The statistical mechanics of traveling salesman type problems

David S. Dean[(1,2)], David Lancaster[(3)] and Satya N. Majumdar[(2,4)]
(1) DAMTP, CMS, University of Cambridge, Cambridge, CB3 0WA, UK
(2) Laboratoire de Physique Théorique, UMR CNRS 5152, IRSAMC, Université Paul Sabatier, 118 route de Narbonne, 31062 Toulouse Cedex 04, France
(3) Harrow School of Computer Science, University of Westminster, Harrow, HA1 3TP, UK
(4) Laboratoire de Physique Théorique et Modèles Statistiques, UMR 8626, Université Paris Sud, Bât 100, 91045 Orsay Cedex, France
(Dated: 3 November 2004)

We study the finite temperature statistical mechanics of Hamiltonian paths between a set of N quenched randomly distributed points in a finite domain $\mathcal{D}$. The energy of the path is a function of the distance between neighboring points on the path, an example is the traveling salesman problem where the energy is the total distance between neighboring points on the path. We show how the system can be analyzed in the limit of large N without using the replica method.

arXiv:cond-mat/0411111 v1 4 Nov 2004

In this Letter we consider a system where N points with quenched positions $x_1^{(q)},\ x_2^{(q)} \cdots x_N^{(q)}$ are independently distributed on a finite domain $\mathcal{D}$ with a probability density function $p_q(x)$. In general, the domain $\mathcal{D}$ is multidimensional and the points $x_i^{(q)}$ are vectors in the corresponding Euclidean space. Inside the domain $\mathcal{D}$ we consider a polymer chain composed of N monomers whose positions are denoted by $x_1,\ x_2,\ \ldots,\ x_N$. Each monomer x_i is attached to one of the quenched sites $x_i^{(q)}$ and only one monomer can be attached to each site.The state of the polymer is described by a permutation $\sigma \in \Sigma_N$ where Σ_N is the group of permutations of N objects. The position of the ith monomer may thus be written as $x_i = x_{\sigma(i)}^{(q)}$. The Hamiltonian for the system is given by

$$H(\sigma) = \sum_{i=1}^{N} V\left(x_{\sigma(i)}^{(q)} - x_{\sigma(i-1)}^{(q)}\right). \tag{1}$$

Here V is the interaction between neighboring monomers on the polymer chain. For convenience the chain is taken to be closed, thus we take the periodic boundary condition $x_0 = x_N$.

A physical realization of this system is one where the $x_i^{(q)}$ are impurities where the monomers of a polymer loop are pinned. The potential V represents effective interaction between neighboring monomers on the chain. For instance $V(x) = \lambda x^2/2$ corresponds to the Rouse model of a polymer chain[1]. Another application of this model occurs in combinatorial optimization: if one takes $V(x)$ to be the norm, or distance, of the vector x then $H(\sigma)$ is the total distance covered by a path which visits each site $x_i^{(q)}$ exactly once. The problem of finding σ^* which minimizes $H(\sigma)$ is known as the traveling salesman problem (TSP) [2]. If one takes $V(x) = |x|$ (the Euclidean norm) then the combinatorial optimization problem is called the Euclidean TSP [3]. The choice $V(x) = -|x|$ means that one is looking for the longest path, this is the so called Maximal TSP or taxicab rip-off [2]. The analogy with the physical polymer system is particularly useful. First one may use the techniques of simulated annealing [4] to search for the optimal path σ^* by introducing a temperature in the system and then incorporating a dynamics respecting detailed balance. The optimal path corresponds to the ground state or zero-temperature energy E_{GS} of H. By slowly cooling the system one may find this state, though in the presence of many local minima or metastable states this procedure may not be efficient. Secondly, and this is the approach taken here, one may try to determine the full temperature dependence of the free energy averaged over the disorder ensemble and then take the zero temperature limit to determine the average value E_{GS} [5, 6, 7]. Depending on the form of V, E_{GS} may not be extensive in N. In such cases, for example for the Euclidean TSP, the temperature needs to be rescaled with N in order to have an extensive ground state energy [5, 8]. In this letter we study the problem with a fixed domain size and no rescaling of the temperature with N. The TSP is often studied in this form and in the thermodynamic limit the ground state energy per site is strictly zero.

