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Article *in* Physical Review E · December 2004

DOI: 10.1103/PhysRevE.70.057701 · Source: PubMed

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Quantum annealing of the Traveling Salesman Problem

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(Dated: February 2, 2008)

We propose a path-integral Monte Carlo quantum annealing scheme for the symmetric Traveling Salesman Problem, based on a highly constrained Ising-like representation, and we compare its performance against standard thermal Simulated Annealing. The Monte Carlo moves implemented are standard, and consist in restructuring a tour by exchanging two links (2-opt moves). The quantum annealing scheme, even with a drastically simple form of kinetic energy, appears definitely superior to the classical one, when tested on a 1002 city instance of the standard TSPLIB.

PACS numbers: 02.70.Uu,02.70.Ss,07.05.Tp,75.10.Nr

Quantum annealing (QA) – that is using quantum mechanics to optimize, through annealing, hard problems of everyday life, including those that have nothing to do with quantum mechanics – is a relatively new and fascinating idea, with important physical implications and potential impact in a variety of areas, from technological applications to other disciplines of science, wherever optimization of a complex system is the issue.

The idea of QA is an offspring of the celebrated thermal *simulated annealing* (SA) [1, 2], where the problem of minimizing a certain cost (or energy) function in a large space of configurations is tackled, through a statistical mechanics analogy, by the introduction of an artificial temperature variable which is slowly reduced to zero in the course of a Monte Carlo (MC) or Molecular Dynamics simulation. This device allows to explore the configuration space avoiding trapping into local minima, often providing a more effective and less biased search for the minimal "energy" than standard gradient-based minimization methods.

Why not using quantum mechanics for the same purpose? Quantum mechanics works with wave-functions that can equally well sample wide regions of phase-space. Instead of thermal fluctuations, one exploits here the *quantum fluctuations* provided by a suitably introduced – and equally artificial – kinetic energy. Annealing is then performed by slowly reducing to zero the amount of quantum fluctuations introduced. Quantum fluctuations have, in many respects, an effect similar to that of thermal fluctuations – they cause, for instance, solid helium to melt even at the lowest temperatures – but they differ considerably in other respects. In particular, quantum systems can *tunnel through* classically impenetrable potential barriers between energy valleys, a process that might prove more effective than waiting for them to be overcome thermally, as in SA.

Formulated in the mid 90's [3], the idea of QA picked up momentum only recently, through experimental work such as that of Brooke *et al.* [4, 5], where it was shown that in the disordered Ising ferromagnet $LiHo_{0.44}Y_{0.56}F_4$, QA is both experimentally feasible and apparently superior to thermal annealing. Stimulated by these findings we recently carried out a benchmark comparison of classical and path-integral MC annealings on the two-dimensional random Ising model [6, 7]. In that study, we confirmed the superiority of QA. We also presented a simple theory based on Landau-Zener tunneling [6] for that. While other theoretical efforts had also reported some success with QA for other problems [8, 9, 10, 11], it is nonetheless fair to say that our overall experience with tackling hard problems by QA is still very limited. The Traveling Salesman Problem (TSP), a classic hard optimization problem, provides an ideal playground for a further test of QA in comparison with SA. In this Letter we report an application of QA to TSP, where we find that again it is superior to SA.

Given N cities with set inter-city distances d_{ij}, TSP consists in finding the shortest route connecting them, visiting each city once and returning to the starting point. The literature on TSP is vast, and *e.g.* Ref. 12 can be consulted for an account of the algorithms proposed. SA, although never a winning scheme when compared to some of the ad-hoc algorithms specifically tailored to the TSP problem, is known to be a very flexible, simple, and competitive algorithm for the TSP as well [12]. The natural question is now: can QA do better than SA, with a comparable computational effort? We will now show that this is indeed the case.

