Simulated Quantum Computation of Global Minima

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Abstract

Finding the optimal solution to a complex optimization problem is of great importance in practically all fields of science, technology, technical design and econometrics. We demonstrate that a modified Grover's quantum algorithm can be applied to real problems of finding a global minimum using modest numbers of quantum bits. Calculations of the global minimum of simple test functions and Lennard-Jones clusters have been carried out on a quantum computer simulator using a modified Grover's algorithm. The number of function evaluations N reduced from $O(N)$ in classical simulation to $O(\sqrt{N})$ in quantum simulation. We also show how the Grover's quantum algorithm can be combined with the classical Pivot method for global optimization to treat larger systems.

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Rational drug design, molecular modeling, quantum mechanical calculations and mathematical biological calculations are but a few examples of fields that rely heavily upon the location of a global minimum in a multiple-minima problem[1–4]. Several global optimization methods have been developed over the past decades. However, the large computational cost of finding the global minimum for large number of variables limited the applications of such algorithms[5–8]. Quantum algorithms on the other hand known to speed up the computation compared to classical ones[11–14]. For example, the calculation time for the energy of atoms and molecules scales exponentially with system size on a classical computer but polynomially using quantum algorithms[9, 10].

Quantum computation is generally regarded as being more powerful than classical computation. The evidence for this viewpoint begins with Feynman's pioneering observation [15] that the simulation of a general quantum evolution on a classical computer appears to require an exponential overhead in computational resources compared to the physical resources needed for a direct physical implementation of the quantum process itself. Subsequent work by Deutsch [16], Bernstein and Vazirani [17], Simon [18], Grover [19], Shor and others[20, 21] showed how quantum evolution can be harnessed to carry out some useful computational tasks more rapidly than by any known classical means. For some computational tasks (such as factoring) quantum physics appears to provide an exponential benefit, but for other tasks (such as NP complete problems [22]) the quantum benefits appear to be inherently more restricted, giving at most a polynomial speedup [23–28].

Grovers's quantum algorithm can find an object in a unsorted database containing N objects in $O(\sqrt{N})$ quantum mechanical steps instead of $O(N)$ steps[29, 30]. The problem we are given is a function $f(x)$ with $x = 1, 2, ..., N$. The function has the property that it is 0 for all values of x except for a particular x_p, for which the function $f(x_p) = 1$. The task is to find x_p. The basic idea is to place our register in an equal superposition of all states, and then selectively invert the phase of the marked state, and then perform an inversion about average operation a number of times which has the effect of increasing the amplitude of the marked state[29, 30]. Grovers' search algorithm has been implemented by using nuclear magnetic resonance (NMR) techniques for a system with four states[31] and more recently using quantum optical methods[32]. An efficient quantum algorithm for global optimization can find applications in a wide range of fields[33].

In this paper, we will demonstrate that a modified Grover's quantum algorithm can be

applied to real problems of finding a global minimum using modest numbers of quantum bits. We will simulate the revised quantum search algorithm using a classical computer. The limitation of computer resource such as the memory and speed of CPU will prohibit a large scale quantum computer algorithm simulation on a classical computer. Thus, first we implement the algorithm for simple test functions and small size Lennard-Jones clusters. The quantum search circuit is shown in Fig. 1. In this figure, we divided the register into three groups, where the Hadamard gates are operated on the initialized registers, then we applied the Grover iteration to rotate the superposition states into target states. The measurement result after the iteration is used to update the threshold value in the Grover iteration steps. Grover oracle is replaced by the adapted threshold to search all the states which $f(x_1, x_2, ..) \leq M_{n-1}$, where M_{n-1} gives the minimum measurement value. The iteration number during each search will be preselected. After each iteration, the result will be measured and compared with the other measured results to setup a new threshold value.

