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Enclosure 1

Final Report: Gaitan—DAAD 19-02-1-0051

Frank Gaitan

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Contents

1 Problem Statement and Activities

The goal of our research has been to study the effects of decoherence on: (1) the performance of a geometric quantum computer; and (2) the quantum adiabatic search (QuAdS) algorithm of Farhi et. al. [1]. To achieve this goal we have studied the adiabatic dynamics of a quantum system coupled to a classical control field that contains noise. Such control fields are used to drive the dynamics of both a geometric quantum computer and QuAdS, with the noise acting to introduce decoherence. This study evolved into 3 research activities which were carried out concurrently.

Geometric Quantum Computer: This activity studied how noise, introduced through the control field that drives the dynamics of a geometric quantum computer (GQC), would cause a dephasing of the off-diagonal elements of a GQC's density matrix (decoherence). We were especially interested in seeing whether this effect would: (1) for a single qubit, lead to a dephasing of the observable consequences of the adiabatic geometric phase; and (2) for the 2-qubit controlled phase gate used in a GQC, lead to dephasing of entangled states. This activity was successful and its results are discussed in section 2. Study of other dynamical models which introduce decoherence into the dynamics of a GQC will be carried out in collaboration with Melique Hoover who has recently joined my research group. This activity is expected to form a substantial portion of his PhD thesis work.

Twisted Rapid Passage: While examining the decoherence of a GQC, I stumbled onto very interesting quantum interference effects that occur during a type of non-adiabatic rapid passage which we have called twisted rapid passage (TRP). TRP causes a qubit to pass through resonance multiple times during a single TRP sweep, and in combination with the temporal phase coherence of the quantum state, leads to controllable quantum interference effects which allow for direct control over qubit transitions. This activity has looked into whether TRP could be used to produce a universal set of non-adiabatic quantum gates whose error probability falls below the accuracy threshold needed for the set to be used as part of a fault tolerant scheme of quantum computation. This work was not part of our ARO proposal, but it was discovered while carrying out activities associated with that proposal. These quantum interference effects have the potential to significantly impact efforts to build highly reliable quantum logic gates. Building such highly reliable quantum gates is the essential task to be accomplished if a working quantum computer is to be built. Consequently, we decided to pursue this potentially high payoff application of TRP. To do this, we numerically simulate the non-adiabatic Schrodinger dynamics generated by TRP. These simulations allow us to assess how well TRP is able to implement the universal set whose elements are the Hadamard, Phase, $\pi/8$, and CNOT gates. The error probability for each gate is determined and compared with the accuracy threshold needed for fault tolerant quantum computing. I carried out the first phase of this activity, while the remainder of this work has been done in collaboration with my graduate student Ran Li. This work will form the bulk of her PhD thesis work. The results of this activity (to date) are reported in section 2.

Noisy Quantum Adiabatic Search: We simulated the effects of decoherence on the QuAdS algorithm of Farhi et. al. [1]. Their work suggests that an isolated quantum computer might be able to solve an NP-Complete computational problem in polynomial-time. If true, this would indicate that the computational complexity classes P and NP are the same on a quantum computer, with enormous consequences for theoretical computer science. Our aim was to examine the robustness of this algorithm to noise. We simulated application of QuAdS to finding solutions to instances of the NP-Complete problem N-Bit Exact Cover 3 (EC3) in the presence of noise. The goal of these simulations being to determine how rapidly the exponent b in the scaling relation $\overline{T}(N) = aN^b$ varied with noise power and polarization. Here $\overline{T}(N)$ is the algorithm's median runtime and N is the number of bits in the EC3 instance. This variation would provide a direct measure of the robustness of QuAdS to noise, and would also determine which noise polarizations are most problematic for the algorithm. Our simulation code has been run on the TeraGrid cluster through time allotted by the National Center for Supercomputing Applications in Urbana, IL. This activity has been successful and further simulation runs are planned to begin in May, 2005. See section 2 for a discussion of our results.

The above activites have led to a number of invited and contributed talks.

- Invited talk at the *Xth International Conference on Quantum Optics, 2004* in Minsk, Belarus: May 30-June 3, 2004.
- Invited talk at the *34th Winter Colloquium on the Physics of Quantum Electronics* in Salt Lake City, Utah: January 4-8, 2004.
- Invited talk at the *Theory in Quantum Computing* meeting in Harper's Ferry, West Virginia: June 9-10, 2003.
- Invited talk at the Department of Physics, Indiana University, Bloomington, Indiana: April 12, 2002.
- Talk presented at the *Army Research Office Quantum Computing Program Review* in Nashville, Tennessee: August 18-22, 2003.
- Talk presented at the *Army Research Office Quantum Computing Program Review* in Nashville, Tennessee: August 19-23, 2002.
- Contributed talks presented at the APS March Meeting in 2002 and 2004.