The main technical problem associated with the second approach above is to perform the average over the quenched disorder.The replica method and cavity methods have been used previously to perform the quenched average for the TSP [8, 9, 10, 11, 12], notably in the random link version of the problem where the distances between sites i and j are assumed to be independent. This 'random link' assumption considerably facilitates carrying out the disorder average within the replica/cavity formalism. However, in the Euclidean TSP problem the distances between the sites are evidently correlated (for instance the triangle inequality must be respected). In this Letter we present an exact approach that (i) does not require the use of the replica method, (ii) fully takes into account the correlations between the distances and (iii) moreover provides us with exact asymptotic results at all temperatures.

The canonical partition function is given by the sum over all permutations

$$Z_N = \frac{1}{N!} \sum_{\sigma \in \Sigma_N} \exp\left(-\beta H(\sigma)\right). \tag{2}$$

Since the number of permutations grows as $N!$, the entropy is of order $N \ln N$ and we insert a factor of $1/N!$ to absorb it. To simplify our formulas we take unit domain size.

We define the density of quenched sites on $\mathcal{D}$ as

$$\rho_q(x) = \frac{1}{N} \sum_{i=1}^{N} \delta(x - x_i^{(q)}). \tag{3}$$

The partition function Z_N only depends on $\rho_q(x)$. If x_i is the site visited by the monomer i then the partition function of the permutation problem can be written up to constant factors as

$$Z_N = \frac{1}{N!} \int \prod_{i=1}^{N} dx_i \left[\prod_x \delta \left(N\rho_q(x) - \sum_i \delta(x - x_i) \right) \right] \exp\left(-\beta \sum_i V(x_i - x_{i-1}) \right). \tag{4}$$

The delta function constraint above ensures that the monomers x_i have the same density as the quenched points and thus visit only the quenched points and with the correct degeneracy. Using a Fourier representation of the functional constraint gives, up to temperature independent constants,

$$Z_N = \int d[\mu] \exp\left(N \int dx \mu(x) \rho_q(x) \right) \mathcal{Z}_N. \tag{5}$$

The object $\mathcal{Z}_N$ is the annealed partition function for a *free* ring polymer whose monomers can attain any point in $\mathcal{D}$ but with an x dependent chemical potential. It is defined as:

$$\mathcal{Z}_N = \int \prod_{i=1}^{N} dx_i \ \exp\left(-\beta \sum_{i=1}^{N} V(x_i - x_{i-1}) - \sum_{i=0}^{N} \mu(x_i) \right). \tag{6}$$

The partition function $\mathcal{Z}_N$ may be evaluated by operator techniques: $\mathcal{Z}_N = \mathrm{Tr}\ T^N$ where T is the symmetric operator

$$T(x, y) = \exp\left(-\frac{\mu(x)}{2} - \frac{\mu(y)}{2} - \beta V(x - y) \right). \tag{7}$$

The full partition function Eq. (5) can be evaluated by the saddle point method in the limit where $N \to \infty$ keeping the size of $\mathcal{D}$ fixed. The saddle point equation is

$$\rho_q(x) = -\frac{1}{N} \frac{\delta \ln \mathcal{Z}_N}{\delta \mu(x)} = \frac{1}{N} \langle \sum_{i=1}^{N} \delta(x - x_i) \rangle = p_a(x). \tag{8}$$

where the above expectation, is for the system with partition function $\mathcal{Z}_N$ defined in Eq. (6), so $p_a(x)$ is the, annealed, density of points (monomers) for the free ring polymer. Physically this approach can be thought of as choosing a site dependent chemical potential μ which fixes the density of the annealed calculation to be the same as that of the quenched one, *i.e.* so that $\rho_q(x) = p_a(x)$. The approach has some similarity with the constrained annealing approximation [14, 15], but fixes the whole distribution rather than individual moments.

The ground state eigenfunction, corresponding to the maximal eigenvalue λ_0 of T obeys

$$f_0^{(q)}(x) = \lambda_0^{-1} \int dy \ T(x, y) f_0^{(q)}(y), \tag{9}$$

and for large N the annealed density of points in $\mathcal{D}$ is given by

$$p_a(x) = -\frac{\delta \ln(\lambda_0)}{\delta \mu(x)} = \left[f_0^{(q)}(x) \right]^2. \tag{10}$$

Substituting this into the saddle point equation and writing $\exp(-\frac{\mu(x)}{2}) = \sqrt{\rho_q(x)}/s_{\lambda_0}(x)$ we find that $s_{\lambda_0}(x)$ obeys

$$s_{\lambda_0}(x) = \lambda_0^{-1} \int dy \ \exp\left(-\beta V(x - y) \right) \frac{\rho_q(y)}{s_{\lambda_0}(y)}. \tag{11}$$