We first applied the adapted quantum search algorithm to test a simple analytical function used in global optimization: the Goldstein-Price function(GP) which is given by[8]

$$\begin{aligned} f(x_1, x_2) \;=\; & [1 + (x_1 + x_2 + 1)^2(19 - 14x_1 + 3x_1^2 - 14x_2 + 6x_1x_2 + 3x_2^2)][30 + (2x_1 - 3x_2)^2 \\ & (18 - 32x_1 + 12x_1^2 + 48x_2 - 36x_1x_2 + 27x_2^2)], \end{aligned} \tag{1}$$

where $-2 \leq x_i \leq 2$. The GP function is an excellent test function for any global optimization method. The global minimum for the GP function is equal to 3, which is located at(0,-1), also there are four local minima in the minimization region. The potential surface near the global minimum is shown in Fig. 2. The location of minimum value $f(x_1, x_2) = 3$ is also shown in Fig. 2. We used 8 qubits as the registers. The registers will be divided into two groups to present the variable x_1 and x_2. The searching range is $x_{1,2} \in [-2, 1.75]$. After applying the Hadamard gate, the registers group will be initialized into the superposition state, each will be used to cover 2^4 discrete points in the searching range, namely, each basis function will be mapped to the number within the searching domain. Then, the measurement will be performed to obtain the first threshold value after selected number of Grover iterations was applied. The number of iterations before each measurement is important to reduce the total iteration number. We chose the sequence: $0, 0, 0, 1, 1, 0, 1, 1, 2, 1, 2, 3, 1, 4, 5, 1, 6, 2, 7, 9, 11, 13, 16, 5...$, as the iteration number before each measurement, i.e. for step 1 we measure the state without any Grover itera-

tion, for step 4, we measure the state after one Grover iteration. This sequence has been proposed in Ref. [34] to reduce the Grover iteration numbers for adopted Grover search method. During each iteration, the state function will be rotated towards the threshold value, which is always the best measurement result at previous steps. The new obtained value will be compared with the old threshold value. The threshold value will be reset to the new value if the old threshold value is larger than the new measurement result, otherwise it is unchanged. The iteration will continue until convergence is reached. The quantum search yields the same result(high probability) as the classic method with about 16 steps. In Fig. 3, we show the probability distribution of the state function before the iteration steps. The top left panel is the initial state, where the state function is the superposition for every possible state, and the measurement result yields 118094.0237 after step one without any Grover iteration. In Fig.3, panel (b) is the state function after total 2 Grover iterations at step 5, where the measurement result yields 2157.1992. As we can see the probabilities for smaller function values become larger, meanwhile the eigenfunction corresponding to larger function values start decreasing. When we increase the measurement step to 10 and Grover iteration number to 7, the probability distribution further localized in an eigenfunction which corresponds to the global minimum value. At step 13 with total 13 Grover iteration, we reach the global minimum value 3 at $x_1 = 0$ and $x_2 = -1$ as shown in panel (d) of Fig. 3.

Let us further illustrate this approach by considering a real and practical optimization problem: finding the global minimum of Lennard-Jones clusters, clusters of atoms or molecules that interact with each other through the Lennard-Jones potential. The Lennard-Jones potential (referred to as the L-J potential or 6-12 potential) is a simple mathematical model that describes the long range attractive van der Waals force and the short range Pauli repulsion force. The L-J potential is of the form:

$$V_{LJ}(r) \; = \; 4\epsilon[(\frac{\sigma}{r})^{12} \; - \; (\frac{\sigma}{r})^{6}], \tag{2}$$

where ϵ is the well depth, σ is the hard sphere radius and r is the relative distance between two particles. These parameters can be fitted to reproduce experimental data or deduced from results of accurate quantum chemistry calculations. The L-J potential is a relatively good approximation and due to its simplicity often used to describe the properties of gases, and to model dispersion and overlap interactions in molecular models. It is particularly accurate for noble gas atoms and is a good approximation at long and short distances