2 Project Results

2.1 Findings

Geometric Quantum Computer: We examined the adiabatic dynamics of a quantum system coupled to a noisy classical control field. A stochastic phase shift was shown to arise in the off-diagonal elements of the system's density matrix which can cause decoherence. We derived the condition for onset of decoherence, and identified the noise properties that drive decoherence. We showed how this decoherence mechanism causes: (1) a dephasing of the observable consequences of the adiabatic geometric phase; (2) the dephasing of entanglement in maximally entangled states such as the Bell states; and (3) the loss of computational efficiency of the Shor factoring algorithm when run on a sufficiently noisy geometric quantum computer. A paper describing this work has been submitted to Physical Review Letters.

Twisted Rapid Passage: As mentioned in section 1, while examining the decoherence of a geometric quantum computer, I stumbled onto very interesting quantum interference effects that arise during a type of non-adiabatic rapid passage that I have called twisted rapid passage (TRP). Using analytical and numerical studies, we showed that TRP causes a quantum system to pass through resonance multiple times during a single TRP sweep. The time separating the multiple resonances can be altered by varying the TRP sweep parameters, producing controllable quantum interference effects which allow for direct control over qubit transitions. I worked out the original theoretical analysis and experimental predictions in reference [2]. The predictions were confirmed experimentally using liquid-state NMR by Zwanziger, Werner-Zwanziger, and Gaitan [3]. This work led to invited talks at the: (1) 34th Winter Colloquium on the Physics of Quantum Electronics, Salt Lake City, Utah, January 4-8, 2004; and (2) Xth International Conference on Quantum Optics 2004, Minsk, Belarus, May 30-June 3, 2004. The content of these talks appears in Gaitan [4]; and R. Li and F. Gaitan [5], respectively. In collaboration with my research student Ran Li, we have some interesting findings which are almost ready to submit for publication, and which I will preview here. We have been examining whether TRP could be used to implement a universal set of quantum logic gates which: (i) are non-adiabatic; and (ii) have error probabilities which fall below the accuracy threshold needed for the set to be used as part of a fault-tolerant scheme for quantum computation. Why this is important will be discussed in section 2.2. We have found that TRP can produce the following universal set of quantum gates: Hadamard, phase, $\pi/8$, and CNOT. TRP can implement all gates in this set non-adiabatically, and for all gates except the CNOT, TRP sweep parameters have been found which produce gate error probabilities that fall below the accuracy threshold. The simulation code for the CNOT gate is still not sufficiently numerically stable to allow us to reach the level of precision needed to determine whether TRP can implement a non-adiabatic CNOT gate that beats the accuracy threshold. We are working hard to stabilize the CNOT code and hope to complete this work in the coming months.

Noisy Quantum Adiabatic Search: We have recently completed the most detailed simulation of the quantum adiabatic search algorithm in the presence of noise that has been carried out to date. The algorithm was applied to the NP-Complete problem N-Bit Exact Cover 3 (EC3). The noise was assumed to be Zeeman-coupled to the qubits and its effects on the algorithm's performance was studied for various levels of noise power, and for 4 different types of noise polarization. We determined the scaling relation between the number of bits N (EC3 problem-size) and the algorithm's noise-averaged median run-time $\overline{T}(N)$. Clear evidence was found of the algorithm's sensitivity to noise. Two fits to the simulation results were done: (1) power-law scaling $\overline{T}(N) = aN^b$; and (2) exponential scaling $\overline{T}(N) = a\left[\exp(bN) - 1\right]$. Both types of scaling relations provided excellent fits. The scaling parameters a and b varied with noise power, and with the type of noise polarization. This sensitivity of the scaling exponent b to noise polarization allows, for the first time, a determination of which noise polarizations are most problematic for quantum adiabatic search. A paper describing this work has been submitted to Physical Review A. A discussion of the significance of these results is given in section 2.2.

2.2 Contributions Within Discipline

As described in section 1, our work in connection with this grant has fallen into three areas of activity. I discuss below how each has contributed to progress in physics (discipline) and in quantum computing (field).