Considering the case of a uniform distribution of the points, $x_i^{(q)}$, and substituting back into the action we obtain

$$-\frac{\beta F_N}{N} = 2 \int dx \ \ln\left(s_{\lambda_0}(x) \right) + \ln(\lambda_0) + \text{terms indep. of } \beta. \tag{12}$$

From Eq. (11) we see that there is a family of solutions $\{s_{\lambda_0}(x), \lambda_0\}$ which are related by $s_{\lambda_0} = a^{1/2} s_{a\lambda_0}$, for $a > 0$ and in addition these solutions all have the same action. This apparent zero mode is an artifact introduced by the fact that the constraint $N = N \int dx \ \rho_q = \int dx \ \sum_i \delta(x - x_i)$ is automatically satisfied. Thus we may chose $\lambda_0 = 1$, leading to our final result for the average energy per site

$$\begin{aligned} \epsilon &= -2 \frac{\partial}{\partial \beta} \left[\int dx \ \ln\left(s(x) \right) \right] \\ &= \int dx \ dy \ \frac{V(x - y) \exp\left(-\beta V(x - y) \right)}{s(x) s(y)}, \end{aligned} \tag{13}$$

where s obeys

$$s(x) = \int dy \ \frac{\exp\left(-\beta V(x - y) \right)}{s(y)}. \tag{14}$$

In general Eq. (14) can be solved by an iterative numerical procedure. The average energies obtained in this way for the one dimensional TSP on the unit interval $[0, 1]$ and the conventional two dimensional TSP on the square domain $[0, 1]^2$ are shown as continuous lines in Fig. (1). To test these predictions we have carried out Monte Carlo simulations of this TSP for system sizes of $N = 2000$ and compared the average energy measured after equilibrating the system over 10^6 Monte Carlo steps and measuring the average energy over a subsequent 10^6 Monte Carlo steps. The basic move in the dynamics was a

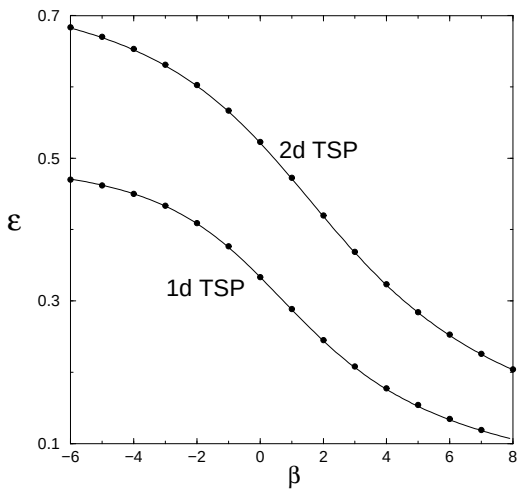

FIG. 1: Theoretical prediction for the average energy ϵ for one and two dimensional TSP as a function of β (solid line) compared with the Monte Carlo simulations (solid circles). Negative β corresponds to the maximal TSP problem. Error bars based on 20 realizations of the quenched points are smaller than the symbol sizes.

transposition of a pair of points in the permutation, and the acceptance criterion was the Metropolis rule. The simulation points are also shown as solid circles on Fig. (1) and we see that for all temperatures the agreement with the theoretical prediction is excellent.

For the one dimensional ring and two dimensional torus or sphere, where the Euclidean distance is taken to be the shortest way round the domain, Eq. (14) admits a constant solution. This indicates that in these cases, the annealed approximation is exact without the need for any chemical potential to force the density of the annealed points to be uniform. In the case of the ring we find

$$\epsilon = \frac{1}{\beta} - \frac{1}{2(e^{\beta/2}-1)}, \tag{15}$$

for both positive and negative β. This result, and the corresponding one for the torus and sphere are confirmed by Monte Carlo simulations, and moreover support the correctness of the iterative procedure used to numerically solve Eq. (14) [13].

In one dimension the Euclidean TSP amounts to a sorting problem, but even when the quenched points are regularly spaced, no simple expression for the partition function is known [16]. For the unit interval $\mathcal{D} = [0,1]$ we have obtained the low temperature expansion

$$\begin{aligned} \epsilon &= \frac{1}{\beta} - \frac{\pi^2 - 6\ln^2(2)}{6\beta^2} \quad \beta \to \infty, \\ \epsilon &= \frac{1}{2} - \frac{\pi^2}{6\beta^2} \quad \beta \to -\infty, \end{aligned} \tag{16}$$

which agrees with our numerical results. We have also considered the one-dimensional potentials $V(x) = x^2$ and $V(x) = -\ln(|x|)$, the latter was only considered at positive temperature as it is ill defined at negative temperature. In all these cases, the comparison with simulation results confirms the predictions of our method.