for neutral atoms, molecules and clusters. Lennard-Jones clusters are excellent for testing the efficiency of global optimization algorithms. Homogeneous Lennard-Jones clusters have well-established minima and regular minimum-energy structures for very large clusters [35]. However, the number of local minima apparently grows as $\exp(N^2)$ and finding the global minimum in Lennard-Jones clusters is an NP-hard problem [36]. Several global optimization methods have been applied to the energy function of Lennard-Jones clusters. The total energy for a Lennard-Jones cluster of N particles is: $E_N = \sum_{i=1}^{N-1} \sum_{j=i+1}^{N} V_{LJ}(r_{ij})$, where r_{ij} is the distance between the i-th and the j-th particles and $V_{LJ}(r)$ is the Lennard-Jones two-body potential. We start simulating the process of searching the global minimum for $N = 3$ particles. A total of 9 register qubits were separated into two groups for presenting three variable B_1, B_2, and A_1, where B_1 is the bond length between the atom 0 and 1, B_2 is the bond length between atom 0 and 2, and A_1 is the bond angle of atom 0, 1 and 0, 2 as shown in Fig. 4. Five qubits will be used as the first register to cover the space $B_1 = B_2$, and four qubits will be used as the second register for A_1. The searching range for $B_{1,2} \in [0.0001, 2]$ and for $A_1 \in [0.0001, \pi]$. The classical search yields the minimum value -2.9094 at $B_1 = 1.032$, $B_2 = 1.032$ and $A_1 = 60^o$. Unlike the search method for GP function, where the number of iterations is preselected based upon the proposed sequence, here we increase the number of iterations after every measurement to study the importance of the iteration sequence. In Fig. 4, we show the search results and the total iteration steps. From the histogram of total number of iterations for 100 independent searches, we found that the average number of iteration is about 21. This indicates that the running time of adapted search algorithm is still the same as the Grover search algorithm $O(\sqrt{N})$. The configuration corresponding to the minimum for LJ cluster is also shown in Fig. 4.

In order to expand the adapted quantum search algorithm to search the global minimum for larger number of variables and to overcome the limit of using large number of qubits in the computation, we combined the classical pivot search method[7, 8] with the quantum Grover's search algorithm. The basic scheme is as following: *Step (1)*: Generate N random probes, then shift it into superposition of the entire state space by applying the Hamiltonian (a designed Hamiltonian to represent the function to be optimized). *Step (2)*: Use the quantum Grover algorithm mentioned before to do the comparison. Select and keep about the smallest 15% of the original N random probes as pivot probes. *Step (3)*: Initialize the quantum computer with the state associated with these pivot probes, apply a series of

controlled Hadamard gates to produce the superposition state with points near the selected probes. $x_{R,i} = x_{B,i} + \Delta x_i$, where Δx_i is a randomly generated vector according to a particular distribution such as Gaussian distribution [7]. *Step (4)*: Redo *Step (2)*and keep going until the criteria of convergence is satisfied. Using this procedure, it is possible to cover the entire searching space by a small number of qubits. Moreover, this small number of qubits is sufficient to cover each subdomain to yield the desired resolution. To illustrate this combined approach, we search the global minimum for the Shubert test function, which is given by[8]:

$$f(x_1, x_2) = [\sum_{i=1}^{i=5} i \cos[(i+1)x_1 + i]] \times [\sum_{i=1}^{i=5} i \cos[(i+1)x_2 + i]] \tag{3}$$

with $-10 \leq x_{1,2} \leq 10$, which has 760 local minima, 18 of which are global with $f(x_1, x_2) = -186.7309$. The surface potential of this function is shown in Fig.5. Ten qubits were used to do this simulation, each X was assigned 5 qubits. Following the same procedure mentioned above, we initially generated $2^{10}(1024)$ random points. Then 15% minimum of these points was picked up by quantum Grover algorithm, they worked as pivots. After that, we arranged the pivots based on the weight of the optimized function $(\exp(-f(x_1, x_2)/kT))$, where kT is just a fixed parameter. On the behave of the weight, we generated the other points according to the Gaussian distribution. We ran this simulation for 98 times, the researched minimum values are between -30.56 and -186.73. Over 80% points are located in -186.73, which is exact global minimum for this function. It also covers all 18 global minima and the average iteration is 1300. The simulation result is shown in Fig. 5, where the black dots are measurement results on the contour of the surface potential with red dots as global minima. From this simulation result, it can be seen that our combined quantum search method is very powerful in finding global minima.

