Solving NP-complete problem by simulations.

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Abstract.
The mathematical formalism of quantum resonance combined with tensor product decomposability of unitary evolutions is mapped onto a class of NP-complete combinatorial problems. It has been demonstrated that nature has polynomial resources for solving NP-complete problems and that may help to develop a new strategy for artificial intelligence, as well as to re-evaluate the role of natural selection in biological evolution.

1.Introduction.
In this work an attempt is made to simulate combinatorial optimization that is the main obstacle to artificial intelligence. It is a well-established fact that nature exploits combinatorial optimization for natural selection. It is also known that even ants collectively solve combinatorial problems (such as the shortest path to food in a labyrinth) more efficiently than man-made artificial devices. That is why combinatorial problems are not only an obstacle, but is the greatest challenge to artificial intelligence. In this work, a new approach to simulation of NP-complete problems is introduced: combinatorial properties of tensor product decomposability of unitary evolution of many-particle quantum systems are mapped to solutions of NP-complete problems, while the reinforcement and selection of a desired solution is executed by quantum resonance.

2. Quantum Resonance.
Consider a quantum system characterized by a discrete spectrum of energy eigenstates subject to a small perturbing interaction, and let the perturbation be switched on at zero time. The Hamiltonian of the system can be presented as a sum of the time-independent and oscillating components

$$H = H_0 + \varepsilon_0 H_1 \int_\omega \xi(\omega) \sin \omega t d\omega \qquad (1)$$

where H_0 and H_1 are constant Hermitian matrices, ω is the frequency of perturbations, and $\xi(\omega)$ is the spectral density.

The probability of transition from state *k* to *q* in the first approximation is proportional to the product, [1]

$$P_{kq} \propto |\varphi^*_k H_1 \varphi_q|^2 \frac{[\sin \frac{1}{2}(a_{qk} - \omega)t]^2}{(a_{qk} - \omega)} \qquad (2)$$

Here φ_i are the eigenstates of H_0:

$$H_0 \varphi_j = E_j \varphi_j, \qquad j = 1,2,..n. \qquad (3)$$

where E_i are the energy eigenvalues,

$$\hbar a_{kq} = E_k - E_{q,} \quad k,q = 1,2,..n \qquad (4)$$

and $\hbar$ is the Planck constant.

The resonance, i.e., a time-proportional growth of the transition probability P_{kq} occurs when $\omega = a_{qk}$:

$$P_{kq} \propto |\varphi^*_k H_1 \varphi_q| \xi^2(\omega) t \qquad (5)$$

3. Combinatorial problems.
Combinatorial problems are among the hardest in the theory of computations. They include a special class of so called NP-complete problems which are considered to be intractable by most theoretical computer scientists. A typical representative of this class is a famous traveling-salesman problem (TSP) of

determining the shortest closed tour that connects a given set of n points on the plane. As for any of NP-complete problem, here the algorithm for solution is very simple: enumerate all the tours, compute their lengths, and select the shortest one. However, the number of tours is proportional to $n!$ and that leads to exponential growth of computational time as a function of the dimensionality n of the problem, and therefore, to computational intractability.

It should be noticed that, in contradistinction to continuous optimization problems where the knowledge about the length of a trajectory is transferred to the neighboring trajectories through the gradient, here the gradient does not exist, and there is no alternative to a simple enumeration of tours.

The class of NP-complete problems has a very interesting property: if any single problem (including its worse case) can be solved in polynomial time, then every NP-complete problem can be solved in polynomial time as well. But despite that, there is no progress so far in removing a curse of combinatorial explosion: it turns out that if one manages to achieve a polynomial time of computation, then the space or energy grow exponentially, i.e., the effect of combinatorial explosion stubbornly reappears. That is why the intractability of NP-complete problems is being observed as a fundamental principle of theory of computations which plays the same role as the second law of thermodynamics in physics.