The crucial point in devising a QA scheme is how to describe the Hilbert space of the problem, and how to write and implement a quantum Hamiltonian $H_{TSP} = H_{pot} + H_{kin}$. Here H_{pot} represents the classical potential energy of a given configuration (in our case, the length of a tour), and H_{kin} is a suitable kinetic energy operator providing the necessary quantum fluctuations, and eventually annealed to zero. The route we followed (certainly not unique, or even the most efficient) goes through the mapping to a highly constrained Ising-like system, some-

what reminiscent of the Hopfield-Tank mapping of TSP as a neural network [13]. (See also Ref. 14.) Formally, each configuration of the system (a valid tour) is associated to a $N \times N$ matrix $\hat{T}$ with 0/1 entries in the following way: For every directed tour (an ordered sequence of cities) $\hat{T}_{i,j} = 1$ if the tour visits city i immediately after city j, and $\hat{T}_{i,j} = 0$ otherwise. $\hat{T}$ has N entries equal to 1, all other elements being 0, and obeys the typical constraints of a permutation matrix, i.e.: *a)* All diagonal elements vanish, $\hat{T}_{i,i} = 0$; *b)* There is a single 1 in each row i and in each column j. For the *symmetric* TSP problem we want to consider (a TSP where the distance matrix is symmetric $d_{ij} = d_{ji}$), a directed tour represented by a $\hat{T}$, and the reversed tour, represented by the transposed matrix $\hat{T}^t$, have exactly the same length. It is convenient, as will be apparent in a moment, to introduce the symmetric matrix $\hat{U} = \hat{T} + \hat{T}^t$ as representative of *undirected* tours, the non-zero elements of $\hat{U}$ being given by $\hat{U}_{i,j} = 1$ if i is connected to j in the tour, i being visited before or after j. One can be readily convinced that there is no loss of information in working with $\hat{U}$ instead of $\hat{T}$. Given the matrix $\hat{U}$ there is no ambiguity in extracting the directed tour, represented by $\hat{T}$, which originated it. The length of a tour can be expressed in terms of the $\hat{U}_{i,j}$, as follows:

$$H_{pot}(\hat{U}) = \frac{1}{2}\sum_{(ij)} d_{ij}\hat{U}_{i,j} = \sum_{\langle ij\rangle} d_{ij}\hat{U}_{i,j} \ , \qquad (1)$$

where $d_{ij} = d_{ji}$ is the distance between city i and city j, and $\langle ij\rangle$ signifies counting each link only once. H_{pot} is the potential energy we will finally seek to minimize.

Since there is no natural physical kinetic energy in the problem we have to devise a suitable one. This choice is arbitrary, and many simple forms, such as transposition of two neighboring cities in a tour, could provide one or another kind of quantum fluctuations. Reasonably, however, the choice of H_{kin} should also encompass the important elementary "moves" of the problem, determining which configurations are to become direct neighbors of a given configuration, a choice which in turn influences the problem's effective landscape [15]. A very important move that is often used in heuristic TSP algorithms is the so-called *2-opt move*, consisting in eliminating two links in the current tour, $(c_1 \rightarrow c_2)$ and $(c_{1'} \rightarrow c_{2'})$, and rebuilding a new tour in which the connections are given by $(c_1 \rightarrow c_{1'})$ and $(c_2 \rightarrow c_{2'})$. This is illustrated with a 8-city example in Fig. 1, were (left part) the tour $(1 \rightarrow 2 \rightarrow 5 \rightarrow 8 \rightarrow 7 \rightarrow 6 \rightarrow 3 \rightarrow 4)$, represented by the matrices $\hat{T}_{\rm in}$ and $\hat{U}_{\rm in}$, is rebuilt by eliminating the two links $(c_1 = 2 \rightarrow c_2 = 5)$ and $(c_{1'} = 3 \rightarrow c_{2'} = 4)$, and forming (see right part of Fig. 1) two new links $(c_1 = 2 \rightarrow c_{1'} = 3)$ and $(c_2 = 5 \rightarrow c_{2'} = 4)$. The matrices $\hat{T}_{\rm fin}$ and $\hat{U}_{\rm fin}$ in the lower right part of Fig. 1 represent the final (directed and undirected) tour obtained after the 2-opt move. A 2-opt move implies that a whole section of the original tour (between the two removed links $(c_1 \rightarrow c_2)$ and $(c_{1'} \rightarrow c_{2'})$) gets reversed in the new tour, yielding a long series of bit flips in the matrix $\hat{T}$ (dotted circles in Fig. 1). If we associate a spin variable $+1$ (-1) to each entry 1 (0), and represent a 2-opt move in terms of spin-flip operators acting on the configuration $\hat{T}_{\rm in}$, we would need a whole string of spin-flip operators (a non-local object) to enforce a trivial operation – reversing a piece of tour – which does not affect the tour length at all. The advantage of working with $\hat{U}$ is that it represents, in a symmetric way, the direct and the reverse tour, so that all the entries corresponding to the section of reversed tour are completely untouched. The whole 2-opt move, when working with $\hat{U}$ matrices, can be represented by just four spin-flip operators:

$$S^+_{\langle c_{1'},c_1\rangle} S^+_{\langle c_{2'},c_2\rangle} S^-_{\langle c_2,c_1\rangle} S^-_{\langle c_{2'},c_{1'}\rangle} \ ,$$

where, by definition, each $S^{\pm}_{\langle i,j\rangle}$ flips an Ising spin variable (defined as $S^z_{\langle i,j\rangle} = (2\hat{U}_{i,j} - 1) = \pm 1$) at position (i,j) and at the symmetric position (j,i), i.e., $S^{\pm}_{\langle i,j\rangle} = S^{\pm}_{i,j} S^{\pm}_{j,i}$.

The quantum Hamiltonian for the TSP which implements the 2-opt moves is:

$$H_{TSP} = H_{pot}(\hat{U}) + H_{kin} = \sum_{\langle ij\rangle} d_{ij} \frac{\left(S^z_{\langle i,j\rangle} + 1\right)}{2} - \frac{1}{2}\sum_{\langle ij\rangle}\sum_{\langle i'j'\rangle} \Gamma(i,j,i',j';t) \left[S^+_{\langle i',i\rangle} S^+_{\langle j',j\rangle} S^-_{\langle j,i\rangle} S^-_{\langle j',i'\rangle} + H.c.\right] . \qquad (2)$$

Here the quantum coupling Γ is a real positive function depending, in principle, on the links, as well as, in the annealing problem, on time. The link dependence of Γ can be restricted to a dependence on the distances between the cities involved in the two links created by the 2-opt move, in such a way as to realize a *neighborhood pruning* [12], by discouraging (or forbidding altogether) the creation of links between distant cities. In so doing, we mapped the symmetric TSP problem onto a highly constrained Ising spin problem with $N(N-1)/2$ sites – one for each pair of (i,j), with $i > j$, due to the symmetry $(i,j) \leftrightarrow (j,i)$, which we denote by $\langle i,j\rangle$ –, with

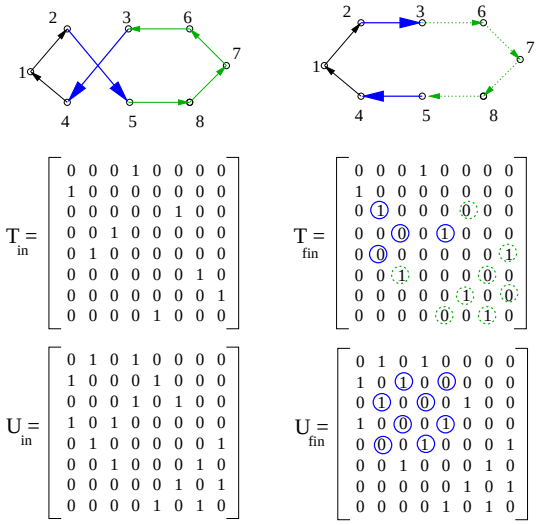

FIG. 1: Left: Representation of an 8-city tour, with the corresponding matrix $\hat{T}_{\rm in}$ and $\hat{U}_{\rm in} = \hat{T}_{\rm in} + \hat{T}^t_{\rm in}$. Right: The final tour obtained when a 2-opt move is performed, with a whole section reversed (dotted line). The matrices $\hat{T}_{\rm fin}$ and $\hat{U}_{\rm fin}$ are shown, the circles indicating the entries that have been switched ($0 \leftrightarrow 1$) by the 2-opt move. The dotted circles in $\hat{T}_{\rm fin}$ are entries related to the trivial reversal of a section of the tour.