From an optimization point of view, besides the algorithm for discovering it, the most interesting quantity is the length or energy of the optimum path *i.e.* E_{GS}; thus we now focus on the zero temperature limit. First, let us recall that our treatment computes an extensive ground state energy. On the other hand, we expect that for the Euclidean TSP in d dimensions, the length of the shortest path should scale as $N^{1-1/d}$ [3]. In this Letter, rather than attempt to pursue finite size corrections to our formalism [13], we study models which do have an extensive ground state energy. This is the case in the maximal TSP problem and for problems where the potential $V(x)$ between neighboring monomers is repulsive. We reformulate Eq. (13) to work directly at zero temperature by writing $s(x) = \exp(-\beta w(x))$. Then in the limit $\beta \to \infty$ we find

$$w(x) = \min_{y\in(0,1)} \{V(x-y) - w(y)\}. \tag{17}$$

The ground state energy is then given according to Eq. (13) as

$$\epsilon_{GS} = 2\int dx\ w(x). \tag{18}$$

The Eq. (17) seems in general quite difficult to solve, however we can make progress in some specific cases in one dimension. First there is the obvious case of what happens when the minimum value of $V(x)$ occurs at $x = 0$, as is the case for the positive temperature TSP. Clearly $\epsilon_{GS} = V(0)$ here as the optimal solution connects all the sites in ascending (or descending) order and the distance between each site $\sim 1/N \to 0$. In this case we see that Eq. (17) clearly has a solution $w(x) = V(0)/2$ and thus Eq. (18) implies indeed that $\epsilon_{GS} = V(0)$.

When V is a monotonically decreasing function (so the monomers prefer to be as far from each other as possible) a possible strategy for obtaining the ground state energy is a greedy algorithm where one starts at the leftmost point and goes to the rightmost point, then to the second leftmost point and so on. This leads to an energy of

$$\epsilon_{GA} = \int dx\ V(x). \tag{19}$$

Obviously the solution $w(x)$ to Eq. (17) should be symmetric about $x = \frac{1}{2}$ thus $w(x) = u(|x - \frac{1}{2}|)$ and u obeys

$$u(x) = \min_{y\in(-\frac{1}{2},\frac{1}{2})} \{V(x-y) - u(y)\}. \tag{20}$$

Inspired by the greedy algorithm we postulate that the minimization on the right-hand side of Eq. (20) is achieved by $y = -x$. This leads to a solution of Eq. (20) $u(x) = \frac{1}{2}V(2x)$, which is valid when $V''(2x) < 0$, *i.e* when V is concave, for all $x \in [0,1]$. The energy of this

solution is given by Eq. (19) and is thus attained by the greedy algorithm. We cannot guarantee that this solution is unique but it is in agreement with the simulations for the potentials $V(x) = -|x|$ and $-x^2$ [13].

Another ansatz for solving Eq. (20) is $u(x) = a|x| + b$. The Eq. (20) is solved by this form when $V''(1/2) > 0$ (and thus does not work for concave potentials) and one finds $a = V'(\frac{1}{2})$ and $b = \frac{1}{2}\left(V(\frac{1}{2}) - \frac{1}{2}V'(\frac{1}{2})\right)$. The ground state energy predicted by this solution is $\epsilon_{GS} = V(\frac{1}{2})$ A potential where the above solution is possible is $V(x) = -\ln(|x|)$. Numerical solution of Eq. (14) at low temperatures converges to the solution found above. The predicted value of the ground state energy is $\epsilon_{GS} = \ln(2)$, this value is compatible with the simulations for this potential [13]. This energy is achieved by making jumps from site to site where the jump size is a random variable Δ very close to $1/2$ *i.e.* if the current position is $x < 1/2$ one jumps to $x + \Delta$, otherwise one jumps to $x - \Delta$. This halfjump-algorithm will generate an energy per site of $\epsilon_{HA} = V(1/2)$ and it will also generate the required uniform quenched distribution of points on $[0, 1]$. To summarize, the greedy and half-jump algorithms will achieve energies per site:

$$\epsilon_{GA} = \int dx\ V(x); \quad \epsilon_{HA} = V(\frac{1}{2}). \tag{21}$$