Furthermore, following the same steps, we also applied this combined method to search optimized structure for LJ cluster. We tried 5 atoms and got the exact same result as the classical method. The detailed procedure for the 3 atoms simulation is as following: we first set 5 qubits for $B_{1,2}$ and 5 qubits for A_1. The same previous range, which is $B_{1,2} \in [0.0001, 2]$ and for $A_1 \in [0.0001, \pi]$. We first generated 2^5 random $B_{1,2}$ and 2^5 random A_1 in the above range. Then we used the combined classical pivot method and Grover's search algorithm which was mentioned in previous paragraph. After the search, we got the global minimum structure for the 3 atoms cluster (the same structure shown in Fig. 4). The distance between each atom is 0.99889 and the total potential for this structure is -2.9999, which is exact the

same as the classical result. Furthermore, based on the optimized structure of 3 atoms, we added another atom to form the 4 atoms cluster. We also used 10 qubits to do this simulation, 4 qubits for X axis, 3 qubits for Y axis and the rest 3 qubits for Z axis. In order to save simulation steps, we set $X \in [-0.5, 0.5]$, $Y \in [0.01, 1.01]$ and $Z \in [0.01, 1.01]$. Then we followed the same steps as 3 atoms, generated random points and started the search. In order to illustrate this procedure, we used two variables to get the probability image, which is shown in Fig. 6. In this picture, we fixed the X coordinate of the 4th atom at 0.0 and let Y and Z coordinates totally free between 0.01 and 1.01. The final LJ potential for this cluster is -5.9926, which is exact the same as the classical result. After that, we added the fifth atom to the 4 atoms system and did the simulation. The searched structure is also shown in Fig. 6 and the energy is -9.0952, also the same as the classical result.

It is known that the $\sqrt{N}$ is the optimal running time for quantum Grover search algorithm. The combined search method does not reduce the total rotation steps, but does reduce the required number of qubits to do the simulation. Due to the limited available qubits in the classical computer, we can only simulate small number of LJ clusters. However, if a quantum computer exists, we will be able find the global minimum for large numbers of LJ clusters. Moreover, for larger LJ clusters, if we had larger qubits, we can incorporate the partial knowledge that we had by starting with the structure of the smaller $(N-k)$ clusters and adding k additional particle at random. In any "growing" problem, such as minimum energy configuration of clusters, self-avoiding walks, protein folding, etc., this systematic approach to solving the structure of large clusters can be incorporated. One of the powerful features of this combined algorithm is that information such as this can be built into the initialization of the probes.

We have used an adapted quantum search algorithm to search the global minima for test functions and LJ clusters. Our quantum computer simulations on the classical computer yield the same global minimum values as the classical search method with high probability. We also show how to combine the classical Pivot method with the adapted quantum search algorithm to search for the global minimum in larger domains. Recently, Jordan[37] proposed a fast quantum algorithm for estimating numerical gradient with one query. One can use this method to search the potential gradient with zero value. This will rotate the entire space towards the state function which corresponds to all minima. The measurement will yield one of the minima in stead of any point in the search domain. Combining this

with our search method will greatly reduce the number of rotations needed for finding the global minimum. This method was tested using a test function in a large search domain, and the result agrees very well with the classical search method with fewer searching steps. With further improvements in the quantum search algorithms, we expect to see solutions of previously intractable global optimization problems in many different fields.

