Geometric Phase Based Quantum Computation Applied to an NP-Complete Problem

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We present a new approach to quantum computation involving the geometric phase. In this approach, an entire computation is performed by adiabatically evolving a suitably chosen quantum system in a closed circuit in parameter space. The problem solved is the determination of the solubility of a 3-SAT Boolean Satisfiability problem. The problem of non-adiabatic transitions to higher levels is addressed in several ways. The avoided level crossings are well defined and the interpolation can be slowed in this region, the Hamiltonian can be scaled with problem dimension resulting in a constant gap size and location, and the prescription here is sufficiently general as to allow for other suitably chosen Hamiltonians. Finally, we show that with \( n \) applications of this approach, the geometric phase based quantum computation method may be used to find the solution to the 3-SAT problem in \( n \) variables, a member of the NP-complete complexity class.

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I. INTRODUCTION

Geometric phases have been proposed in the context of quantum computation, specifically in the proposal of fault-tolerant gates\(^1\)\(^2\)\(^3\). Here we discuss the possibility of performing an entire computation using a single application of the geometric phase. This approach uses the geometric phase phenomenon in conjunction with the adiabatic approach of Farhi, et. al. \(^4\). With a single application, the problem solved is determining the solubility of a Boolean satisfiability 3-SAT problem in \( n \) variables. With \( n \) applications of this approach, the geometric phase based quantum computation method may be used to find the solution to the 3-SAT problem itself. This last problem is of the NP-complete complexity class\(^2\).

II. ADIABATIC QUANTUM COMPUTATION

Farhi and coworkers\(^4\) presented an approach to quantum computation, Adiabatic Quantum Computation (AQC). The AQC approach involves an adiabatic interpolation from the ground state of an initial Hamiltonian \( (H_i) \) to the ground state of a final Hamiltonian \( (H_p) \) that encodes the solution to the problem of interest. The method involves adiabatically evolving the Hamiltonian \( H(z) = zH_i + (1-z)H_p \), while remaining in the ground state. In this approach, the problem solved is an NP-Complete problem, the 3-SAT Boolean Satisfiability problem containing \( n \) clauses in \( n \) variables. In our construction, each eigenstate of the \( N = 2^a \) dimensional \( H_p \) encodes a possible solution to the problem. The energy of each level of \( H_p \) corresponds to the number of clauses that have been violated by that possible solution, with the ground state \( E=0 \) level corresponding to a solution of the problem (0 violated clauses).

In the context of AQC, it was shown that in the case of a computationally hard instance of the 3-SAT problem, there exists a parameter region in which the spectrum is irregular, the spectral fluctuation distribution taking the form of the Wigner distribution\(^6\). In these regions, it was shown the interpolation was susceptible to non-adiabatic transitions from the ground state leading to an interpolation time that scales exponentially with problem size. The question arises whether similar AQC ideas could be implemented without interpolating through the irregular spectral region. Namely, by adding a second parameter dependence and interpolating around an appropriately modified final Hamiltonian, the geometric phase may be used and a computation performed without traversing through a problematic region.

III. GEOMETRIC PHASE

Berry\(^7\) noted that an eigenstate having a parameter dependence acquires, in addition to the familiar dynamical phase, a geometric phase (Berry phase) when the state is adiabatically evolved in a cyclic manner near a level degeneracy, termed a diabolical point. In the special case of a real Hamiltonian, cyclic evolution of the parameters produces a phase of \( \pi \), an overall sign change in the eigenstate being transported.

