Simulation and Analysis of the Knapsack Problem in Adiabatic Quantum Computation

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Introduction
Adiabatic Quantum Computation (AQC) has been a method of interest that sets out to solve many NP-hard and NP-complete problems. The time evolution of a quantum state $|\psi(t)\rangle$ is described by the Schrödinger equation
\[
i\hbar \frac{\partial |\psi(t)\rangle}{\partial t} = \hat{H}|\psi(t)\rangle
\]
where $\hat{H}$ is the Hamiltonian operator which describes the total energy of a physical system. Eigenvalues of the Hamiltonian describe the energy and the eigenvectors describe the state of the system. The adiabatic theorem states that for a slow transformation from $\hat{H}_{\text{init}}$ to $\hat{H}_{\text{final}}$ if the system is in the ground-state (lowest energy) of $\hat{H}_{\text{init}}$ it will also be in the ground-state of $\hat{H}_{\text{final}}$. AQC utilizes this for computation in the following steps:

• Create an initial state $|\psi(0)\rangle$ of qubits (two-state systems) which will be used to calculate the result of a computation.
• Start with an initial Hamiltonian, and vary it adiabatically such that it transforms into a final Hamiltonian whose ground-state encodes the solution to the problem.

An interpolation Hamiltonian $\hat{H}(t)$ is used to describe the transformation
\[
\hat{H}(t) = \hat{H}_{\text{init}}(1 - \frac{t}{T}) + \frac{t}{T} \hat{H}_{\text{final}} \quad T >> \frac{1}{\Delta E_{\text{min}}}^2
\]
The theorem holds if the transformation occurs slowly relative to the smallest difference between energy eigenvalues. AQC allows one to solve many NP optimization problems such as knapsack problem, number partitioning problem, etc. by constructing final Hamiltonians whose ground-states form a string of bits which we interpret as our solution to the problem at hand.

Motivation
AQC is a multi-disciplinary field spanning mathematics, computer science, and physics with it’s potential power drawing plenty of interest. The prospect of solving multiple famous NP optimization problems in complexity theory in a new context yet equivalent is promising and also with laboratory feasibility makes AQC an attractive subject. The Knapsack problem is one of particular interest as it has major application in economics, and the classical algorithm to solve the problem is widely popular and highly needed. We set out to explore the AQC method of solving the Knapsack problem, demonstrate correctness described in [2], and begin to quantify the problems complexity (difficulty) in AQC through many numerical experiments.

The Integer Knapsack Problem
The Knapsack problem is a NP-hard problem in combinatorial optimization that asks the following:

Given a set of $N$ objects, each with an integer weight $w_\alpha$ and cost $c_\alpha$, determine the objects to include in a collection so that the total weight is less than or equal to a given constraint weight $W$ and the total cost is optimized.

We let $x_\alpha$ be a binary variable denoting whether (1) or not (0) the object is contained in the Knapsack, and let $y_n$ for $1 \leq n \leq W$ denote an auxiliary binary value which is 1 if the final weight of the knapsack is $n$, and 0 otherwise. The final Hamiltonian whose ground state encodes the solution is
\[
\hat{H}_{\text{final}} = \hat{H}_A + \hat{H}_B^2
\]
\[
\tilde{H}_A = A(1 - \sum_{n=1}^{W} y_n)^2 + A \left( \sum_{n=1}^{N} n y_n - \sum_{\alpha} w_\alpha x_\alpha \right)^2
\]
\[
\hat{H}_B = -B \sum_{\alpha} c_\alpha x_\alpha \quad 0 < B \max(c_\alpha) < A
\]

Results
We demonstrated effective simulation of the above Hamiltonian, and verified the solution using a dynamic programming classical algorithm. Plotted and examined the ground state energies, first excited state energies, and also the energy gap through out the adiabatic transformation with
\[
s = \frac{t}{T}
\]

Methods
Using Mathematica we simulated the many NP problems. For construction of our initial and final Hamiltonians we used an Ising model formulation. A model consisting of $N$ discrete atomic spin variables, usually a lattice, from which we say we have $N$ qubits.

\[
\tilde{H}(\sigma_1^z, \ldots, \sigma_N^z) = - \sum_{\alpha=1} N n j_i \sigma_i^z - \sum_i h_i \sigma_i^z
\]

Here we have $\sigma^z$ the Pauli spin-$z$ operator, and in order to relate these with binary variables define the following:
\[
x_\alpha \equiv \sigma_\alpha^z + \frac{1}{2} \quad y_n \equiv \frac{\sigma_\alpha^z + 1}{2}
\]

So we have our problem Hamiltonian expressed in terms of spin-$z$ operators, and we construct our initial simply as
\[
\tilde{H}_{\text{initial}} = -h_0 \sum_{\alpha=1} N \sigma_\alpha^z \quad h_0 \approx \max(c_\alpha)
\]

These Hamiltonians are represented as large $2^N \times 2^N$ matrices, but with clever use of lists we can reduce the computational time with these objects. We simulated the problem Hamiltonian for multiple NP difficult problems by:

• Constructing the final Hamiltonian
• Solving for the ground-state
• Interpreting the ground-state as a solution string of bits

We then analyzed the full interpolation Hamiltonian $\tilde{H}(t)$ by solving for the ground-state energy and first excited energy (2nd lowest) at discrete time steps throughout the evolution in an attempt to study how time to solve the problem changes.

Discussion & Future Work
The Knapsack and other problem Hamiltonian do correctly encode the solution to the problem in their ground-states, which was tested with multiple cases with problem conditions and total number of qubits. The major issue encountered is computation time as the problems scale numerically by $2^N$. This fact has been our draw back when attempting to characterize the complexity of the problem. We would also like to study the effects of introducing a intermediate Hamiltonian, and use a non-linear interpolation to increase the minimum energy gap.

References