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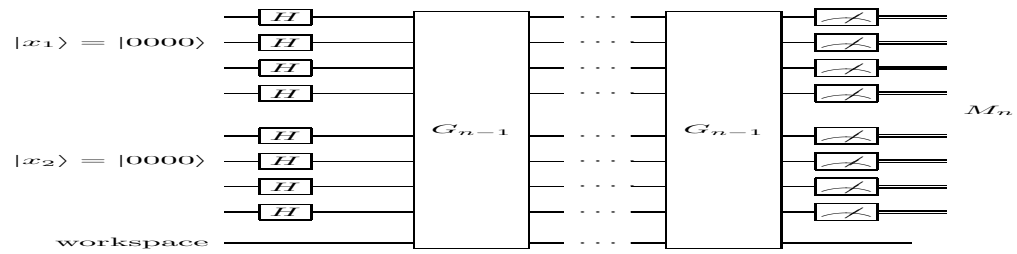

FIG. 1: Quantum Circuit for searching the global minimum. The G_{n-1} is the oracle to rotate the vector toward the state with $f(x_1, x_2, ...) \leq M_{n-1}$, where M_{n-1} is the minimum of all measurement results. The registers will be initialize to $|x_1\rangle = |0000\rangle$ and $|x_2 = |0000\rangle$ for variable $x_1$and x_2, after using the Hadamard gates to convert the initial state into the superposition state, the adapted grover operators will applied iteratively to rotate the superposition state in the specific states. The threshold value of grover operator will be updated based on the measurement result after certain number of iterations.

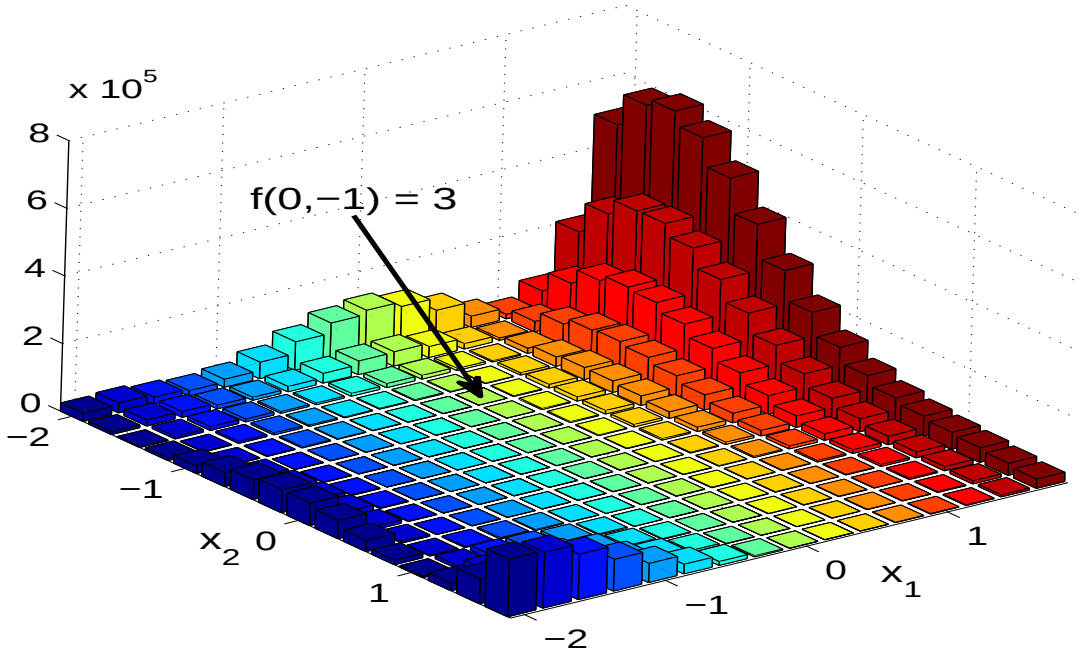

FIG. 2: The potential surface near the global minimum of the GP function (See the text). $f(0,-1)=3$ is the global minimum as indicated by the arrow.