In the current approach, we use a construction similar to that of AQC - although instead of interpolating in one parameter (\( z \)) from \( H_i \) (\( z = 1 \)) to \( H_p \) (\( z = 0 \)), we use two parameters (\( x, z \)) and evolve the system in a closed circuit in the two dimensional parameter space about the point (0,0). To illustrate the method, we show how the Berry phase phenomena yields a test for solubility of the 3-SAT using \( H_p \) itself. \( H_p \) encodes a particular 3-SAT
problem instance in \( n \) variables and is constructed easily without a priori knowledge of the solution.\(^3\)

The Hamiltonian for this problem is constructed in such a way that a level degeneracy only exists at the point \((0,0)\) if a solution exists, and no level degeneracy exists if a solution does not exist. When the system is transported along the closed path encircling the point \((0,0)\), the state accrues a Berry phase if a solution exists and accrues no phase if a solution does not exist. Since the Hamiltonian is real, the accrued phase becomes \( \pi \) in the event of the existence of a solution.\(^7\)

IV. GEOMETRIC PHASE BASED QUANTUM COMPUTATION

The Hamiltonian we use for this problem is the direct sum of two Hamiltonians with the addition of interaction terms. The first Hamiltonian, \( H_a \), is constructed by adding \( \frac{2z}{4} \mathbb{I} \) to the \( H_p \) above: \( H_a = H_p + \frac{2z}{4} \mathbb{I} \), which has \( N = 2^n \) dimensions, where \( n \) is the number of variables in the 3-SAT problem instance. We construct \( H_a \) in such a way that relies on no a priori knowledge of which state is the solution. This definition of \( H_a \) is selected for certain simplifications, although many forms for \( H_a \) may be chosen. In fact, it is worth noting that \( H_a \) can be chosen to be \( H_p \) identically. In the following, we demonstrate the method for a soluble 3-SAT instance, with the generalization to non-solvable cases being straightforward. We arrange the basis states of \( H_a \) such that \( H_{p,i} \neq 0 \), \( 1 \leq i \leq N-1 \); and \( H_{p,N} = 0 \) (the solution state). The second Hamiltonian under consideration, in addition to \( H_a \), is the Hamiltonian \( H_b = -\frac{2z}{4} \mathbb{I} \), having dimension 1. We define the unperturbed Hamiltonian for the problem to be \( H^{(0)} = H_a \bigoplus H_b \). The unperturbed states \( \left| \psi_i \right\rangle, \left| \psi_a \right\rangle \) and \( \left| \psi_b \right\rangle \) are defined by:

\[
\begin{align*}
H^{(0)} | \psi_i \rangle &= H^{(0)}_{ii} | \psi_i \rangle = \left( \frac{z}{4} + H_{p,i} \right) | \psi_i \rangle, \quad (i < N) \\
H^{(0)} | \psi_a \rangle &= H^{(0)}_{NN} | \psi_a \rangle = \frac{z}{4} | \psi_a \rangle \\
H^{(0)} | \psi_b \rangle &= H^{(0)}_{N,N+1} | \psi_b \rangle = -\frac{z}{4} | \psi_b \rangle.
\end{align*}
\]

(1)

The final form for the Hamiltonian used in the geometric phase computation includes between \( H_b \) and all states of \( H_a \) through the additional parameter \( x \). In the unperturbed basis of Eq. (1), the general matrix representation of \( H \) that determines the 3-SAT solubility through the geometric phase phenomenon is

\[
\begin{align*}
H_{ii} &= H_{a,ii} + \frac{z}{4} + H_{p,ii} \quad (i < N) \\
H_{NN} &= H_{a,NN} + \frac{z}{4} + H_{p,NN} \\
H_{IN} &= H_{N,i} = x \quad (i < N) \\
H_{N+1,N+1} &= H_b = -\frac{z}{4},
\end{align*}
\]

(2)

where no particular problem instance has yet been chosen for \( H_p \).

The problem to be solved is determining the existence of a solution to the 3-SAT problem, or 3-SAT solubility. Evolving the ground state of Eq. (2) adiabatically in a closed circuit in the parameters \((x,z)\) results in one of two possible outcomes: no geometric phase in the case of no solution, or a geometric phase = \( \pi \) in the case of the existence of a solution to the 3-SAT problem.

