Award Number:1037992
Project Title: Centers for Chemical Innovation, Phase I: Quantum Information and Computation for Chemistry
Report Type: Final Project Report
PI: Sabre Kais
Awardee: Purdue University
Program Officer Name: Katharine J. Covert
Program Officer Email:kcovert@nsf.gov
Program Officer Phone Number:(703)292-4950

Quantum Information for Quantum Chemistry (QIQC)

PI: Sabre Kais (Purdue)
Alan Aspuru-Guzik (Harvard)
Ken Brown (Georgia Tech)
Daniel Lidar (USC)
Peter Love (Haverford)

The Center of Quantum Information for Quantum Chemistry brought together leaders in the frontier area of chemical research: experts in theoretical chemistry and experts in quantum information processing to work in close collaboration to develop quantum algorithms and research structure that can respond to experimental realization of quantum computers and the quantum information revolution in a manner that would be beyond the scope of individual investigators

In the early twentieth century, the new field of quantum chemistry was formed by the interaction of chemists, physicists, applied mathematicians and computer scientists. This project aims to **catalyze the creation of a new field** from the intersection of modern theoretical physical chemistry with the twenty-first century ideas stemming from the fields of physics and computer science, which are rooted in quantum information theory. We pursued immediate applications of the ideas in this field to a) understand the role of quantum information in molecular systems; b) construct quantum algorithms and quantum information processors for chemistry; c) re-envision quantum spectroscopy and control; and d) impact other fields such as chemical engineering and scientific computing.

*contact email: kais@purdue.edu

In Phase I, we have made important steps towards reaching the aspirations of the QIQC center, as clearly articulated in our mission statement:

> **Mission Statement:** To understand chemistry from the viewpoint of quantum information, to develop techniques and quantum computers to solve important problems in chemistry, and to inspire a new generation of scientists with the power of technology built on quantum effects.

These step have been accomplished by a commitment to research excellence and a desire to spread quantum information to the broader chemistry community.

Summary of Major Research Activities/Accomplishments

QIQC Center research has been very active in Phase I. The group has already published 42 papers in top rated, peer-reviewed journals. In addition to these paper advancing the field of quantum chemistry and quantum information, we have also produced a number of review articles that broaden the accessibility of this new area. Center Director Sabre Kais has also edited a special issue of Advanced Chemical Physics for Quantum Information in Quantum Chemistry. The motivation for the special issue may be summarized by two questions. First, what can chemistry contribute to quantum information? Second, what can quantum information contribute to the study of chemical systems? Of the 17 total chapters, six were contributed by members of the QIQC.

This research advances were made possible by the Centers support for undergraduate students, graduate students, and postdocs. As a center we are particularly proud of the contribution of undergraduates to the research program and they have co-authored papers. These results stems directly from the undergraduate research program piloted with students from Haverford.

Our main findings are in three areas, representing the three goals of the Phase I center. The first area is *quantum information for chemical systems* in which we seek to use insights and techniques arising from our expertise in both chemistry and quantum information to advance the field of chemistry. The second area is *quantum algorithms for quantum chemistry*, in which we seek new techniques by which future quantum computers can be used to address problems in chemistry that are too difficult for any conceivable classical computer to solve. In this area we also seek to implement early examples of these algorithms on experimental quantum computers that exist now. The third area is *quantum control for quantum simulation* in which we address issues of protection of quantum algorithms for chemistry from the effects of errors. Our progress in these three areas can be summarized as follows:

In the area of *quantum information for chemical systems* we have focused on energy transport in light harvesting complexes from the point of view of open quantum systems, entanglement and quantum process tomography. We have developed new simulation techniques, have developed new techniques for computing entanglement and applied them to the FMO system, and we have developed new experimental protocols based on reinterpreting nonlinear

optical spectroscopy in terms of a standard technique in quantum information science: Quantum Process Tomography. We have also exploited the emergence of large commercial adiabatic quantum optimization devices to address lattice-model protein folding problems. Over the period of the Phase I grant this hardware has progressed sufficiently that this effort, which began in the area of quantum algorithms for quantum chemistry, may now be considered as an application of quantum information technology for chemical systems, as we explain in detail below.

In the area of *quantum algorithms for quantum chemistry* we have made significant progress on elucidating, optimizing and implementing ground state algorithms, in particular electronic structure problems on quantum computers. We have also developed methods based on quantum algorithms for solving linear equations, specifically Poisson's equation. Relative to the state of quantum algorithms for quantum chemistry at the start of the CCI, we have found orders of magnitude improvement in the length of the algorithm (circuit depth) by finding more efficient ways to emulate the wavefunction evolution on a quantum computer.

In the area of *quantum control for quantum simulation* we have extensively developed and investigated dynamical decoupling methods. We have also collaborated to see these methods implemented experimentally in diamond at room temperature, and to protect a quantum memory in NMR. We have investigated use of the quantum Zeno effect for control, developed a general framework for compensated pulse sequences, and worked on more easily simulated models of quantum errors. These improvements can be extended to a number of physical implementations of quantum computers from NMR to ion traps.

Summary of Integrative QIQC Activities

Education

Phase I has resulted in successful education programs at the high-school, undergraduate, and graduate levels. At the high-school level, we focused on teacher workshops and development days that provided materials for high-school teachers to add quantum mechanics to their curriculum. At the undergraduate level, our flagship program was the research opportunities for Haverford undergraduates. At the graduate level, the center has provided a number of opportunities for the career development from workshops on innovation to networking opportunities at QIQC sponsored conferences.

K-12 Education

In July 2011, Prof. Brown organized a professional development day for physical science teachers in the Atlanta area in coordination with our CCI and the DAMOP annual meeting. Teachers were given materials to take back to their classroom and lead through one exercise on diffraction and one exercise on laser light lead by Dr. Heide Doss. Aaron Buikema, a Haverford undergraduate visiting the Brown lab as part of the CCI, helped organize materials and participated in the laser workshop with the teachers.

Figure 1: Quantum information and quantum computing on NanoDays, May 2012.

In February 2012 the center hosted a High School Conference intended to introduce the field to the lay public Organized by Bill Bayley and Sabre Kais. The conference covered topics such as: benefits of quantum technology, quantum mechanics in nature, and introductions to the physical concepts of quantum computers. Also taught and given to the teachers was the game Quantum Tic-Tac-Toe - a game which exemplifies concepts within quantum mechanics, such as: superposition, collapse, and entanglement; this was intended to give the teachers something which they could take back to the classroom and teach their students as a means of inspiring interest. Since then Nick Mack, from McCutcheon High School, Lafayette, Indiana, joined the center for his summer project on using the Quantum Tic-Tac Toe game in high school. He is working at assisting the generation of a workable code for the game and testing it. The intent of his presence is both of have him work on this project and teach him the necessary concepts in quantum mechanics.