Geometric Quantum Computer: The system of interest is a quantum system coupled to an adiabatically-evolving noisy classical control field. We suspected that such a control field would lead to decoherence, and specifically, to dephasing of the observable consequences of the adiabatic geometric phase. Since many quantum systems in physics and chemistry develop adiabatic geometric phases, such a decoherence mechanism would have impact both within our discipline (physics), as well as outside it (chemistry). One of the fundamental questions we wanted to address was, in quantum systems that develop an adiabatic geometric phase, what type of external disturbance would cause the observable consequences of this phase to disappear? We were drawn to this problem by past work we had done on vortices moving in superconducting thin films where the adiabatic geometric phase caused a force to act on a moving vortex which was seen to disappear at sufficient high impurity concentration and/or temperature. Another quantum system where this type of decoherence might be important is a geometric quantum computer where the adiabatic geometric phase is used to encode conditional phase shifts. We suspected that this decoherence mechanism would impact the performance of a geometric quantum computer. We found, as part of our activity associated with this grant, that a noisy classical control field does cause decoherence, and the mechanism by which this occurs is as follows. For systems for which the dephasing time T_2 is much shorter than the thermal relaxation time T_1 (the common case), we showed that the noisy control field causes a stochastic phase shift to appear in the off-diagonal elements of the quantum system's density matrix. Averaging over the noise causes these off-diagonal elements to be strongly suppressed (decoherence). We derived the condition for the onset of decoherence and identified the noise properties that drive this decoherence. We showed how this decoherence causes the disappearance of the observable consequences of the adiabatic geometric phase. To the best of our knowledge, this is the first time anyone has tried to understand how the effects of the adiabatic geometric phase are washed out by noise present in the control field that generates this phase. We also showed how this mechanism leads to loss of quantum entanglement, and how it causes the Shor factoring algorithm to loose its computational efficiency when it is run on a sufficiently noisy geometric quantum computer. This is also the first time such an analysis has been done.

Twisted Rapid Passage: During the course of examining the decoherence of a geometric quantum computer, we discovered very interesting quantum interference effects that arise during a type of non-adiabatic rapid passage that we have called twisted rapid passage (TRP). It was found that TRP can cause a qubit to pass through resonance multiple times during a *single* TRP pulse. The time separating successive resonances can be altered by varying the TRP pulse parameters, leading to controllable quantum interference effects that allow for highly precise control of a quantum state [2]. Experimental confirmation of these quantum interference effects was done using liquid-state NMR, with excellent agreement between theory and experiment [3]. I have also worked out how to generate TRP pulses using electric fields, opening the door to using this class of pulses to precisely control the electronic states of atoms and molecules. We have also found that we can use TRP to generate the following universal set of quantum gates: Hadamard, phase, $\pi/8$, and CNOT. TRP is able to implement them non-adiabatically, and as pointed out in section 2.1, pulse parameter values have been found for all these gates (except the CNOT) which yield quantum operations with error probabilties that fall below the accuracy threshold for the gates to be used as part of a fault-tolerant scheme for quantum computation. The simulation code for the CNOT gate is still not sufficiently numerically stable to allow us to reach the level of precision needed to test whether TRP can produce a non-adiabatic CNOT gate that beats the accuracy threshold. Efforts to stabilize this code are underway. In physics and chemistry, generally, and in quantum computing, specifically, any technique which allows for highly precise control of atomic and molecular systems is highly desired. TRP pulses show real promise for providing a means to achieve such precise control. In fact, in the context of quantum computing, the degree of precision needed is quantified by the accuracy threshold for fault-tolerant quantum computing. TRP pulses are the only class of *non-composite* pulses that we are aware of that can produce a non-adiabatic universal set of quantum gates, and which we believe will be able to do this with error probabilities that fall below the accuracy threshold. The task of producing such a universal set of quantum gates is one of the major challenges facing the field of quantum computing that must be met if an actual working quantum computer is to be built. TRP shows strong potential for providing a means to meet this challenge. Because each gate in this universal set is produced be a specific choice of the TRP pulse parameters, experimentalists can focus their efforts on producing this one class of pulses well to be able implement a universal set of quantum gates which achieve the accuracy threshold. In summary, TRP shows strong potential to significantly impact the field of quantum computing. It also has the potential to strongly impact efforts to control quantum states in atomic and molecular physics, and in quantum chemistry. We will continue working to develop applications of this class of control pulses.

