Tailoring Many-Body Interactions to Solve
Hard Combinatorial Problems

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Abstract

A quantum machine consisting of interacting linear clusters of atoms is proposed for the 3SAT problem. Each cluster with two relevant states of collective motion can be used to register a Boolean variable. Given any 3SAT Boolean formula the interactions among the clusters can be so tailored that the ground state(s) (possibly degenerate) of the whole system encodes the satisfying truth assignment(s) for it. This relates the 3SAT problem to the dynamics of the properly designed glass system.

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Equipped with powerful algorithms, today’s electronic computers solve many problems amazingly fast. Yet there are problems hard to them in the sense that the best algorithms essentially take exponential running time. Many of the hard problems are NP even NP-complete [1]. A problem is NP provided that it can have its answer checked in polynomial time. If the problem has the further property that all problems in the NP class can be translated into it by algorithms taking polynomial time, it is NP-complete [1].

Recently attempts to search for novel machines with greater computational power are stimulated by the growing evidence that no general efficient polynomial time solution running in classical computers exists for any NP-complete problem. DNA computers have been proposed to solve the directed Hamiltonian path problem [2] and the satisfiability problem [3]. These proposals took the advantage of the enormous parallelism of solution-phase chemistry. However, the number of molecules required rises exponentially as the complexity of the problem increases, which stops the application of the DNA computation to large scale problems [4,5,6]. Quantum computers may also solve some problems fast by virtue of the so-called quantum parallelism [7,8]. But this quantum parallelism seems difficult to harness. So far no fast quantum algorithm has been found for any NP-complete problem [9]. Furthermore, it is a thorny issue to construct a quantum computer and maintain the quantum coherence to achieve any useful computation [10,11]. Nevertheless, recent studies reveal the essential role of physics in computer science. People realize more and more that, what can be computed and how fast it can be computed is not only a problem of pure computer science, but a question posed to physics as well.

The satisfiability problem (SAT) is among the first known NP-complete problems. Consider formulas over a set of Boolean variables

\[ V = \{v_1, v_2, ..., v_m\} \]

where each variable can only have values 0 (false) and 1 (true). All variables \(v_i\) and their negations \(\bar{v}_i\) are called literals over \(V\). A clause is a formula of the form

\[ l_1 \lor l_2 \lor \cdots \lor l_k \]

where each \(l_i\) is a literal (\(\lor\) is the logical OR operation, \(\land\) is the logical AND correspondingly). It is said that a clause is satisfied if and only if at least one of its member literals has the value 1 so that the clause gets the value 1. The famous SAT problem is to ask whether there is a truth assignment that satisfies a formula of the form

\[ F = C_1 \land C_2 \land \cdots \land C_n \]  \hspace{1cm} (1)

where each \(C_i\) is a clause. The 3SAT problem is just the restricted SAT problem in which all clauses have exactly three literals.

In this letter, a quantum search machine consisting of linear clusters of atoms is proposed to encode the 3SAT problem. Each cluster has two relevant states of collective motion which can be used to register a Boolean variable. It will be shown that the interactions among the clusters can be so tailored that the ground state of the whole system encodes an assignment of Boolean values which solves the satisfaction problem. Later it will be clear that the restricted structure of 3SAT greatly simplifies the tailoring of many-body interactions. If in some situation, the system could quickly relaxes to the ground state, the solution can
be read out fast. However, in the worst cases, the system will be trapped in local energy minima, the relaxation is exponentially slowed down. Anyway, our model machine provides a direct connection between an NP-complete problem and a properly designed glass system. Studying the dynamics of the glass system bears significance on learning how to solve the NP problem.

If each Boolean variable is registered by an individual atom or electron, it won’t be easy to tailor the many-body interactions in the desired way. Specifically for the 3SAT problem, a Boolean variable may enter many clauses, it is convenient to encode a variable into the collective motion of a chain of atoms (called a linear cluster of atoms). For example, a one-dimensional ferromagnetic chain does the favor, the two directions of magnetization of the chain can be used to store binary information. Lent et al. have proposed a binary wire consisting of interacting quantum-dot cells [12,13]. Although this kind of binary wire is by no means the only possible candidate for implementing the search machine, it serves as a very good illustration. In this letter, whenever the term binary wire appears, it refers to the wire proposed by Lent et al., and more specifically the wire consisting of rotated cells [13]. In a binary wire, the two ways of cell polarizations are used to encode binary information. A remarkable advantage of the binary wire system is that it is very easy to achieve logic fan-out. The quantum machine encoding a simple 3SAT problem

\[ F = (\bar{x}_1 \lor x_2 \lor x_4) \land (x_1 \lor \bar{x}_3 \lor x_4) \]