QIQC members participated NanoDays events on May 8th, 2012. NanoDays is a Purdue hosted event for all regional school student from 5th grade to high school. Ross Hoehn spoke to a collected group of High School students about introductory topics in quantum mechanics such as: superposition, entanglement and collapse - also showed them the game Quantum Tic-Tac-Toe. Other group members assisted in the variously hosted events for the local school students.

Undergraduate Education

The most successful program has been the pilot undergraduate research program where undergraduate students from Haverford and Bryn Mawr are paired with a mentor at another QIQC institute. So far, eleven undergraduate students have participated in the program, which is organized by Peter Love. Three students, Sam Rodriques, Alex Vargo, and Susan Xia, have co-authored papers with their respective mentors. Sam is starting graduate school at UC Berkeley, Alex is interning in the quantum information group at IBM, and Susan is a senior at Bryn Mwar. The success of our student research program across all participating institutions lays the foundation for an expanded program in Phase II which can draw both from the expanded pool of students available to a larger center and to specific partners that serve the diversity and outreach goals of the center.

Course Development: In Spring 2011 Peter Love taught Advanced Quantum Mechanics at

Haverford College. A number of aspects of this course were additions to more standard treatments pf the subject, including a presentation of supersymmetry in one-dimensional quantum mechanics and treatment of the Hydrogen atom from a ladder operator perspective. In order to help disseminate these aspects of the course Love recorded podcasts of a number of the lectures in the course. These, together with the lecture notes are posted on the CCI website.

Figure 2: Explaining quantum information and computing at Science Cafe, June 2012.

Graduate Education

Professional Development: CCI Grad students attended and participate in the number of conferences organized by the CCI. The Winter School in particular gave the students an opportunity to network with leaders in the field and attend tutorials on the basic elements of quantum information.

Innovation Education: The center hosted CCI Research to Innovation (R2I) Workshop on Monday, April 23rd, 2012. Sabre Kais hosted, at Purdue, the NSF R2I workshop in which attendees focused on several selections from the QIQC's research goals and discussed means by which these goals can be grown into marketable products, companies can be formed and benefit from the QIQC's works and how to take such goals to market.

Course Development: Sabre Kais taught quantum information for quantum chemistry at Purdue University, the course attracted students from all science and engineering departments. Daniel Lidar taught a graduate level course on quantum error correction.

Public Outreach

Sabre Kais, Center Director, and graduate student Ross Hoehn at the Center discussed quantum computers at the Science Cafe series, 6:30-8 p.m., at K Dees Coffee & Roasting Co. Sabre Kais speaks to a general public audience about the use of quantum technology and how it can benefit the public through secure communications and secure computing technologies; afterward Ross Hoehn discussed the game Quantum Tic-Tac-Toe as a means of lightening the event and giving the public an approachable means to learn the concepts previously discussed.

Figure 3: 241st National ACS Meeting in March 2011, Anaheim, CA.

Conferences

The center independently organized a 2012 Winter School on Quantum Information for Chemistry. The Winter School highlighted the first two years of progress of the QIQC Center and brought together Phase I and future Phase II members as well as outside speakers to discuss the future of quantum information for chemistry. The addition of these individuals into the QIQC provides the Center with a new found communal ability, allowing us to address new challenging problems in chemistry with new and inventive solutions. It also provided an important opportunity for graduate students in the center to network with leaders of the fields.

Center participants also organized four additional meetings on quantum information and quantum chemistry ranging from small workshops at Banff to symposia in the National ACS meeting. All the conferences are listed below.

- *Quantum Information for Quantum Chemistry (11frg014*), Organized by Sabre Kais and Alan Aspuru-Guzik, June 5-12, 2011 at the Banff International Research Station, Banff, Canada.
- *Quantum Information and Computation in Chemistry: Experiment and Theory 241st* NATIONAL ACS MEETING, Organized by Kenneth Brown and Alan Aspuru-Guzik, Anaheim, CA March 27-31, 2011.
- *QEC11, the Second International Conference on Quantum Error Correction*, Organized by Daniel Lidar, University of Southern California, Dec. 5-9, 2011.
- *Winter School on Quantum Information for Quantum Chemistry in January 2012*, Palm Springs, CA
- *Tutorial: Quantum Information and Computation for Quantum Chemistry*, APS March Meeting 2013. March 18-22, 2013. Baltimore. Organized by Daniel Lidar with tutorials from Kenneth Brown and Peter Love.

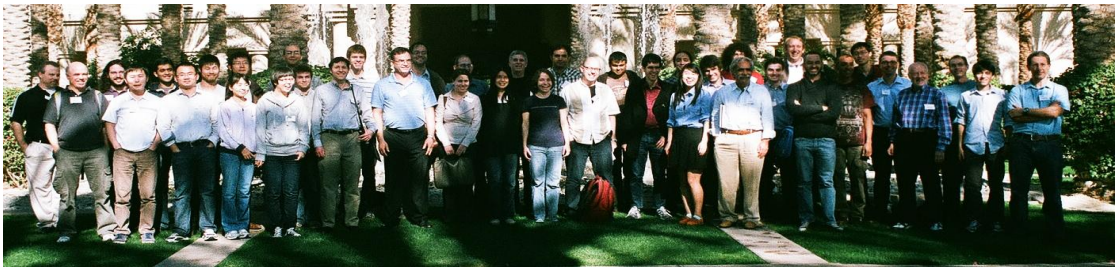


Figure 4Participants of Winter School on "Quantum Information for Quantum Chemistry" in January 2012, Palm Springs

2011-2014
Cumulative Published: 46
Collaborations amongst CCI PIs: 10
Undergraduate Authors: 6
Books: 1

Published

Article title: Analysis of the Quantum Zeno Effect for Quantum Control Computation

Authors: Jason M Dominy, Gerardo A Paz-Silva, A T Rezakhani, and **Daniel A. Lidar**.