Our numerical analysis uses the specific case of \( n=7 \), \( N=128 \). In addition, we choose a specific problem instance encoded by \( H_p \). We choose the highly degenerate case of \( H_p \) having a solution state (\( E=0 \)) and \( N-1 \) degenerate states (\( E=1 \)). Specifically, \( H_{p,i} = 1 \), \( i < N \) and \( H_{p,N} = 0 \). Although somewhat unrealistic from a problem standpoint, this case produces the smallest minimum gap size at the avoided level crossings (see Fig. 1g) where a non-adiabatic transition may occur, and so represents the worst case situation. This is discussed further below.

We start the system in the ground state of the system at \((x,z)=(0,1)\) (see Fig. 1h); this corresponds to the unperturbed state \( | \psi_b \rangle \), with the eigenvalue equation.
\[ H(0, 1) |\psi_b(0, 1)\rangle = -\frac{1}{4} |\psi_b(0, 1)\rangle. \] This state is then adiabatically evolved around the following parametric circuit: \((x, z) = (0, 1) \rightarrow (-1, 1) \rightarrow (-1, -1) \rightarrow (1, -1) \rightarrow (1, 1) \rightarrow (0, 1).\)

The approach may be viewed graphically in the following manner. The spectrum generated by Eq. (2) with the particular instance of \(H_p\) so defined is shown in Fig. 1. This choice of \(H_p\) produces a spectrum of three energy levels. The highest energy sheet has a degeneracy \((N-1)\), and the two lowest are nondegenerate. These lowest two energy sheets are responsible for the generation of the geometric phase.

If the 3-SAT problem encoded in \(H_p\) has a solution, then the ground state energy of \(H_p\) is 0, and there will be a degeneracy in the two lowest energy sheets at the origin in parameter space, \((x = 0, z = 0)\) (see Figs. 1c, 1d). When the ground state is evolved adiabatically in a closed circuit in parameter space about this point, this will give a Berry phase = \(\pi\) (see Figs. 1a, 1b, 1e, 1f).

If \(H_p\) is chosen such that no solution exists, there is no degeneracy, and the closed circuit does not encircle a diabolical point resulting in no Berry phase.

### V. AVOIDED LEVEL CROSSINGS

We now consider the problem of avoided level crossings: gap size and location.

In order to encircle the origin and accrue the Berry phase, the state must remain on the ground state energy sheet and not make a transition at the avoided level crossing (eg. by way of Landau-Zener transition) (see Fig. 1g). Simulations have shown that the avoided crossing gap size produced by Eq. (2) with \(H_p\) defined above decreases exponentially with increasing problem size. This is similar to difficulties in the AQC approach.

Even so, unlike other approaches, the location of the avoided level crossings is well defined, can be predicted to some extent, and the interpolation slowed in that region to prevent a level transition.

We gain insight into the Hamiltonian in Eq. (2) by calculating the approximate location of the avoided level crossings using perturbation theory. We consider the Hamiltonian in Eq. (2) with \(H_p\) defined above evaluated at \(z = -1\) and \(x\) small (corresponding to Fig. 1g). In this case, the unperturbed states are given by Eq. (11), taking \(x\) as the perturbation parameter. As \(x\) does not appear as a diagonal entry in the perturbation matrix, there is no first order correction. The second order correction is easily evaluated using the following unperturbed energies:

\[
\begin{align*}
E_i^{(0)} &= H_i^{(0)} = H_{ii} = 1 + \frac{3}{4} (i < N) \\
E_a^{(0)} &= H_{NN}^{(0)} = H_{NN} = \frac{3}{4} \\
E_b^{(0)} &= H_{N+1,N+1}^{(0)} = -\frac{3}{4}
\end{align*}
\]

We are interested in the second order perturbative corrections to \(E_a^{(0)}\) and \(E_b^{(0)}\), and we denote these energies by \(\Delta_a^{(2)}\) and \(\Delta_b^{(2)}\). The second order correction is given by the familiar formula

\[
\Delta^{(2)} = \sum_{n \neq m} \frac{|H'_{n,m}|^2}{E_n^{(0)} - E_m^{(0)}},
\]

where \(H'\) is the perturbation matrix containing only off diagonal terms equal to \(x\) \((H'_{N+1, i} = x, i < N)\).