is shown in Fig.1 as an example. There are four Boolean variables which are registered by four horizontal binary wires labeled by \( x_1, x_2, x_3 \) and \( x_4 \) respectively. It is assumed that the system is at low enough temperature so that any free wire stays at the two-fold degenerate ground state, no higher energy collective mode can be excited. Hence for the four bit register, the only relevant states are those \( 2^4 \) expanded states called the working modes which are degenerate. The register is connected by vertical transmission wires to three-literal clause evaluators (3CEs). Notice these inverters on some transmission wires (it is easy to implement a logic inverter [13]). Also notice that both the transmission lines and the inverters conserve the energy degeneracy among the working modes. The energy degeneracy conservation will be broken when the 3CEs are connected. Actually the 3CE is a device inside which the relevant three binary wires are brought close to interact and the interactions are properly tailored so that the energy degeneracy among the eight working modes expanded by the three related literals is lifted according to whether they satisfy the corresponding clause or not. As long as the clause is satisfied, the energy remain lower, otherwise the energy is pushed higher. Specifically, for a 3CE connecting to three literals \( (l_1, l_2, l_3) \), the expanded eight states fall into two energy levels: if at least one of the literals has the value 1, the clause \( l_1 \lor l_2 \lor l_3 \) is satisfied, the system remains at the lower energy level; when all the values of the three literals are 0, the system will be raised to a higher energy level. A concrete implementation of the 3CE will be shown later. At this stage let’s see how the search machine works provided that the three-literal clause evaluators behaving as desired are available. Generally, a 3SAT problem has \( m \) Boolean variables and \( n \) 3-clauses involved (there is an obvious upper bound for \( n \), i.e. \( n < C_3^m \)). One may construct a quantum search machine with an \( m \) bit register, \( n \) 3CEs, a sufficient number of transmission wires, and some inverters. The working modes associated with the \( m \) bit register consist of the \( 2^m \) degenerate ground states. Because the register, the transmission wires, and the
inverters conserve the energy degeneracy among the working modes, while the 3CEs lift the energy degeneracy according to whether the corresponding clauses are satisfied or not, the whole system of the search machine will be in its ground state(s) if and only if all 3-clauses are satisfied. When the system is in the ground state, one measures the register and gets the solution for the SAT problem if only it exists, otherwise the measurement result will tell that there is no truth assignment at all which satisfies all the given clauses.

Now it is time to show how the 3CE can be really implemented. One may symmetrically arrange the binary wires so that the Hamiltonian for the 3CE is invariant under any permutation of the three literals. There are eight states expanded by the three literals \((l_1, l_2, l_3)\) which serve the labels for the states at the same time. The permutation symmetry divides the eight states into four classes

\[
\text{class 0 : (000)}
\]

\[
\text{class 1 : (001), (010), (100)}
\]

\[
\text{class 2 : (110), (101), (011)}
\]

\[
\text{class 3 : (111)}
\]

Without the tailored interactions, all these states are degenerate. The purpose of interaction tailoring is to lift the degeneracy into two energy levels, keep the seven states in class 1, 2, and 3 at the lower level while raise the state in class 0 to a higher energy level. The Hamiltonian of the 3CE for three given literals \((l_1, l_2, l_3)\) includes one-body terms \(H_i^{(1)}\), two-body terms \(H_{ij}^{(2)}\) and a three-body term \(H_{123}^{(3)}\),

\[
H_{3CE} = \sum_i H_i^{(1)} + \sum_{i \neq j} H_{ij}^{(2)} + H_{123}^{(3)}
\]  

where the one-, two-, and three-body terms are given by

\[
H_i^{(1)} = 2A \left( \frac{1}{2} - l_i \right)
\]

\[
H_{ij}^{(2)} = 2B \left( l_i \oplus l_j - \frac{1}{2} \right)
\]

\[
H_{123}^{(3)} = \sqrt{D^2 + \left( E + F \sum_{i=1}^3 l_i \right)^2}
\]

where \(i, j = 1, 2, 3, i \neq j, l_i\) and \(l_j\) are Boolean variables that can have the value 0 or 1, \(\oplus\) is the exclusive-OR operation, and \(A, B, D, E,\) and \(F\) are parameters characterizing the many-body interactions. To make a one-body term \(H_i^{(1)}\) is straightforward: applying a bias electric field, its side effect splits the two degenerate ground states of a binary wire. Notice that \(A\) is easily adjustable. It is also easy to have a two-body interaction, simply draw the two binary wires \(l_i\) and \(l_j\) close, the Coulomb interaction between their charge distributions gives the desired \(H_{ij}^{(2)}\). The only tricky implementation is for \(H_{123}^{(3)}\). As shown in Fig.2, one may place in the same plane, say \((x, y)\) plane, the three binary wires symmetrically with their ends sitting at a same circle (the readers may notice at once the fact that there are inevitably two-body interactions when the three wires are brought close). At a point \(P\) out of \((x, y)\) plane just above the center of the circle, the \(z\)-component of the electric field due to the charge distribution of each binary wire \(l_i\) is
\[ E_i = Fl_i + \text{constant}, \quad i = 1, 2, 3 \]  