Journal: Journal of Physics A: Math Theor. Vol 46 075306

Publication date: Jan. 7, 2013

Abstract: Within quantum information, many methods have been proposed to avoid or correct the deleterious effects of the environment on a system of interest. In this work, expanding on our earlier paper (Paz-Silva et al 2012 Phys. Rev. Lett. 108 080501), we evaluate the applicability of the quantum Zeno effect as one such method. Using the algebraic structure of stabilizer quantum error correction codes as a unifying framework, two open-loop protocols are described which involve frequent non-projective (i.e. weak) measurement of either the full stabilizer group or a minimal generating set thereof. The effectiveness of the protocols is measured by the distance between the final state under the protocol and the final state of an idealized evolution in which system and environment do not interact. Rigorous bounds on this metric are derived which demonstrate that, under certain assumptions, a Zeno effect may be realized with arbitrarily weak measurements, and that this effect can protect an arbitrary, unknown encoded state against the environment arbitrarily well.

Article title: Quantum algorithm and circuit design solving the Poisson equation

Authors: Yudong Cao, Anargyros Papageorgiou, Iasonas Petras, **Joseph Traub** and **Sabre Kais**

Journal: New Journal of Physics Vol. 15.1

Publication date: Jan. 2013

Abstract: The Poisson equation occurs in many areas of science and engineering. Here we focus on its numerical solution for an equation in d dimensions. In particular we present a quantum algorithm and a scalable quantum circuit design which approximates the solution of the Poisson equation on a grid with error ε. We assume we are given a superposition of function evaluations of the right-hand side of the Poisson equation. The algorithm produces a quantum state encoding the solution. The number of quantum operations and the number of qubits used by the circuit is almost linear in d and polylog in ε−1. We present quantum circuit modules together with performance guarantees which can also be used for other problems.

Article title: Approximation of real errors by Clifford channels and Pauli measurements

Authors: Mauricio Gutiérrez, Lukas Svec, Alexander Vargo, and **Kenneth R. Brown**

Journal: Phys. Rev. A 87, 030302

Publication date: March 2013

Abstract: The Gottesman-Knill theorem allows for the efficient simulation of stabilizer-based quantum error-correction circuits. Errors in these circuits are commonly modeled as depolarizing channels by using Monte Carlo methods to insert Pauli gates randomly throughout the circuit. Although convenient, these channels are poor approximations of common, realistic channels like amplitude damping. Here we analyze a larger set of efficiently simulable error channels by allowing the random insertion of any one-qubit gate or measurement that can be efficiently simulated within the stabilizer formalism. Our new error channels are shown to be a viable method for accurately approximating real error channels.

Article title: Identifying Single Molecular Ions by Resolved Sideband Measurements

Authors: James E. Goeders, Craig R. Clark, Grahame Vittrorini, Kenneth Wright, C. Ricardo Viteri, and **Kenneth R. Brown**

Journal: J. Phys. Chem. A 117(39) 9725

Publication date: April 2013

Abstract: The masses of single molecular ions are non-destructively measured by co-trapping the ion of interest with a laser-cooled atomic ion, 40Ca+. Measurement of the resolved sidebands of a dipole forbidden transition on the atomic ion reveals the normal mode frequencies of the two ion system. The mass of two molecular ions, 40CaH+ and 40Ca16O+, are then determined from the normal mode frequencies. Isotopes of Ca+ are used to determine the effects of stray electric fields on the normal mode measurement. The future use of resolved sideband experiments for molecular spectroscopy is also discussed.

Article title: A Universal Quantum Circuit Scheme For Finding Complex Eigenvalues of Non-Unitary Matrices: Simulation of Resonance States

Authors: Anmer Daskin, Ananth Grama, and **Sabre Kais**

Source: Quantum Information Processing 13(2) 333

Publication date: Feb. 2014

Abstract: We present a general quantum circuit design for finding eigenvalues of non-unitary matrices on quantum computers using the iterative phase estimation algorithm. In particular, we show how the method can be used for the simulation of resonance states for quantum systems.

Article title: Experimental realization of quantum algorithm for solving linear systems of equations

Authors: Jian Pan, Yudong Cao, Xiwei Yao, Zhaokai Li, Chenyong Ju, Xinhua Peng, **Sabre Kais**, and Jiangfeng Du

Journal: Phys. Rev. A 89, 022313

Publication date: Feb. 2014

Abstract: Quantum computers have the potential of solving certain problems exponentially faster than classical computers. Recently, Harrow, Hassidim and Lloyd proposed a quantum algorithm for solving linear systems of equations: given an N N matrix A and a vector ~b, find the vector ~x that satisfies A~x =~b. It has been shown that using the algorithm one could obtain the solution encoded in a quantum state jxi using O(logN) quantum operations, while classical algorithms require at least O(N) steps. If one is not interested in the solution ~x itself but certain statistical feature of the solution hxjMjxi (M is some quantum mechanical operator), the quantum algorithm will be able to achieve exponential speedup over the best classical algorithm as N grows. Here we report a proof-of-concept experimental demonstration of the quantum algorithm using a 4-qubit nuclear magnetic resonance (NMR) quantum information processor. For all the three sets of experiments with different choices of ~b, we obtain the solutions with over 96% fidelity. This experiment is a first implementation of the algorithm. Because solving linear systems is a common problem in nearly all fields of science and engineering, we will also discuss the implication of our results on the potential of using quantum computers for solving practical linear systems.

Article title: Using Quantum Games To Teach Quantum Mechanics, Part 1

Authors: Ross D. Hoehn, Nick Mack, and Sabre Kais

Journal: J. Chem. Educ, 91, 417−422

Publication date: 2014

Abstract: The learning of quantum mechanics is contingent upon an understanding of the physical significance of the mathematics that one must perform. Concepts such as normalization, superposition, interference, probability amplitude, and entanglement can prove challenging for the beginning student. Several class activities that use a nonclassical version of tic-tac-toe are described to introduce several topics in an undergraduate quantum mechanics course. Quantum tic-tac-toe (QTTT) is a quantum analogue of classical tic-tac-toe (CTTT) and can be used to demonstrate the use of superposition in movement, qualitative (and later quantitative) displays of entanglement, and state collapse due to observation. QTTT can be used to aid student understanding in several other topics with the aid of proper discussion.