We begin with \(\Delta_b^{(2)}\). The sum in this case can be split into two terms, one involving the \((N-1)\) states with energy \(E_{n}^{(0)}\) and one involving the state with energy \(E_{a}^{(0)}\).

In both cases the matrix element yields \(|H'_{b,n}|^2 = x^2(n \leq N)\). \(\Delta_b^{(2)}\) simplifies directly since \(H'_{a,i} = 0\) for \(i \neq N+1\), and the sum reduces to one term. Evaluation of these sums, using Eq. (4), yields

\[
\begin{align*}
\Delta_a^{(2)} &= -2x^2 \\
\Delta_b^{(2)} &= \frac{-2(N-1)x^2 - 2x^2}{2 + z}.
\end{align*}
\]

Inserting \(N = 128, z = -1\) into Eqs. (3) the energies to 2nd order are:

\[
\begin{align*}
E_a &= -\frac{1}{4} - 2x^2 \\
E_b &= \frac{1}{4} - 252x^2.
\end{align*}
\]

This is consistent with Fig. 1e and Fig. 1g. The differences are attributed to higher order perturbations, which become more pronounced with increasing \(x\). The intersection of these two parabolas gives the approximate location of the avoided level crossings to second order, \(x_{gap} \approx \pm 0.045\) (see Fig. 1g).

Earlier we chose the Hamiltonian \(H_p\) such that \(H_{p,i} = 1, i < N\) and \(H_{p,N} = 0\). The reason results from the perturbation theory calculation above: each level above 0 contributes to the level repulsion on state \(|\psi_b\rangle\) (see Fig. 1g). In this case for \(|x| < x_{gap}\), \((N-1)\) levels contribute to the level repulsion downward, and one state \(|\psi_a\rangle\) repels the state upward. In the general case, the sum is dominated by the closest levels. The \(H_p\) chosen has \(N-1\) levels located at the closest energy corresponding to a non-solution (\(E=1\)). This results in the situation having the strongest level repulsion, and in this sense represents the worst case situation in terms of the avoided level crossings. Other choices of 3-SAT problem instances for \(H_p\) result in weaker level repulsion.

### VI. SCALING

In addition to varying the interpolation speed near the avoided level crossings, the problem can be scaled with \(N\) such that the minimum gap size remains \(N\) independent for all problem sizes. We choose the scaling such that \(\Delta^{(2)}\) is \(N\) independent for large \(N\) in Eq. (4). This may be accomplished by scaling \(z\) or by scaling \(x\) appropriately. If \(z\) is chosen to scale with \(N\) such that \(z \rightarrow Nz\), the perturbative corrections \(\Delta_a^{(2)}\) and \(\Delta_b^{(2)}\) approach a constant.
for large $N$. Explicitly, the Hamiltonian containing this scaling is the following (cf. Eq. (2)):

$$
\begin{align*}
H_{ii} &= H_{a_{ii}} = z/4 + NH_{p_{ii}}, \quad 1 < i < N \\
H_{NN} &= H_{a_{NN}} = z/4 + NH_{p_{NN}} \\
H_{iN} &= H_{N_{i}} = x, \quad 1 < i < N \\
H_{kk} &= H_{b_{k}} = -z/4, \quad k = N + 1.
\end{align*}
$$

(6)

We have used $n=7$, $N=128$ in the numerical simulation of Eq. (6), with the results shown in Fig. 2 (cf. Fig. 1). The scaling was checked numerically for $3 \leq n \leq 9$. For these values, a constant minimum gap size ($\Delta_{gap} \approx 0.5$) and constant gap location ($x_{gap} \approx 0.0$) was found.