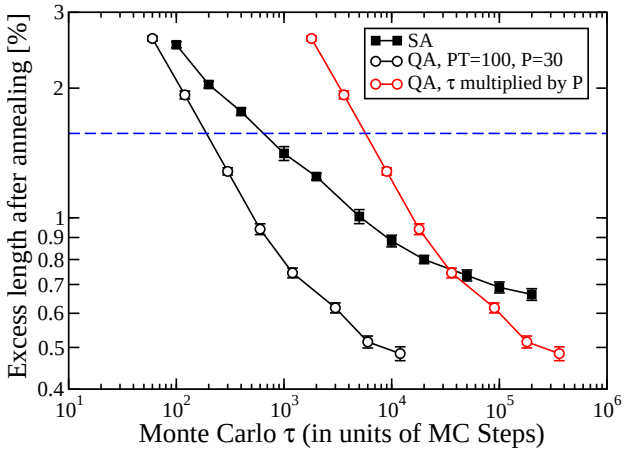

FIG. 2: Average residual excess length found after Monte Carlo annealing for a total time τ (in MC steps), for the $N = 1002$ instance pr1002 of the TSPLIB. Notice how quantum annealing (QA) provides residual excess lengths decaying faster than classical annealing (SA).

a four-spin-flip kinetic term providing the 2-opt quantum fluctuations. The potential energy H_{pot} appearing in H_{TSP} (tour length), represents, in the Ising language, a (random) external magnetic field at each site $\langle i,j\rangle$ depending on the inter-city distance d_{ij}. The constraints on the Hilbert space are such that the matrix $\hat{U}_{i,j} = (S^z_{\langle i,j\rangle} + 1)/2$ represents a valid tour. In particular, the system lives in a subspace with a fixed magnetization – exactly N spins are up ($\hat{U}_{i,j} = 1$) among the $N(N-1)/2$ – and the 2-opt kinetic term conserves the magnetization.

As in the past [6], we will not attempt an actual Schrödinger annealing evolution of the quantum Hamiltonian proposed – out of the question due to the large Hilbert space. On the contrary, we shall address the quantum problem by Quantum Monte Carlo (QMC), where annealing will take place in the fictitious "time" represented by the number of MC steps. Path-integral Monte Carlo (PIMC) provides a natural tool, due to its simplicity. However, attacking H_{TSP} by PIMC meets with a first difficulty, namely Trotter discretization of the path-integral [16]. That requires calculation of the matrix elements of the exponential operator $\langle C'|\exp -\epsilon H_{kin}|C\rangle$ between arbitrary configurations $|C\rangle$ and $|C'\rangle$ of the system [16], a complicated affair for the H_{kin} in Eq. (2). To circumvent this difficulty without giving up the simplicity of PIMC, we introduce a drastic simplification to our kinetic energy term, replacing it altogether with a standard transverse Ising form:

$$\tilde{H}_{TSP} = \sum_{\langle ij\rangle} d_{ij} \frac{\left(S^z_{\langle i,j\rangle} + 1\right)}{2} - \Gamma(t) \sum_{\langle ij\rangle} [S^+_{\langle j,i\rangle} + H.c.] \,, \tag{3}$$

This form is trivially Trotter-discretized, as in the standard Ising system in transverse field [16], since the spin-flip term acts independently on single spins at each time-slice. Strictly speaking this simplified form of kinetic energy would no longer fulfill the constraint to take a valid tour to another valid tour. However, so long as we constrain the MC dynamics strictly within the valid tour subspace – a restriction that comes automatically if we use exclusively 2-opt moves in the MC algorithm, and no single spin-flip moves – that problem does not arise. That this way of bypassing the difficulty in treating the original Hamiltonian (2) should eventually produce a working QA scheme is a priori far from obvious. We will eventually find that it indeed does. The simplified single spin-flip kinetic term $\tilde{H}_{kin}$ in Eq. (3) enters only in calculating the weights of configurations of the Trotter discretized system, and not in the actual MC dynamics, which relies on the 2-opt moves and hence conserves the constraints. The details of the remaining implementation are identical to those reported for the random Ising case [6, 7, 17].