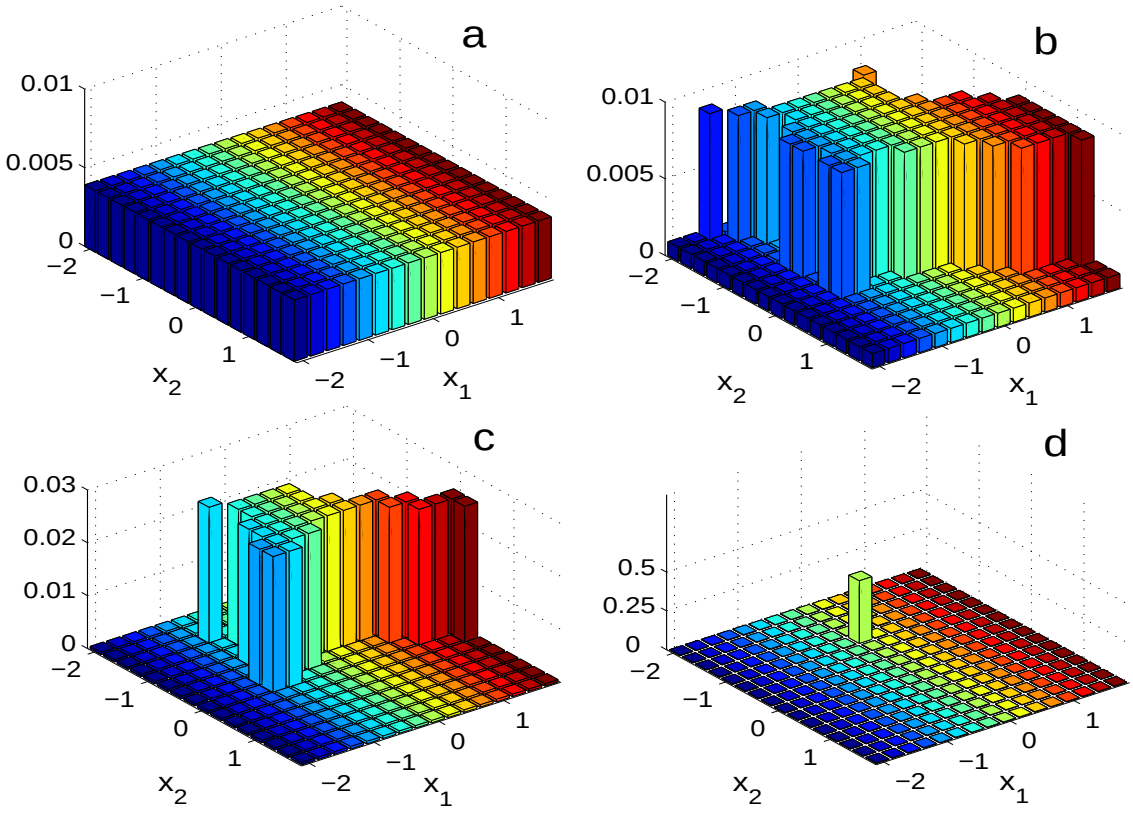

FIG. 3: Probability distribution of the state function before the measurement for the GP function. The panel a is the initial state corresponding to the superposition of all possible states, the panels b, c and d are the distributions of step 5, 10 and 13 respectively.