Noisy Quantum Adiabatic Search: In 2001, Farhi and co-workers [1] applied the quantum adiabatic search (QuAdS) algorithm to the NP-Complete problem N-Bit Exact Cover 3. They simulated the algorithm on a classical computer and found that their results for the median runtime $\overline{T}(N)$ for the algorithm to succeed versus the number of bits N could be fit with a quadratic scaling relation: $\overline{T}(N) \sim N^2$. Because a quantum computer cannot be efficiently simulated on a classical computer, their simulations were restricted to $7 \leq N \leq 20$. They noted that, should this scaling behavior persist to large N, quantum adiabatic search would provide a polynomial-time algorithm for an NP-Complete problem. This would imply that the computational complexity classes P and NP would be equal on a quantum computer, suggesting that quantum computers might be more powerful than their classical counterparts. Their simulations assumed that the quantum computer was perfectly isolated from noise. We decided to examine the robustness of this algorithm to noise. To that end, we carried out the most detailed simulation of the QuAdS algorithm in the presence of noise that has been done to date. We also applied the algorithm to Exact Cover 3. The noise was assumed to Zeeman-couple to the qubits and its effects on the algorithm's performance was studied for various levels of noise power, and for 4 different types of noise polarization. As noted in section 2.1, we determined the scaling relation between the number of bits N and the algorithm's noise-averaged median runtime $\langle T(N) \rangle$. Clear evidence was found of the algorithm's sensitivity to noise. Power-law and exponential fits were done to the simulation results. This was the first time such a comparison of fits was carried out. Both types of scaling relations provided excellent fits. This is surprising as power-law scaling suggests that the QuAdS algorithm might provide a polynomial-time algorithm for an NP-Complete problem, while exponential scaling indicates that it does not. Farhi et. al. [1] never carried out a comparison exponential fit to their data. Exponential scaling also provides an excellent fit to our *noiseless* simulation results. The ambiguity related to which of these two scaling relations provides the best fit to the data is a consequence of the small size of the set of simulation results. This small size is itself due to the computational inefficiency of simulating a quantum computer on a classical computer. One will need to be allocated substantial amounts of supercomputer time to be able to expand the size of this data-set beyond what we have so far managed to do. Our results raise the question of just how definitively the simulation results for QuAdS found to date imply that this algorithm gives a polynomial-time algorithm for an NP-Complete problem. At sufficient noise power one expects a quantum computer to crossover to classical behavior, and the NP-like exponential scaling to provide a better fit than the P-like polynomial scaling (assuming $P \neq NP$). We may already be seeing first signs of this crossover in our current results for noisy QuAdS, though further simulations at higher noise power are needed to properly address this question. Our results clearly impact the question of whether a quantum computer is more powerful than a classical computer, a fundamental question for both quantum computation and for theoretical computer science. We will be applying for a large scale allocation of time on the TeraGrid cluster through the Partnership for Advanced Computation Infrastructure (PACI) to push our simulations to higher noise power levels and larger number of bits N to see whether we can unambiguously observe the above crossover.

2.3 Contributions Outside Discipline

Contributions made to other disciplines by activites associated with this grant are discussed below. Please see sections 1 and 2 for background discussion concerning the remarks below.

Geometric Quantum Computer: The decoherence mechanism produced by a noisy classical control field used to drive a quantum system that develops an adiabatic geometric phase applies to all such systems for which the dephasing time T_2 is much less than the thermal relaxation time T_1. Many such systems are known in physics and in quantum chemistry. Our work on this mechanism should be relevant to areas of quantum chemistry that work with such systems (e. g. NMR and ESR).

Twisted Rapid Passage: Over the past 15 years there has been a significant effort in quantum chemistry to control the dynamics of atoms and molecules. Twisted rapid passage (TRP) pulses allow for highly precise control of the electronic and magnetic states of these systems and so should be of interest to researchers in quantum control, as well as to NMR and ESR chemists. In fact, TRP was first observed experimentally using liquid-state NMR. I have recently understood how to generate TRP pulses using electric fields. I will begin reaching out to chemists working on ESR and quantum control in an effort to bring the merits of TRP pulses to their attention and to interest them in adding it to their experimental toolbox.

Noisy Quantum Adiabatic Search: Our work here is connected with efforts that aim at determining whether quantum computers are more powerful than classical computers. Results from this activity should have a direct impact on theoretical computer science.

3 Publications and Reports

3.1 Peer-Reviewed Publications

1. R. Li and F. Gaitan, "Controlling Qubits Transitions Through Quantum Interference During Non-Adiabatic Rapid Passage", to appear in *Optics and Spectroscopy*

2. F. Gaitan, "Controlling Qubit Transitions During Non-Adiabatic Rapid Passage Through Quantum Interference", J. Mod. Optics **51**, 2415 (2004).

3. F. Gaitan, "Temporal Interferometry: A Mechanism for Controlling Qubit Transitions During Twisted Rapid Passage with a Possible Application to Quantum Computing", *Phys. Rev. A* **68**, 052314 (2003).

4. J. W. Zwanziger, U. Werner-Zwanziger, and F. Gaitan, "Non-Adiabatic Rapid-Passage", *Chem. Phys. Lett.* **375**, 429 (2003).