Article title: Using Quantum Games To Teach Quantum Mechanics, Part 2

Authors: Ross D. Hoehn, Nick Mack, and Sabre Kais

Journal: J. Chem. Educ. 91, 423−427

Publication date: **2**014

Abstract: Introductory courses in computational and quantum chemistry introduce topics such as Hilbert spaces, basis set expansions, and observable matrices. These topics are fundamental in the practice of quantum computations in chemistry as most computational methods rely on basis sets to approximate the true wave function. The mechanics of these topics can easily and intuitively be shown through the use of the game quantum tic-tac-toe (QTTT). Herein we propose a series of activities, using the mechanics of both classical tic-tac-toe (CTTT) and QTTT, intended to assist in the student's understanding of these quantum chemistry topics by exploiting their intuitive comprehension of the game. Quantum tic-tac-toe QTTT is a quantum analogue of CTTT and can be used to demonstrate the use of superposition in movement, qualitative (and later quantitative) displays of entanglement, and state collapse due to observation. QTTT can be used for the benefit of the student's comprehension in several other topics with the aid of proper discussion. This paper is the second in a series on the topic published in this Journal.

Article title: Implementation of quantum logic gates using polar molecules in pendular states

Authors: Jing Zhu, **Sabre Kais**, Qi Wei, **Dudley Herschbach,** Bretislav Friedrich

Journal: Journal of Chemical Physics, Vol. 138, Issue 2

Publication date: Dec. 2012

Abstract: We present a systematic approach to implementation of basic quantum logic gates operating on polar molecules in pendular states as qubits for a quantum computer. A static electric field prevents quenching of the dipole moments by rotation, thereby creating the pendular states; also, the field gradient enables distinguishing among qubit sites. Multi-target optimal control theory is used as a means of optimizing the initial-to-target transition probability via a laser field. We give detailed calculations for the SrO molecule, a favorite candidate for proposed quantum computers. Our simulation results indicate that NOT, Hadamard and CNOT gates can be realized with high fidelity, as high as 0.985, for such pendular qubit states.

Article title: Universality Proof and Analysis of Generalized Nested Uhrig Dynamical Decoupling

Authors: Wan-Jung Kuo, Gregory Quiroz, Gerardo Paz-Silva, and **Daniel A. Lidar**

Journal: Journal of Mathematical Physics Vol 53 122207

Publication date: Dec. 2012

Abstract: Nested Uhrig dynamical decoupling (NUDD) is a highly efficient quantum error suppression scheme that builds on optimized single axis UDD sequences. We prove the universality of NUDD and analyze its suppression of different error types in the setting of generalized control pulses.

We present an explicit lower bound for the decoupling order of each error type, which we relate to the sequence orders of the nested UDD layers. We find that the error suppression capabilities of NUDD are strongly dependent on the parities and relative magnitudes of all nested UDD sequence orders. This allows us to predict the optimal arrangement of sequence orders. We test and confirm our analysis using numerical simulations.

Article title: Ground-state stability and criticality of two-electron atoms with screened Coulomb potentials using the B-splines basis set

Authors: Pablo Serra, **Sabre Kais**

Journal: Journal of Physics B: At. Mol. Opt. Phys., Vol 45 235003

Publication date: Dec. 2012

Abstract: We applied the finite-size scaling method using the B-splines basis set to construct the stability diagram for two-electron atoms with a screened Coulomb potential. The results of this method for two-electron atoms are very accurate in comparison with previous calculations based on Gaussian, Hylleraas and finite-element basis sets. The stability diagram for the screened two-electron atoms shows three distinct regions, i.e. a two-electron region, a one-electron region and a zero-electron region, which correspond to stable, ionized and double ionized atoms, respectively. In previous studies, it was difficult to extend the finite-size scaling calculations to large molecules and extended systems because of the computational cost and the lack of a simple way to increase the number of Gaussian basis elements in a systematic way. Motivated by recent studies showing how one can use B-splines to solve Hartree–Fock and Kohn–Sham equations, this combined finite-size scaling using the B-splines basis set might provide an effective systematic way to treat criticality of large molecules and extended systems. As benchmark calculations, the two-electron systems show the feasibility of this combined approach and provide an accurate reference for comparison.

Article title: Universal Programmable Quantum Circuit Schemes to Emulate an Operator

Authors: Anmer Daskin, Ananth Grama, Giorgos Kollias, and **Sabre Kais**

Journal: The Journal of Chemical Physics Vol 137, Issue 23

Publication date: Nov. 30, 2012

Abstract: Unlike fixed designs, programmable circuit designs support an infinite number of operators. The functionality of a programmable circuit can be altered by simply changing the angle values of the rotation gates in the circuit. Here, we present a new quantum circuit design technique resulting in two general programmable circuit schemes. The circuit schemes can be used to simulate any given operator by setting the angle values in the circuit. This provides a fixed circuit design whose angles are determined from the elements of the given matrix–which can be non-unitary–in an efficient way. We also give both the classical and quantum complexity analysis for these circuits and show that the circuits require a few classical computations. For the electronic structure simulation on a quantum computer, one has to perform the following steps: prepare the initial wave function of the system;

present the evolution operator $U = e^{-iHt}$ for a given atomic and molecular Hamiltonian H in terms of quantum gates array and apply the phase estimation algorithm to find the energy eigenvalues. Thus, in the circuit model of quantum computing for quantum chemistry, a crucial step is presenting the evolution operator for the atomic and molecular Hamiltonians in terms of quantum gate arrays. Since the presented circuit designs are independent from the matrix decomposition techniques and the global optimization processes used to find quantum circuits for a given operator, high accuracy simulations can be done for the unitary propagators of molecular Hamiltonians on quantum computers. As an example, we show how to build the circuit design for the hydrogen molecule.

Article title: High-fidelity Adiabatic Quantum Computation via Dynamical Decoupling

Authors: Gregory Quiroz and **Daniel A. Lidar**

Journal: Physical Review A Vol **86** 042333

Publication date: Oct., 2012

Abstract: We introduce high-order dynamical decoupling strategies for open-system adiabatic quantum computation. Our numerical results for the random-unitary map model demonstrate that a judicious choice of high-order dynamical decoupling method, in conjunction with an encoding which allows computation to proceed alongside decoupling, can dramatically enhance the fidelity of adiabatic quantum computation in spite of decoherence.

Article title: Multipartite Quantum Entanglement Evolution in Photosynthetic Complexes

Authors: Jing Zhu, **Sabre Kais, Alán Aspuru-Guzik**, Sam Rodriques, Ben Brock et al.