At the same time, one has to recognize that the theory of computational complexity is an attribute of a digital approach to computations, which means that the monster of NP-completeness is a creature of the Turing machine. As an alternative, one can turn to an analog device which replaces digital computations by physical simulations. Indeed, assume that one found such a physical phenomenon whose mathematical description is equivalent to that of a particular NP-complete problem. Then, incorporating this phenomenon into an appropriate analog device one can simulate the corresponding NP-complete problem. In this connection it is interesting to note that, at first sight, NP-complete problems are fundamentally different from natural phenomena: they look like man-made puzzles and their formal mathematical framework is mapped into decision problems with yes/no solutions. However, one should recall that physical laws can also be stated in a "man-made" form: The least time (Fermat), the least action (in modifications of Hamilton, Lagrange, or Jacobi), and the least constraints (Gauss).

In this work we will describe how to map a combinatorial decision problem into the physical phenomenon of quantum resonance on a conceptual level, and propose a possible circuit implementation.

Let us turn to the property (5) that can be mapped into several computational problems, and, for the purpose of illustration, choose the following one: given m different items to be distributed over n places; the cost of a β^{th} item put in a γ^{th} place is $\lambda_{\beta}^{(\gamma)}$; in general, the costs (the number of which is nm) can be positive or negative (but not zero), and there are no restrictions to how many different items can be put at the same place. Find yes/no answer to the following question: is there at least one total cost whose absolute value falls into an arbitrarily given interval.

This problem is typical for optimal design. Since the cost of a particular distribution is expressed by the sum

$$E_j = \sum_{\beta=1}^{n} \lambda^{\gamma_\beta}{}_{\beta}, \qquad j = 1,2...N = m^n \tag{6}$$

classically one has to compute all the m^n sums (1) in order to find is there at least one E_q such that

$$a_1 \le \mid E_q \mid \le a_2; \qquad a_2 > a_1, \tag{7}$$ (I.3.3.2)

where a_1 and a_2 are arbitrarily prescribed positive numbers.

Since costs $\lambda_{\beta}{}^{\gamma_\beta}$ can be positive or negative, the absolute value in Eq. (7) represents a global constraint, and therefore our problem belongs to the class of so called constraint satisfaction problems that are the hardest among other optimization problems. The constraint (7) prevents one from decomposing the solution into smaller-size sub-problems. It can be shown that this problem is mapped into the partition problem, [2] , and therefore, it is NP-complete.

Now we will demonstrate how this problem can be solved by the quantum device described above in one computational step.

First, let us represent the unitary matrix U_0 corresponding to the time-independent Hamiltonian

$$U_0 = e^{iH_0 t} \tag{8}$$ (I.3.3.3)

as a tensor product of n diagonal unitary matrices of the size $m \times m$

$$U_0 = U_1 \otimes U_2 \otimes ... \otimes U_n, \qquad (9) \qquad \text{(I.3.3.4)}$$

This corresponds to the direct sum decomposition of H_0

$$H_0 = H^{(1)}{}_0 \otimes 1_m \otimes ... \otimes 1_m + 1_m \otimes H^{(2)}{}_0 \otimes ... \otimes 1_m + ...$$
$$+ 1_m \otimes ... \otimes 1_m \otimes H_0{}^{(n)} \qquad (10) \qquad \text{(I.3.3.5)}$$

where 1_m is an $m \times m$ unit matrix.

Here

$$H_0{}^{(r)} = \begin{bmatrix} \lambda_1{}^{(r)} 0...0 \\ ..... \\ 0.....0 \lambda^{(r)}{}_m \end{bmatrix} \qquad U_r = \begin{bmatrix} e^{i\lambda^{(r)}{}_1 r} 0...0 \\ ..... \\ 0.....0 e^{i\lambda_n{}^{(r)}} \end{bmatrix} \qquad (11) \qquad \text{(I.3.3.6)}$$

Then the unitary matrix U_0 in (9) will be also diagonal and

$$H_0 = \begin{bmatrix} E_1 0...0 \\ ..... \\ 0.....0 E_N \end{bmatrix}, N = m^n \qquad (12) \qquad \text{I.3.3.7)}$$

while E_j is expressed by Eq. (6).