3.2 Submitted Manuscripts

1. F. Gaitan, "Simulation of Quantum Adiabatic Search in the Presence of Noise", submitted to *Phys. Rev. A*.

2. F. Gaitan, "Noisy Control, the Adiabatic Geometric Phase, and Destruction of the Efficiency of Geometric Quantum Computation", submitted to *Phys. Rev. Lett.* .

4 Personnel

4.1 Training and Development

The following students have worked on the activities associated with this grant.

Torrance (T. J.) Flynn: T. J. worked with me for two semesters. This was his first experience doing research. He was a graduate student in computer science who was intrigued by the idea of a quantum computer. He had no background in quantum mechanics or quantum computing so I gave Saturday morning lectures explaining the basics of these topics which he and Gabe Shaughnessey (see below) attended. T. J. contributed to the early writing of simulation code. After two semester's, T. J. found a summer internship at Oak Ridge National Laboratory. At the end of the summer, T. J. was offered a programming job at Oak Ridge which he accepted.

Gabe Shaughnessey: Gabe was an undergraduate student in physics and he worked with me for two semesters. He had previously worked with an experimental research group in the Physics department here at Southern Illinois University (SIU). Working on this quantum computing project, however, was his first exposure to doing research in theoretical physics. Gabe sat in with T. J. Flynn on the Saturday morning lectures (see above) which aimed to explain the basics of quantum mechanics and quantum computing. Gabe contributed to the early writing of simulation code. After two semesters, Gabe graduated from SIU and went on to do graduate work at Cornell University.

Ran Li: Ran has been working with me for two years. She is midway through her PhD thesis work. She has been helping me develop applications for twisted rapid passage control pulses (see sections 1 and 2.1). The focus has been to determine whether twisted rapid passage can be used to implement a universal set of quantum gates that are: (i) non-adiabatic; and (ii) have error probabilities that fall below the accuracy threshold needed for the set to be used as part of a fault-tolerant scheme for quantum computing. I anticipate that she'll be ready to graduate in another 24 months.

Melique Hoover: Melique did a reading course with me on quantum computing while he was an undergraduate double-major in physics and electrical engineering at SIU. He graduated in May, 2004 and began graduate studies in August, 2004 here at SIU. He is the recipient of a fellowship from the NSF program *Bridge to the Doctorate* which aims to increase the number of minority students receiving doctorates in science, technology, engineering, and mathematics. He has been focusing on classwork during his first academic year (Fall, 2004 and Spring, 2005) and will begin doing research with me this summer. I have also had him keep abreast of the work I have been doing with Ran Li. I have given him papers to read on the adiabatic geometric phase, geometric quantum computers, and decoherence. He will work with me examining a number of models of environments that introduce decoherence into the dynamics of a geometric quantum computer. This work is expected to form the bulk of his PhD thesis work.

4.2 Contributions to Education

In this section I will describe how the activities associated with this grant have contributed to the development of human resources in science.

1. Providing opportunities for research in science.

The activities associated with this grant have provided opportunities for 4 students to do research in the frontier field of quantum computing. Three were/are graduate students (Ran Li, Melique Hoover, and T. J. Flynn), and the fourth was an undergraduate (Gabe Shaughnessey). All 4 had no previous experience doing research in theoretical physics, although Gabe had previously worked in an experimental physics group doing research on carbon nanotubes. T. J. and Gabe worked with me for 2 semesters. T. J. moved on to a job at Oak Ridge National Laboratory, and Gabe to graduate study at Cornell University.

Ran has worked with me as a graduate research student for two years and is approximately halfway through her PhD thesis work. Melique is finishing his first year of graduate school and will begin doing research this summer (2005).

2. Improving performance, skills, or attitudes of members of under-represented groups that will improve their access to or retention in research and teaching careers.

Both Ran Li and Melique Hoover are members of under-represented groups in science. Ran is a woman and Melique is a black American. Melique is currently funded through the NSF program *Bridge to the Doctorate* which aims to increase the number of minority students receiving doctorates in science, technology, engineering, and mathematics. Both are expected to complete PhD degrees, and to be qualified to teach physics at a 4-year college or to work in industry. Both have expressed interest in trying to land postdoctoral fellowships upon graduating, though success along this route will depend on factors that are hard to predict at this time. Neither had considered research in physics as a career prior to involvement in the activities of this grant. Their research work on these activities will form the bulk of their PhD thesis work, leading to their doctoral degrees, and (one hopes) to careers in physics doing research and/or teaching.

5 Bibliography

1. E. Farhi et. al. , *Science* **292**, 472 (2001).

2. F. Gaitan, *Phys. Rev. A* **68**, 052314 (2003).

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