(5)

The resultant electric field \( E_{\text{tot}} \) along the \( z \) direction at point \( P \) due to the three wires and an on purpose applied external field with variable intensity, will be

\[ E_{\text{tot}} = E + F \sum_{i=1}^{3} l_i \]  

(6)

where \( E \) is variable. There is a responser placed at point \( P \) which yields an energy varying according to \( E_{\text{tot}} \) by the virtue of the Stark effect [15]. The responser should be sensitive only to the \( z \)-component of the electric field. A quantum dot made from a symmetric double well along the \( z \) direction can serve as a good responser as desired. In \( x, y \) directions the quantum confinement effect of the dot is very strong leading to large energy spacing, the Stark effect is negligible. While in the \( z \) direction, the symmetric double well leads to a very good two-level system with relatively small energy spacing [16] which is sensitive to perturbations. The Schrödinger equation of a two-level system perturbed by an external field can be exactly solved [17]. The exact eigen-energies are given by

\[ U = \pm \sqrt{D^2 + (pE_{\text{tot}})^2} \]  

(7)

where \( \pm D \) are the energy levels without perturbation, \( p \) is the transition electric dipole. The combination of Eqs.6 and 7 leads to the desired three-body energy term \( H_{123}^{(3)} \), where for simplicity the constant dipole is set to \( p = 1 \). Now, according to Eq.3, the total energies of a 3CE at states of class 0, 1, 2, 3 are respectively \( U_0, U_1, U_2, U_3, \)

\[ U_0 = 3A + 3B - \sqrt{D^2 + (E + 3F)^2} \]

\[ U_1 = A - B - \sqrt{D^2 + (E + F)^2} \]

\[ U_2 = -A - B - \sqrt{D^2 + (E - F)^2} \]

\[ U_3 = -3A + 3B - \sqrt{D^2 + (E - 3F)^2} \]  

(8)

In practice, the parameters \( B, D, \) and \( F \) are usually fixed, not easy to adjust, while \( A \) and \( E \) are ready to vary. It is convenient to measure all the parameters in unit of \( D \). For any given parameters \( B/D \) and \( F/D \), The interaction tailoring actually is to adjust the two parameters \( A/D \) and \( E/D \) so that the following condition holds

\[ U_1 = U_2 = U_3 < U_0 \]  

(9)

The equations can be numerically solved. In Fig.3 the points lying in the black area are of the parameters \( B/D \) and \( F/D \) for which suitable values of \( A/D \) and \( E/D \) (called good 3CE solution) can be found satisfying the condition (9), under which the seven states in classes 1, 2, and 3 are degenerate, while the energy of the only state in the class 0 is lifted sufficiently higher. Actually the black area in Fig.3 is constricted to the points for which the stronger condition is satisfied

\[ U_1 = U_2 = U_3 < U_0 - 0.2D \]  

(10)
The wide black area indicates the fact that for a wide range of $B/D$ and $F/D$, which are fixed upon the completion of the device fabrication, good 3CEs can be achieved by varying $A/D$ and $E/D$ which are directly related to adjustable external bias fields. This fact is particularly advantageous to device fabrication.

The 3CE proposed here is of course not unique. It is only for illustrative purpose. One may implement 3CEs by other means. The key point is to keep the states in the classes 1, 2, and 3 degenerate while lift the state in the class 0 to a higher energy.

In conclusion, it has been showed that a quantum search machine consisting of lines of interacting quantum dots can encode the 3SAT problem efficiently in the sense that the solution is kept in the ground state of the system and the machine contains a number of 3CEs less than $C_{2n}^3$ where $n$ is the number of Boolean variables. The purpose of the present letter is to show the possibility of tailoring the many-body interactions in a “static quantum network” to solve some hard computational problems. The example 3SAT problem is a hard NP problem to classical computers in the sense that with the best algorithm a classical computer needs exponential running time to find the solution. The problem becomes intractable when its input size gets larger [1]. To our machine there is the open question of how to make it relax quickly to the ground state so that it gives us the solution in a short time.
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FIGURE CAPTIONS

Fig.1 The search machine solving the simple 3SAT problem \((\bar{x}_1 \lor x_2 \lor x_4) \land (x_1 \lor \bar{x}_3 \lor x_4)\).
Fig.2 Three binary wires are brought close to yield the three-body interaction.
Fig.3 The area of parameters \(B/D\) and \(F/D\) where good 3CE solutions exist.
Fig. 1
Fig. 3