Hence, if one select $\lambda_\beta{}^{(\gamma)}$ in (8) as the costs of an β^{th} item put in a γ^{th} place, then the eigenstates E_j of the Hamiltonian H_0 represent costs of all $N=n^n$ possible distributions (8).

Without loss of generality, one can assume that $m=2$ since computation of 2^n different sums has also an exponential computational complexity. At the same time, this assumption will simplify the implementation of the simulation device.

Now we have to choose the perturbation of the Hamiltonian, (see Eq. (1)). For that purpose assume that initially the quantum device is in a certain base state k, whose energy E_k does not belong to the interval (7), i.e.,

$$| E_k | < a_1, \qquad or \qquad | E_k | > a_2, \qquad (13) \qquad \text{(I.3.3.8)}$$

and select $\xi(\omega)$ as follows:

$$\xi(\omega) = \begin{cases} \xi_0 = Const & if \ \frac{| E_k - a_2 |}{\hbar} \le \omega < \frac{| E_k - a_1 |}{\hbar} \\ 0 & otherwise \end{cases} \qquad (14) \qquad \text{(I.3.3.9)}$$

The only constraint imposed upon the Hamiltonian H_1 is that all its out-of-diagonal components are non-zeros. Indeed, in this case each element of the matrix (5) will have the form:

$$| \varphi_k{}^* H_1 \varphi_q |^2 = | \lambda_k \lambda_q H_1{}^{(kq)} |^2 \neq 0 \qquad if \qquad k \neq q. \qquad (15) \qquad \text{(I.3.3.10)}$$

and no possible resonance transitions will be missed.

Here, for the sake of concreteness, the initial state E_k was selected such that:

$$| E_k - a_1 | > | E_k - a_2 | \qquad (16) \qquad \text{(I.3.3.11)}$$

Turning to Eq. (1) and taking into account Eqs. (4) and (7), one concludes that Hamiltonian of the system is decomposable only at $t=0$. For $t>0$, the quantum system becomes correlated due to the perturbations.

Suppose that the given interval a_1,a_2 contains at least one total cost $|E_q|$ from the set (6), i.e., $|E_q|$ satisfies the inequality (7). Then, according to Eqs. (5) and (14), the resonance transition from the initial state E_k to the state E_q (or other states satisfying (7)) will occur with the probability one. Indeed, in the presence of a resonance, the probability for non-resonance transitions is vanishingly small if $\varepsilon_0 << 1$ (see Eq. (1)).

However, if the given interval a_1,a_2 does not contain any costs $|E_q|$ from the set (6), then according to Eqs. (5) and (14), there will be no resonance transitions at all, and therefore, with the probability one the quantum device will stay in the initial state.

A mapping of the combinatorial problems onto tensor decomposability of the Schrödinger equation is illustrated in Fig. 1