Clearly when $V''(|x|) > 0$ everywhere in $[0, 1]$, Jensen's inequality tells us that $\langle V(X)\rangle \geq V(\langle X\rangle)$ for X distributed on $[0, 1]$; when this distribution is uniform this implies that $\epsilon_{GA} > \epsilon_{HA}$ and hence the half-jump algorithm is the most efficient. In the case where the potential is concave the greedy algorithm is the most efficient. We note that the case of the maximal TSP is an intermediate case where $V''(x) = 0$ and in this case $\epsilon_{GA} = \epsilon_{HA}$ and the forms of $u(x)$ in these two cases coincide. If $V(x)$ (for $x > 0$) is such that it has a single minimum at $x = x^*$ and where $x^* < 1/2$, then Eq. (17) has a solution $w(x) = V(x^*)/2$ for all x and the ground state energy is $\epsilon_{GS} = V(x^*)$. An algorithm which achieves this is the x^*-jump algorithm, note that this works because when $x^* < 1/2$ the algorithm be applied from any starting position. When $x^* > 1/2$, $w(x) = V(x^*)/2$ is clearly not a solution for all x as it fails in the neighborhood of $x = 1/2$. We note that when $x^* < 1/2$ the jumping algorithm is in fact a greedy algorithm as it always chooses the near optimal jump size and this jump size is independent of its current position. When the optimal jump size $x^* > 1/2$ the strategy clearly does not work for the reasons discussed above. In this case the jump sizes are no longer concentrated around some typical value and the next jump size depends on the current position.

We have discussed the statistical mechanics of models whose phase space is the set of permutations of N objects characterized by quenched positions/sites. The Hamiltonians are functions of the neighboring elements in the sequence, and thus a given sequence can be interpreted as the energy of a polymer or random walk which visits each site once. We showed how the quenched calculation could be carried out and confirmed its predictions with Monte Carlo simulations. Physically the method corresponds to imposing a fictitious site dependent chemical potential on the distribution of the set of dynamical variables x_i in the presence of the original interaction Hamiltonian. This chemical potential is then chosen to ensure that the annealed density of these dynamical x_i is the same as the desired distribution of the quenched random variables $x_i^{(q)}$. The method introduced works in the thermodynamic limit (corresponding to high density where the size of the domain is held constant) for any quenched distribution $p_q(x)$, in any dimension and for any interaction potential $V(x)$. For the problem of a directed polymer in dimensions greater than two a finite temperature phase transition is known to occur [17], it would be interesting to see if this phase transition shows up in the Euclidean TSP in $d > 2$. Finally, the idea of treating quenched variables as effectively annealed variables and then adjusting their Boltzmann weight in order to recover, self consistently, the original quenched distribution may prove useful either as an exact or approximate method, as is the case of Morita's approach [14, 15], in other problems involving quenched disorder.

[1] P.E. Rouse, J. Chem. Phys. **21**, 1272 (1953).
[2] G Gutin and, A. P. Punnen (Eds), The Traveling Salesman Problem and Its Variations (Combinatorial Optimization Series), Kluwer, Boston (2002).
[3] J. Beardwood, J. H. Halton and J.M. Hammersley, Proc. Cam. Phil. Soc. **55** 299 (1959).
[4] S. Kirkpatrick, C.D. Gelatt Jr. and M.P. Vecchi, Science **220** 671 (1983).
[5] M. Mézard, G. Parisi and M.A. Virasoro, Spin Glass Theory and Beyond, World Scientific, Singapore (1987).
[6] Y. Fu and P.W. Anderson, J. Phys. A. **19** 1605 (1986).
[7] O.C. Martin, R. Monasson and R. Zecchina, Theoretical Computer Science **265**, 3 (2001).
[8] J. Vannimenus and M. Mézard, J. Physique Lett. **45** L1145 (1984).
[9] M. Mézard and G. Parisi, Europhys. Lett. **2**, 913 (1986).
[10] W. Krauth and M. Mézard, Europhys. Lett. **8**, 213 (1989).
[11] A.G. Percus and O.C. Martin, Phys. Rev. Lett. **76**, 1188 (1996).
[12] A.G. Percus and O.C. Martin, J. Stat. Phys. **94**, 739 (1999).
[13] D.S. Dean, D. Lancaster and S.N. Majumdar, unpublished.
[14] T. Morita J. Math. Phys. **5**, 1401, (1964).
[15] R. Kühn, Z. Phys. **100**, 231 (1996).
[16] D. Lancaster, J. Phys. A. **37**, 1125 (2004).
[17] B. Derrida and O. Golinelli, Phys. Rev. A. **41**, 4160

(1990).