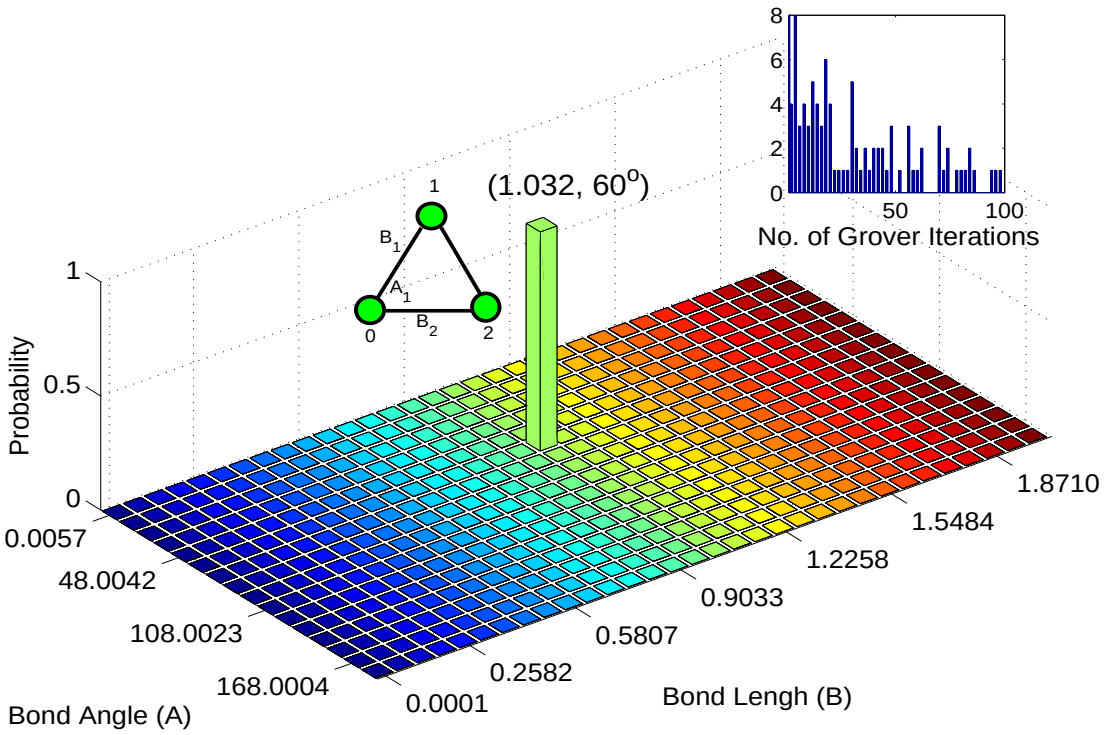

FIG. 4: Final probability distribution of the state function for LJ (N=3). The global minimum located at $B_1 = 1.1429, B_2 = 1.1429$ and $A_1 = 0.8977$. The top panel is the distribution of total measure step before reaching the global minimum for 100 search results. The global minimum and corresponding structure are also shown in figure.