Journal: Journal of Chemical Physics 137, 974112 (2012) doi: 10.1063/1.4742333

Publication date: August 2012 (see reprints)

Abstract: We investigate the evolution of entanglement in the Fenna-Matthew-Olson (FMO) complex based on simulations using the scaled hierarchy equation of motion (HEOM) approach. We examine the role of multipartite entanglement in the FMO complex by direct computation of the convex roof optimization for a number of measures, including some that have not been previously evaluated. We also consider the role of monogamy of entanglement in these simulations. We utilize the fact that the monogamy bounds are saturated in the single exciton subspace. This enables us to compute more measures of entanglement exactly and also to validate the evaluation of the convex roof. We then use direct computation of the convex roof to evaluate measures that are not determined by monogamy. This approach provides a more complete account of the entanglement in these systems than has been available to date. Our results support the hypothesis that multipartite entanglement is maximum primary along the two distinct electronic energy transfer pathways.

Article title: Finding low-energy conformations of lattice protein models by quantum annealing

Authors: Alejandro Perdomo-Ortiz, Neil Dickson, Marshall Drew-Brook, Geordie Rose, and **Alán Aspuru-Guzik**

Journal: Scientific Reports 2, Article 571

Publication date: Aug. 13, 2012

Abstract: Lattice protein folding models are a cornerstone of computational biophysics. Although these models are a coarse grained representation, they provide useful insight into the energy landscape of natural proteins. Finding low-energy threedimensional structures is an intractable problem even in the simplest model, the Hydrophobic-Polar (HP) model. Description of protein-like properties are more accurately described by generalized models, such as the one proposed by Miyazawa and Jernigan (MJ), which explicitly take into account the unique interactions among all 20 amino acids. There is theoretical and experimental evidence of the advantage of solving classical optimization problems using quantum annealing over its classical analogue (simulated annealing). In this report, we present a benchmark implementation of quantum annealing for lattice protein folding problems (six different experiments up to 81 superconducting quantum bits). This first implementation of a biophysical problem paves the way towards studying optimization problems in biophysics and statistical mechanics using quantum devices.

Article title: The Bravyi-Kitaev transformation for quantum computation of electronic structure

Authors: Jacob T. Seeley, Martin J. Richard, and **Peter J. Love**

Journal: The Journal of Chemical Physics 137, 224109

Publication date: Aug. 2012

Abstract: Quantum simulation is an important application of future quantum computers with applications in quantum chemistry, condensed matter, and beyond. Quantum simulation of fermionic systems presents a specific challenge. The Jordan-Wigner transformation allows for representation of a fermionic operator by $O(n)$ qubit operations. Here, we develop an alternative method of simulating fermions with qubits, first proposed by Bravyi and Kitaev [Ann. Phys. 298, 210 (2002)10.1006/aphy.2002.6254; e-print arXiv:quant-ph/0003137v2], that reduces the simulation cost to $O(\log n)$ qubit operations for one fermionic operation. We apply this new Bravyi-Kitaev transformation to the task of simulating quantum chemical Hamiltonians, and give a detailed example for the simplest possible case of molecular hydrogen in a minimal basis. We show that the quantum circuit for simulating a single Trotter time step of the Bravyi-Kitaev derived Hamiltonian for H_2 requires fewer gate applications than the equivalent circuit derived from the Jordan-Wigner transformation. Since the scaling of the Bravyi-Kitaev method is asymptotically better than the Jordan-Wigner method, this result for molecular hydrogen in a minimal basis demonstrates the superior efficiency of the Bravyi-Kitaev method for all quantum computations of electronic structure.

Article title: Population and Coherence Dynamics in Light Harvesting Complex II (LH2)

Authors: Shu-Hao Yeh, Jing Zhu, and **Sabre Kais**

Journal: The Journal of Chemical Physics 137, 084110

Publication date: Aug. 2012

Abstract: The electronic excitation population and coherence dynamics in the chromophores of the photosynthetic light harvesting complex 2 (LH2) B850 ring from purple bacteria (Rhodopseudomonas acidophila) have been studied theoretically at both physiological and cryogenic temperatures. Similar to the well-studied Fenna-Matthews-Olson (FMO) protein, oscillations of the excitation population and coherence in the site basis are observed in LH2 by using a scaled hierarchical equation of motion approach. However, this oscillation time (300 fs) is much shorter compared to the FMO protein (650 fs) at cryogenic temperature. Both environment and high temperature are found to enhance the propagation speed of the exciton wave packet yet they shorten the coherence time and suppress the oscillation amplitude of coherence and the population. Our calculations show that a long-lived coherence between chromophore electronic excited states can exist in such a noisy biological environment.

Article title: Quantum Circuit Design for Solving Linear Systems of Equations

Authors: Yudong Cao, Anmer Daskin, Steven Frankel, and **Sabre Kais**

Journal: Molecular Physics Vol 110, Issue 15-16

Publication date: May 2012

Abstract: Recently, it has been demonstrated that quantum computers can be used for solving linear systems of algebraic equations with exponential speedup compared with classical computers. Here, we present an efficient and generic quantum circuit design for implementing the algorithm for solving linear systems. In particular, we show the detailed construction of a quantum circuit which solves a 4 × 4 linear system with seven qubits. It consists of only the basic quantum gates that can be realized with present physical devices, implying great possibility for experimental implementation. Furthermore, the performance of the circuit is numerically simulated and its ability to solve the intended linear system is verified.

Article title: Decoherence-protected quantum gates for a hybrid solid-state spin register

Authors: T. van der Sar, Z. H.Wang, M. S. Blok, H. Bernien, T. H. Taminiau, D. M. Toyli, **D. A. Lidar**, D. D. Awschalom, R. Hanson & V. V. Dobrovitski

Journal: Nature 484, 82-86

Publication date: April 2012

Abstract: Protecting the dynamics of coupled quantum systems from decoherence by the environment is a key challenge for solid-state quantum information processing[1, 2]. An idle quantum bit (qubit) can be efficiently insulated from the outside world by dynamical decoupling[3], as has recently been demonstrated for individual solid-state qubits[4, 5, 6, 7, 8, 9]. However, protecting qubit coherence during a multi-qubit gate is a non-trivial problem[3, 10, 11]: in general, the decoupling disrupts the interqubit dynamics and hence conflicts with gate operation. This problem is particularly salient for hybrid

systems[12, 13, 14, 15, 16, 17, 18,19, 20, 21, 22], in which different types of qubit evolve and decohere at very different rates. Here we present the integration of dynamical decoupling into quantum gates for a standard hybrid system, the electron–nuclear spin register. Our design harnesses the internal resonance in the coupled-spin system to resolve the conflict between gate operation and decoupling. We experimentally demonstrate these gates using a two-qubit register in diamond operating at room temperature. Quantum tomography reveals that the qubits involved in the gate operation are protected as accurately as idle qubits. We also perform Grover's quantum search algorithm[1], and achieve fidelities of more than 90% even though the algorithm run-time exceeds the electron spin dephasing time by two orders of magnitude. Our results directly allow decoherence-protected interface gates between different types of solid-state qubit. Ultimately, quantum gates with integrated decoupling may reach the accuracy threshold for fault-tolerant quantum information processing with solid-state devices[1, 11]