For a direct test of our QA algorithm against SA we chose a standard benchmark TSP problem, namely the printed circuit board instance pr1002 of the TSPLIB [18]. It is a structured TSP problem with $N = 1002$ cities whose optimal tour length L_{opt} is known exactly by other ad-hoc algorithms [18] to be $L_{opt} = 259045$. Our implementation of SA was a standard Metropolis

MC with a temperature schedule starting from T_0 and going linearly to zero in a MC time τ. We chose an optimal initial temperature T_0 by first performing several SA runs with different (short) cooling times τ starting from sufficiently high temperatures (the ergodic region). This identifies an approximate "dynamical temperature" T_{dyn} below which the cooling curves for different τ's start to differ. For pr1002, we obtained $T_{dyn} \sim 100$. As it turns out, the optimal T_0 for SA approximately coincides with T_{dyn}, $T_0 \sim T_{dyn}$, an implementation feature known for TSP SA as *cold starts* [12]. For QA, we implemented for the Hamiltonian $\tilde{H}_{TSP}$ a similar PIMC to that used previously[6, 7] at a fixed low temperature T (we used $T = 10/3$, see below). The quantum model is mapped onto a classical model with an extra imaginary-time dimension, consisting of P ferromagnetically coupled replicas of the original spin problem, at temperature PT [7, 16] (we used $P = 30$). Since QA requires initial configurations equilibrated at temperature PT [7], an obvious choice is to take $PT \sim T_{dyn}$, i.e., $PT = 100$ for the pr1002 [19]. Finally, the transverse field Γ is annealed linearly in a MC time τ from an initial value $\Gamma_0 = 300$ to a final value of zero. In both SA and QA, we used exclusively 2-opt moves, with a static neighborhood pruning [12], which restricts the attempted 2-opt moves by allowing only a fixed number M (we used $M = 20$) of nearest neighbors of city j to be candidates for j'. Our MC step consisted of MN attempted 2-opt moves (for QA, in each of the P replicas). In both SA and QA, we averaged the best tour length found over up to 96 independent searches.

Fig. 2 shows the results obtained for the residual error (average best-tour excess length) upon annealing for a total MC time τ, $\epsilon_{exc} = (\bar{L}_{best}(\tau) - L_{opt})/L_{opt}$, both with SA (filled squares) and with QA (open circles). As a reference, the best out of 1000 runs of the Lin-Kernighan algorithm (one of the standard local-search algorithms for TSP [12]) gives a percentage excess length of $\epsilon_{exc}^{LK} \approx 1.57\%$ [12] (dashed line in Fig. 2). The results show that QA anneals more efficiently, reducing the error at a much steeper rate than SA. Moreover, even accounting for the extra factor P in the total CPU time required by QA (rightmost open circles), QA is still more convenient than SA at large τ and small excess lengths. The similarity with the previous results on the random 2D Ising magnet [6] is striking. We argued in Ref. [6] that QA is faster for the random Ising case due to the superior ability of quantum physics to cross barriers through Landau-Zener tunneling, as compared to classical physics requiring for them to be overcome thermally: Such feature, although by no means a general property, is apparently shared by the TSP. The upward curvature of the data in Fig. 2 is likely to signal a logarithmically slow annealing for both SA and QA [6]. Also worth mentioning is the effect of the finite value of P, which is likely to be responsible for a saturation effect of the QA data, as shown in Fig. 1 of Ref. 6 for the random Ising case.

Current ad-hoc TSP algorithms do better than either annealings – SA and QA being generic tools – for the same CPU time. Moreover, it is known that combining SA with local search heuristics provides superior results to pure SA for the TSP problem [20]. Nevertheless, the absolute quality of QA and its success in a fair comparison to SA strongly encourages to further applications of QA as a general purpose optimization technique, and to possible improvements of the bare QA scheme by combining it with other local heuristics, in the spirit of Ref. [20]. Equally instructive will be to experiment with other QA schemes, for instance Green's Function QMC, which are able to cope with the 2-opt H_{kin} constructed in Eq. (2) or with other sources of quantum fluctuations. That broadening of the project we must leave for future studies. We believe that gaining further experience with the effects of artificially introduced quantum fluctuations in classical complex problems represents a very promising and challenging route, particularly in view of future developments in quantum computation.

This project was sponsored by MIUR, through COFIN and FIRB, and by INFM/Supercalcolo grant. R.M. acknowledges the hospitality provided by SISSA and ICTP. We thank D. Battaglia, C. Micheletti, and R. Zecchina for discussions.

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