M illuminate the role of other eigenvalues and saddle points.

Consider the case $M = 2$ (figure A1) where a diagonal entry is allowed in the distance matrix as otherwise the path is completely determined. This model can be reinterpreted as a one-dimensional Ising model on a ring with N sites subject to the constraint that states must have zero overall magnetization. The analysis of the Ising model provides additional intuition, but a constrained transfer matrix approach repeats essentially the same technique as in the text. Writing $d = \mathrm{e}^{-\beta J_D}$ for the diagonal term and $n = \mathrm{e}^{-\beta J_N}$ for the neighbor term, the parameters of the system are then d/n and $\rho_- = (\rho_0 - \rho_1)/2$ using the terminology of section 3. The partition function is the sum of the contributions from each of the two eigenvalues $Z = n_0!n_1!(Z_+ + Z_-)$, where

$$Z_\pm = \oint \frac{\mathrm{d}z_0}{2\pi \mathrm{i} z_0} \frac{\mathrm{d}z_1}{2\pi \mathrm{i} z_1} z_0^{n_0} z_1^{n_1} \lambda_\pm^N \tag{A.1}$$

and $\lambda_\pm$ are the two eigenvalues of the transfer matrix

$$\mathbf{T} = \frac{1}{z_0 z_1} \begin{pmatrix} \mathrm{d}z_1 & n\sqrt{z_0 z_1} \\ n\sqrt{z_0 z_1} & \mathrm{d}z_0 \end{pmatrix}. \tag{A.2}$$

In this form, one of the integration variables simply imposes the constraint $n_0 + n_1 = N$ that we will generally make implicit. The constraint is therefore redundant and if we proceeded in this way the two saddle point equations would be linearly dependent and only set z_0 and z_1 proportional to each other. While this approach merely leads to a volume factor, it is clearer to remove the constraint from the start. We therefore insert the factor $2\pi \mathrm{i}\delta(z_0 z_1 - 1)$ (the $2\pi \mathrm{i}$ is the Jacobean factor) into the partition function to obtain a one-dimensional contour integral:

$$Z_\pm = \oint \frac{\mathrm{d}z}{2\pi \mathrm{i} z} z^{N\rho_-/2} \lambda_\pm^N, \tag{A.3}$$

where $\lambda_\pm$ are now the two eigenvalues of the transfer matrix

$$\mathbf{T} = \begin{pmatrix} d/z & n \\ n & \mathrm{d}z \end{pmatrix}, \tag{A.4}$$

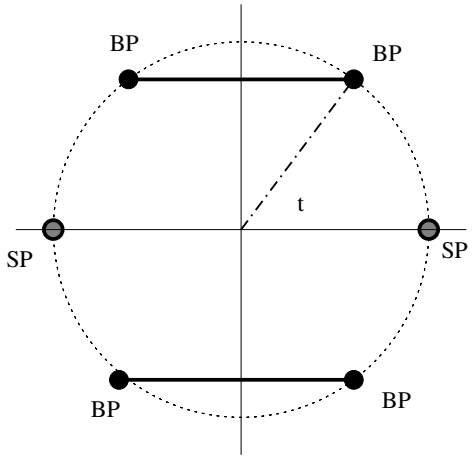

Figure A2. Complex plane for TSP on two sites. For $\rho_- = 0$ and in the region where $n < d$, it is cheaper to revisit a site than to move to the other site. The branch points (BP), cuts and two saddle points (SP) are shown. The angle t is given by $\sin t = n/d$.

that is,

$$\lambda_\pm = \frac{1}{2}\left(d\left(z + \frac{1}{z}\right) \pm \sqrt{d^2\left(z - \frac{1}{z}\right)^2 + 4n^2}\right). \tag{A.5}$$

In this form, it is possible to keep track of the same eigenvalues, labeled by $\pm$ or their relative magnitude at $z = 1$, and not swap between them as z varies around the integration contour. Note that this has involved a choice of sign in moving between (A.2) and (A.4), for example, consider $z = z_0 = z_1 = -1$ (obeying the constraint) in each version of the transfer matrix. The branch points and saddle points in the complex plane are shown in figure A2. For $n < d$, it is possible to choose a contour on the unit circle, but for $n > d$, the contour must be deformed away from the branch cuts.