Article title: Photonic quantum simulators

Authors: **Alán Aspuru-Guzik** and PhilipWalther

Journal: Nature Physics Vol. 8, Issue 4 285-291

Publication date: April 2012

Abstract: Quantum simulators are controllable quantum systems that can be used to mimic other quantum systems. They have the potential to enable the tackling of problems that are intractable on conventional computers. The photonic quantum technology available today is reaching the stage where significant advantages arise for the simulation of interesting problems in quantum chemistry, quantum biology and solid-state physics. In addition, photonic quantum systems also offer the unique benefit of being mobile over free space and in waveguide structures, which opens new perspectives to the field by enabling the natural investigation of quantum transport phenomena. Here, we review recent progress in the field of photonic quantum simulation, which should break the ground towards the realization of versatile quantum simulators.

Article title: Zeno Effect for Quantum Computation and Control

Authors: Gerardo A. Paz-Silva, A. T. Rezakhani, Jason M. Dominy, and **D. A. Lidar**

Journal: Physical Review Letters Vol. 108, Issue 8 080501

Publication date: Feb. 22, 2012 (see reprints)

Abstract: It is well known that the quantum Zeno effect can protect specific quantum states from decoherence by using projective measurements. Here we combine the theory of weak measurements with stabilizer quantum error correction and detection codes. We derive rigorous performance bounds which demonstrate that the Zeno effect can be used to protect appropriately encoded arbitrary states to arbitrary accuracy while at the same time allowing for universal quantum computation or quantum control.

Article title: Experimental Signature of Programmable Quantum Annealing

Authors: **Sergio Boixi**, Tameem Albash, Federico M. Spedalieri, Nicholas Chancellor, and **Daniel A. Lidar**

Journal: Nature Communications 4, 2067

Publication date: 2013

Abstract: Quantum annealing is a general strategy for solving difficult optimization problems with the aid of quantum adiabatic evolution [1, 2]. Both analytical and numerical evidence suggests that under idealized, closed system conditions, quantum annealing can outperform classical thermalization-based algorithms such as simulated annealing [3, 4]. Do engineered quantum annealing devices effectively perform classical thermalization when coupled to a decohering thermal environment? To address this we establish, using superconducting flux qubits with programmable spin-spin couplings, an experimental signature which is consistent with quantum annealing, and at the same time inconsistent with classical thermalization, in spite of a decoherence timescale which is orders of magnitude shorter than the adiabatic evolution time. This suggests that programmable quantum devices, scalable with current superconducting technology, implement quantum annealing with a surprising robustness against noise and imperfections.

Article title: Quantum Coherence and Entanglement in the Avian Compass

Authors: James A. Pauls, Yiteng Zhang, Gennady P. Berman, and **Sabre Kais**

Journal: PHYSICAL REVIEW E 87, 062704

Publication date: 2013

Abstract: The radical pair mechanism is one of two distinct mechanisms used to explain the navigation of birds in geomagnetic fields. However, little research has been done to explore the role of quantum entanglement in this mechanism. In this paper, we study the lifetime of radical pair entanglement corresponding to the magnitude and direction of magnetic fields to show that the entanglement lasts long enough in birds to be used for navigation. We also demonstrate that, due to a lack of orientational sensitivity of the entanglement in the geomagnetic field, the birds are not able to orient themselves by the mechanism based directly on radical-pair entanglement. To explore the entanglement mechanism further, we propose a model in which the hyperfine interactions are replaced by local magnetic fields of similar strength. The entanglement of the radical pair in this model lasts longer and displays an angular sensitivity in weak magnetic fields, both of these factors are not present in the previous models.

Article title: Computational complexity in electronic structure

Authors: James Daniel Whitfield , **Peter John Love** and **Alán Aspuru-Guzik**

Journal: Phys. Chem. Chem. Phys., 2013,15, 397-411

Publication date: 2013

Abstract: In quantum chemistry, the price paid by all known efficient model chemistries is either the truncation of the Hilbert space or uncontrolled approximations. Theoretical computer science suggests that these restrictions are not mere shortcomings of the algorithm designers and programmers but could stem from the inherent difficulty of simulating quantum systems. Extensions of computer science and information processing exploiting quantum mechanics has led to new ways of understanding the ultimate limitations of computational power. Interestingly, this perspective helps us understand widely used model chemistries in a new light. In this article, the fundamentals of computational complexity will be reviewed and motivated from the vantage point of chemistry. Then recent results from the computational complexity literature regarding common model chemistries including Hartree–Fock and density functional theory are discussed

Article title: Optimized Dynamical Decoupling via Genetic Algorithms

Authors: Gregory Quiroz and **Daniel A. Lidar**

Journal: PHYSICAL REVIEW A 88, 052306

Publication date: Nov 2013

Abstract: We utilize genetic algorithms to find optimal dynamical decoupling (DD) sequences for a single-qubit system subjected to a general decoherence model under a variety of control pulse conditions. We focus on the case of sequences with equal pulse-intervals and perform the optimization with respect to pulse type and order. In this manner we obtain robust DD sequences, first in the limit of ideal pulses, then when including pulse imperfections such as finite pulse duration and qubit rotation (flip-angle) errors. Although our optimization is numerical, we identify a deterministic structure underlies the top-performing sequences. We use this structure to devise DD sequences which outperform previously designed concatenated DD (CDD) and quadratic DD (QDD) sequences in the presence of pulse errors. We explain our fundings using time-dependent perturbation theory and provide a detailed scaling analysis of the optimal sequences.