Analogously, we may choose $N$ scaling for $x$, such that $\Delta^{(2)}_a$ and $\Delta^{(2)}_b$ is approximately constant for large $N$. This may be accomplished by choosing $x^2$ to scale with $\frac{1}{\sqrt{N}}$, or $x \rightarrow \frac{1}{\sqrt{N}}\alpha$.

VII. SOLVING THE 3-SAT PROBLEM

The geometric phase based approach above determines the existence of a solution of the encoded 3-SAT problem in $n$ variables. We now show that upon repeated iterations of this approach, the solution to the 3-SAT problem may be searched for and the solution found in $n$ iterations.

As described above, if a solution state exists a geometric phase will be generated. Initially, each eigenvector $|\phi_i\rangle$ of $H_a$ encodes a possible solution to the 3-SAT problem. The collection of these eigenvectors forms the basis of $H_a$ and encodes all possible solutions. This represents the search space under consideration. From among this set we denote the state $|\phi_a\rangle$ as the solution state, if it exists.

Using this $H_a$, we construct $H$ as in Eq. (2). If the Berry phase is generated, then the solution state exists and the search is complete.

In the case of the existence of a solution, we then divide the search space in half, such that $H_a = H^{(1)}_a \bigoplus H^{(1)}_b$, with the basis of each subspace forming a solution space, each containing $\frac{N}{2}$ solutions.

Substituting $H^{(1)}_a$ for $H_p$, in Eq. (2), we construct a new Hamiltonian, $H^{(1)}$, having $\frac{N}{2} + 1$ dimensions. Performing the geometric phase approach with this $H^{(1)}$, the system either accrues a phase, in which case the solution state exists in the basis of $H^{(1)}_a$, or the system accrues no phase, implying the solution lies in the basis of $H^{(1)}_b$.

The Hamiltonian containing the solution state in its basis is then subdivided and used in the next iteration in a similar manner. For example, if $H^{(1)}_a$ generates a phase, then the solution exists in the basis of $H^{(1)}_a$ which is then subdivided into $H^{(2)}_a = H^{(2)}_a \bigoplus H^{(2)}_b$. Substituting $H^{(2)}_a$ for $H_p$ in Eq. (2), we construct a new Hamiltonian, $H^{(2)}$, having $\frac{N}{4} + 1$ dimensions. A single application of the geometric phase approach determines the solution to be in the basis of $H^{(2)}_a$ or $H^{(2)}_b$.

This iterative procedure is a sorting algorithm which halves the search space at each iteration, and locates the half containing the solution in a single evaluation (the geometric phase based procedure). Starting with $N$ states, the search is completed in $\log_2(N)$ evaluations. In the case of the 3-SAT problem in $n$ variables, the initial search space is $N = 2^n$ yielding the solution in $n$ evaluations.

VIII. CONCLUSION

We have illustrated a general approach to solving NP-complete problems using the geometric phase phenomenon in conjunction with the Adiabatic Quantum Computation method.

We first address the problem of whether a Boolean Satisfiability problem (3-SAT) is soluble - if so, the adiabatically evolved eigenstate acquires a geometric phase; if the problem is not soluble, the state does not acquire a phase.

The problem of avoided level crossings having small gap sizes is addressed in several ways. First, the crossings are isolated and well defined, and so the interpolation can be slowed in this vicinity. Second, the Hamiltonian can be scaled with $N$ (see Eq. (6)) to make the gap sizes independent of problem size. Third, as mentioned earlier,
the Hamiltonian (Eq. 2) is not the only choice which leads to a successful approach. This is a particularly simple construction, but there is a large degree of freedom in choosing the Hamiltonian that governs the approach. Other Hamiltonians can be found that also adhere to additional experimental requirements or parameters of a different problem.

Repeated iteration of this procedure results in a search of the set of N basis states encoding the possible solutions that completes in $\log_2(N)$ iterations. For a problem instance having $n$ variables, the solution of the 3-SAT can be found in $n$ iterations of the geometric phase based approach. In this way, we show the geometric phased based approach yields the solution to the 3-SAT, an NP-complete problem.

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