For certain values of the parameters, the integrals can be computed directly. For $d = 0$ or $n = 0$, a contribution is only obtained for certain choices of n_0, n_1. We find $d = 0$ is only possible if $n_0 = n_1 = N/2$ in which case $Z = 2(N/2)!^2 n^N$. For $n = 0$, one of n_0 or n_1 must vanish. These restrictions follow from the integrals but match the expectations from the original geometric problem since the choice of connections must make it possible for paths to visit nodes the required number of times. For $n = d$, one eigenvalue vanishes and we obtain $Z = N!d^N$ irrespective of n_0, n_1 since there are a total of $N!$ paths each of equal weight. The limit of $n \ll d$ is interesting as the corrections to the leading term provide information about the real (not coarse) TSP. In this limit, the diagonal path is short and is always preferred over the neighbor path. By expanding we obtain $Z = n_0!n_1!Nn^2d^{N-2}$ indicating that there are N paths that only flip once between nodes and this matches the combinatorial approach.

Now we take it that neither d nor n vanishes and use the saddle point approach. The stationarity equation is

$$\frac{\rho_-}{z} + \frac{1}{\lambda_\pm}\frac{\mathrm{d}\lambda_\pm}{\mathrm{d}z} = 0 \tag{A.6}$$

which can be solved to find two saddle points for each eigenvalue. These saddle points depend on the sign of ρ_-, but without loss of generality we can always take the sign to be positive.

$$z_{sp}^2 = 1 + 2g^2 \mp \sqrt{g^2 + g^4}, \tag{A.7}$$

$$g^2 = \frac{n^2\rho_-^2}{d^2(1-\rho_-^2)}. \tag{A.8}$$

The upper and lower signs correspond to the two different eigenvalues, while the two separate saddle points for each eigenvalue arise from the sign of z_{sp}.

In general, the saddle points are located at different points depending on the eigenvalue in question. Now consider the symmetric case of $\rho_- = 0$ where $g^2 = 0$, where the location of the saddle points at $z_{sp} = \pm 1$, is the same for each eigenvalue. For Z_+ involving the eigenvalue λ_+, the value of the eigenvalue at the saddle points $z_{sp} = \pm 1$ is $(\pm d + n)$ with eigenvector $(1, 1)$ at each saddle. For the other integral, Z_-, involving eigenvalue λ_-, the value of the eigenvalue at the saddle points $z_{sp} = \pm 1$ is $(\pm d - n)$ with eigenvector $(1, -1)$ at each saddle point. It is already apparent that for each integral, one of the saddle points dominates the other (since we assumed $d \neq 0$), for Z_+ the dominant saddle is at $z_{sp} = +1$, whereas for Z_- it is $z_{sp} = -1$.

These explicit computations match the expectations from the general development in the text. The dominant saddle points come from the real positive solution of equation (17), and the subdominant saddle points arise from a distinct solution of equation (17). The eigenvector associated with the dominant saddle point depends on which integral, $Z_\pm$, is considered.

The asymptotic value of integrals for $Z_\pm$ can be obtained from the dominant saddle point in each case. By expanding about the dominant saddle we find that the contour should pass over it in the imaginary direction, and the contribution from fluctuations can be evaluated. Each of $Z_\pm$ yields the same contribution since N must be even for the symmetric case under consideration. Overall, we obtain

$$Z = (N/2)!^2 \sqrt{\frac{2n}{\pi N d}} (d+n)^N \approx N! \sqrt{\frac{n}{d}} \left(\frac{d+n}{2}\right)^N. \tag{A.9}$$

This expression reproduces the exact result at $n = d$, but the limits $d \to 0$ or $n \to 0$ do not reproduce the known results. In such limits, the simple saddle point calculation fails for technical reasons. The subdominant saddles would be expected to contribute (in which case the contour over them should be in the real direction) and moreover the branch points can approach the saddle points or the cuts can force the contour to be deformed. A more careful approach via a uniform asymptotic expansion [12] may give better results.

In summary, the coarse TSP on two points allows us to carefully track each eigenvalue and find that multiple saddles can occur for each eigenvalue. One saddle point dominates each integral associated with a certain eigenvalue. In the full partition function, each of these eigenvalues contribute equally. The eigenvector corresponding to the dominant saddle depends on the eigenvalue being tracked. Finally, the limit of removing elements of the distance matrix by making them large can be delicate in the saddle point approach. In particular, we are unable to recover the true TSP as a subleading contribution to the $n \ll d$ limit from the saddle point.

Already for the $M = 3$ generalization, the coarse TSP on three sites, the algebra to allow an eigenvalue to be tracked becomes excessive even for $d = 0$ and with the aid of a computer. Additional isolated solutions of the saddle point equations in the text for s_i can be found provided $d \neq 0$.

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