Article title: Quadratic Dynamical Decoupling: Universality Proof and Error Analysis

Authors: Wan-Jung Kuo and **Daniel A. Lidar**

Journal: Physical Review A Vol **84** 042329

Publication date: October 17, 2011

Abstract: We prove the universality of the generalized QDD*N*1*N*2 (quadratic dynamical decoupling) pulse sequence for near-optimal suppression of general single-qubit decoherence. Earlier work showed numerically that this dynamical decoupling sequence, which consists of an inner Uhrig DD

(UDD) and outer UDD sequence using $N1$ and $N2$ pulses, respectively, can eliminate decoherence to $O(TN)$ using $O(N2)$ unequally spaced "ideal" (zero-width) pulses, where T is the total evolution time and $N = N1 = N2$. A proof of the universality of QDD has been given for even $N1$. Here we give a general universality proof of QDD for arbitrary $N1$ and $N2$. As in earlier proofs, our result holds for arbitrary bounded environments. Furthermore, we explore the single-axis (polarization) error suppression abilities of the inner and outer UDD sequences. We analyze both the single-axis QDD performance and how the overall performance of QDD depends on the single-axis errors. We identify various performance effects related to the parities and relative magnitudes of $N1$ and $N2$. We prove that using QDD$N1N2$ decoherence can always be eliminated to $O(T \min\{N1, N2\})$.

Article title: Review of Decoherence Free Subspaces, Noiseless Subsystems, and Dynamical Decoupling

Authors: **Daniel A. Lidar**

Source: Advances in Chemical Physics Volume 154

Publication date: Mar. 2014

Abstract: Quantum information requires protection from the adverse affects of decoherence and noise. This review provides an introduction to the theory of decoherence-free subspaces, noiseless subsystems, and dynamical decoupling. It addresses quantum information preservation as well protected computation.

Article title: Back to the Future: A roadmap for quantum simulation from vintage quantum chemistry

Author: Peter J. Love

Source: Advances in Chemical Physics Volume 154

Publication date: Mar. 2014

Abstract: A discussion of the prospects for quantum computation for quantum chemistry from the point of view of the history of classical calculations of electronic structure.

Article title: Multipartite quantum entanglement evolution in photosynthetic complexes

Authors: Jing Zhu, **Sabre Kais, Alán Aspuru-Guzik**, Sam Rodriques, Ben Brock, and **Peter J. Love**

Journal: J. Chem. Phys. 137, 074112

Source: http://jcp.aip.org/resource/1/jcpsa6/v137/i7/p074112_s1?ver=pdfcov

Publication date: Aug. 21 2012

Abstract: We investigate the evolution of entanglement in the Fenna-Matthew-Olson (FMO) complex based on simulations using the scaled hierarchical equations of motion approach. We examine the role of entanglement in the FMO complex by direct computation of the convex roof. We use monogamy to give a lower bound for entanglement and obtain an upper bound from the evaluation of the convex roof. Examination of bipartite measures for all possible bipartitions provides a complete picture of the multipartite entanglement. Our results support the hypothesis that entanglement is maximum primary along the two distinct electronic energy transfer pathways. In addition, we note that the structure of multipartite entanglement is quite simple, suggesting that there are constraints on the mixed state entanglement beyond those due to monogamy

Article title: Observation of topologically protected bound states in photonic quantum walks

Authors: Takuya Kitagawa, Matthew A. Broome, Alessandro Fedrizzi, Mark S. Rudner, Erez Berg, Ivan Kassal, **Alán Aspuru-Guzik**, Eugene Demler & Andrew G. White

Journal: Nature Communications 3, Article number: 882

Source: doi:10.1038/ncomms1872

Publication date: June 6, 2012

Abstract: Topological phases exhibit some of the most striking phenomena in modern physics. Much of the rich behaviour of quantum Hall systems, topological insulators, and topological superconductors can be traced to the existence of robust bound states at interfaces between different topological phases. This robustness has applications in metrology and holds promise for future uses in quantum computing. Engineered quantum systems—notably in photonics, where wavefunctions can be observed directly—provide versatile platforms for creating and probing a variety of topological phases. Here we use photonic quantum walks to observe bound states between systems with different bulk topological properties and demonstrate their robustness to perturbations—a signature of topological protection. Although such bound states are usually discussed for static (time-independent) systems, here we demonstrate their existence in an explicitly time-dependent situation. Moreover, we discover a new phenomenon: a topologically protected pair of bound states unique to periodically driven systems.

Article title: Progress in compensating pulse sequences for quantum computation

Authors: J. True Merrill and **Kenneth R. Brown**

Journal: Advances in Chemical Physics Volume 154

Publication date: March 2013

Abstract: The control of qubit states is often impeded by systematic control errors. Compensating pulse sequences have emerged as a resource efficient method for quantum error reduction. In this review, we discuss compensating composite pulse methods, and introduce a unifying control-theoretic framework using a dynamic interaction picture. This admits a novel geometric picture where sequences

are interpreted as vector paths on the dynamical Lie algebra. Sequences for single-qubit and multi-qubit operations are described with this method.

Article title: Introduction to Quantum Algorithms for Physics and Chemistry

Authors: Man-Hong Yung, James D. Whitfield, **Sergio Boixo**, David Tempel, and **Alán Aspuru-Guzik**

Journal: Advances in Chemical Physics Volume 154

Publication date: March 2013

Abstract: An enormous number of model chemistries are used in computational chemistry to solve or approximately solve the Schrodinger equation; each with their own drawbacks. One key limitation is that the hardware used in computational chemistry is based on classical physics, and is often not well suited for simulating models in quantum physics. In this review, we focus on applications of quantum computation to chemical physics problems. We describe the algorithms that have been proposed for the electronic- structure problem, the simulation of chemical dynamics, thermal state preparation, density functional theory and adiabatic quantum simulation.

Article title: Rigorous Performance Bounds for Quadratic and Nested Dynamical Decoupling

Authors: Yuhou Xia, Gotz S. Uhrig, and **Daniel A. Lidar**

Journal: Physical Review A Vol. 84, Issue 6

Publication date: December 2011

Abstract: We present rigorous performance bounds for the quadratic dynamical decoupling pulse sequence which protects a qubit from general decoherence, and for its nested generalization to an arbitrary number of qubits. Our bounds apply under the assumptions of instantaneous pulses and of bounded perturbing environment and qubit-environment Hamiltonians such as those realized by baths of nuclear spins in quantum dots. We prove that if the total sequence time is fixed then the trace-norm distance between the unperturbed and protected system states can be made arbitrarily small by increasing the number of applied pulses.