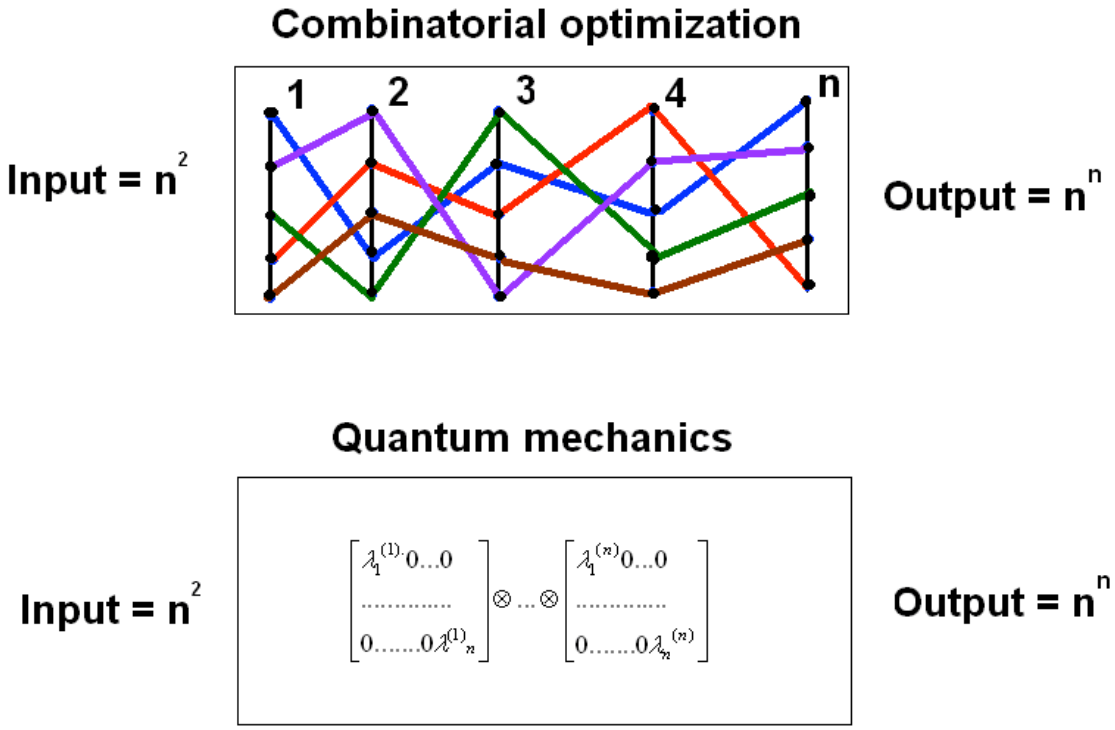

Figure 1. Mapping combinatorial optimization to quantum mechanics.

5. Summary.

Thus, it has been demonstrated how a "man-made" problems of exponential computational complexity which is hard to handle by algorithmic methods are solved by exploiting a strongly pronounced physical phenomena: quantum resonance.

The main advantage of the presented approach is in exponential speedup of solutions to NP-complete combinatorial problems. Three fundamental physical phenomena contribute to it: quantum resonance, entanglement, and tensor-product decomposability of the underlying unitary matrix.

Quantum resonance allows one to represent all the possible solutions to the problem as a set of competing dynamical processes: energy exchanges between pairs of quantum eigenstates. The mathematical formalism of quantum resonance provides storage for these processes: the transition matrix P_{kq} (see Eq. (2)) where each process is labeled through the corresponding transition probability. Quantum entanglement implement the global constraint (7) and
tensor-product decomposability is a fundamental property of the Schrodinger equation for multi-particle systems. Due to its effect, the number of stored solutions, i.e., the number of transitions P_{kq} is exponentially larger than the number of the input parameters (see Eq. (6)) and that is what directly contributes into exponential speedup and capacity.

In order to make these three physical phenomena work together, one has to choose the Hamiltonian of the quantum system such that the optimal solution is the winner in the competition with other solutions, i.e., that its transition probability is the largest. This is achieved by selecting the oscillating part of the Hamiltonian in the form of (14).

Possible implementation of the presented algorithm by a circuit of a polynomial complexityis proposed in [3].

It should be emphasized that the solution of one NP-complete problem opens up a way to solve every NP-complete problem in polynomial time.

References.

1. D. R. Bates, Quantum Theory, Acad. Press, N.Y. 1961, p. 271
2. M. R. Garey and D. S. Johnson, Computers and Intractability, 1979 W. H. Freeman and Co., NY, p. 90
3. M. Zak. From quantum computing to intelligence, Nova, NY, 2011.