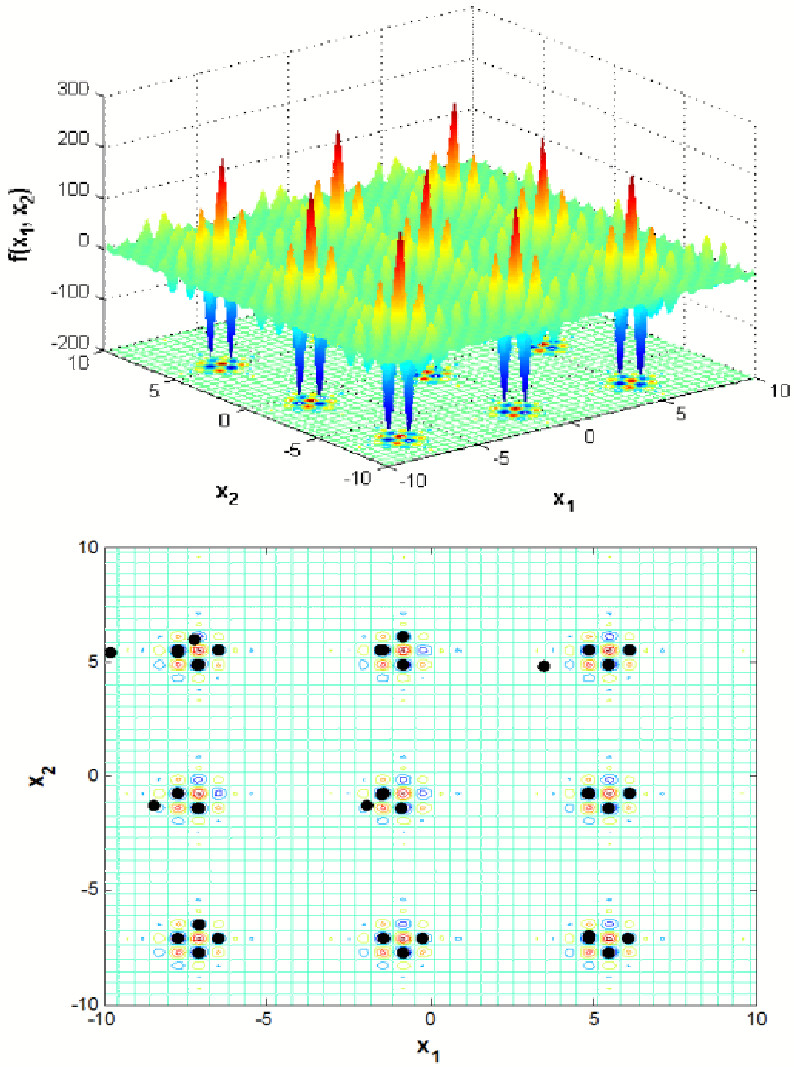

FIG. 5: The surface potential of Shubert function and final quantum search results. The top panel is the surface potential for the Shubert function with the range $x_{1,2} \in (-10, 10)$. The bottom panel is the contour of the function with the quantum search results. The black dots present the measurement results for all search steps.

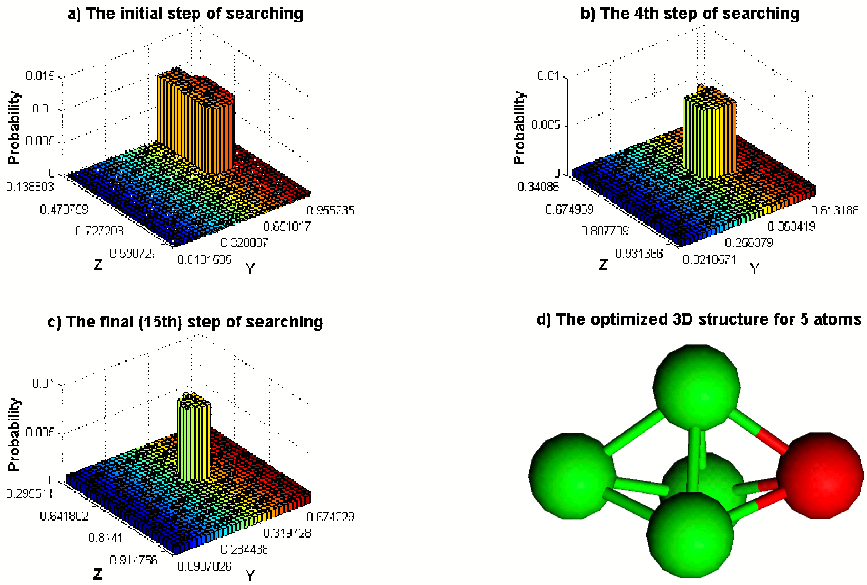

FIG. 6: Probability distribution of the state function for LJ cluster (N=4). The a, b and c are the steps during the searching. The global minimum energy is -5.9926 and the coordinates for the 4th atom are (0.0, 0.28444, 0.81344). Although there are many bars, they are quite close to each other. d is the optimized structure for 5 atoms cluster with the energy of -9.0952. The distances between the red and the green ones are 0.99, 0.99 and 1.00 separately.