Article title: Quadratic Dynamical Decoupling with Non-Uniform Error Suppression

Authors: Gregory Quiroz and **Daniel A. Lidar**

Journal: Physical Review A Vol 86, Issue 4

Publication date: Oct. 2011

Abstract: We analyze numerically the performance of the near-optimal quadratic dynamical decoupling (QDD) singlequbit decoherence errors suppression method [J. West et al., Phys. Rev. Lett.

104, 130501 (2010)]. The QDD sequence is formed by nesting two optimal Uhrig dynamical decoupling sequences for two orthogonal axes, comprising N1 and N2 pulses, respectively. Varying these numbers, we study the decoherence suppression properties of QDD directly by isolating the errors associated with each system basis operator present in the system-bath interaction Hamiltonian. Each individual error scales with the lowest order of the Dyson series, therefore immediately yielding the order of decoherence suppression. We show that the error suppression properties of QDD are dependent upon the parities of N1 and N2, and near-optimal performance is achieved for general single-qubit interactions when N1 = N2.

Article title: Solving Quantum Ground-State Problems with Nuclear Magnetic Resonance

Authors: Zhaokai Li, Man-Hong Yung, Hongwei Chen, Dawei Lu, James D. Whitfield, Xinhua Peng, **Alán Aspuru-Guzik** & Jiangfeng Du

Journal: Scientific Reports 1, 88

Publication date: Sept. 9, 2011

Abstract: Quantum ground-state problems are computationally hard problems for general many-body Hamiltonians; there is no classical or quantum algorithm known to be able to solve them efficiently. Nevertheless, if a trial wavefunction approximating the ground state is available, as often happens for many problems in physics and chemistry, a quantum computer could employ this trial wavefunction to project the ground state by means of the phase estimation algorithm (PEA). We performed an experimental realization of this idea by implementing a variational-wavefunction approach to solve the ground-state problem of the Heisenberg spin model with an NMR quantum simulator. Our iterative phase estimation procedure yields a high accuracy for the eigenenergies (to the 10^{-5}decimal digit). The ground-state fidelity was distilled to be more than 80%, and the singlet-to-triplet switching near the critical field is reliably captured. This result shows that quantum simulators can better leverage classical trial wave functions than classical computers.

Article title: High Fidelity Quantum Memory via Dynamical Decoupling: Theory and Experiment

Authors: Xinhua Peng, Dieter Suter, and **Daniel A. Lidar**

Journal: Journal of Physics B Vol **44**, 063023 (6pp)

Publication date: July 2011

Abstract: Quantum information processing requires overcoming decoherence—the loss of 'quantumness' due to the inevitable interaction between the quantum system and its environment. One approach towards a solution is quantum dynamical decoupling—a method employing strong and frequent pulses applied to the qubits. Here we report on the first experimental test of the concatenated dynamical decoupling (CDD) scheme, which invokes recursively constructed pulse sequences. Using nuclear magnetic resonance, we demonstrate a near order of magnitude improvement in the decay time of stored quantum states. In conjunction with recent results on high fidelity quantum gates using CDD, our results suggest that quantum dynamical decoupling should be used as a first layer of defense

against decoherence in quantum information processing implementations, and can be a stand-alone solution in the right parameter regime.

Article title: Challenges of laser-cooling molecular ions

Authors: Jason H V Nguyen, C Ricardo Viteri, Edward G Hohenstein, C David Sherrill, **Kenneth R Brown,** and Brian Odom

Journal: New Journal of Physics 13, 063023 (28pp)

Publication date: June 2011

Abstract: The direct laser cooling of neutral diatomic molecules in molecular beams suggests that trapped molecular ions can also be laser cooled. The long storage time and spatial localization of trapped molecular ions provides an opportunity for multi-step cooling strategies, but also requires careful consideration of rare molecular transitions. We briefly summarize the requirements that a diatomic molecule must meet for laser cooling, and we identify a few potential molecular ion candidates. We then carry out a detailed computational study of the candidates BH^+ and AlH^+, including improved *ab initio* calculations of the electronic state potential energy surfaces and transition rates for rare dissociation events. On the basis of an analysis of the population dynamics, we determine which transitions must be addressed for laser cooling, and compare experimental schemes using continuous-wave and pulsed lasers.

Article title: Decomposition of unitary matrices for finding quantum circuits: Application to molecular Hamiltonians

Authors: Anmer Daskin and **Sabre Kais**

Journal: The Journal of Chemical Physics

Publication date: April 14, 2011

Abstract: Constructing appropriate unitary matrix operators for new quantum algorithms and finding the minimum cost gate sequences for the implementation of these unitary operators is of fundamental importance in the field of quantum information and quantum computation. Evolution of quantum circuits faces two major challenges: complex and huge search space and the high costs of simulating quantum circuits on classical computers. Here, we use the group leaders optimization algorithm to decompose a given unitary matrix into a proper-minimum cost quantum gate sequence. We test the method on the known decompositions of Toffoli gate, the amplification step of the Grover search algorithm, the quantum Fourier transform, and the sender part of the quantum teleportation. Using this procedure, we present the circuit designs for the simulation of the unitary propagators of the Hamiltonians for the hydrogen and the water molecules. The approach is general and can be applied to generate the sequence of quantum gates for larger molecular systems.

Article title: Group leaders optimization algorithm

Authors: Anmer Daskin and **Sabre Kais**

Journal: Molecular Physics, Vol. 109, Issue 5, (761-772)

Publication date: March 3, 2011

Abstract: We present a new global optimization algorithm in which the influence of the leaders in social groups is used as an inspiration for the evolutionary technique which is designed into a group architecture. To demonstrate the efficiency of the method, a standard suite of single and multi-dimensional optimization functions along with the energies and the geometric structures of Lennard-Jones clusters are given as well as the application of the algorithm on quantum circuit design problems. We show that as an improvement over previous methods, the algorithm scales as $N^{2.5}$ for the Lennard-Jones clusters of N-particles. In addition, an efficient circuit design is shown for a two-qubit Grover search algorithm which is a quantum algorithm providing quadratic speedup over the classical counterpart.

Article title: Simulation of Electronic Structure Hamiltonians Using Quantum Computers

Authors: James D. Whiteld, Jacob Biamonte and **Alán Aspuru-Guzik**

Journal: Molecular Physics Vol 109, Issue 5

Publication date: March 3, 2011

Abstract: Over the last century, a large number of physical and mathematical developments paired with rapidly advancing technology have allowed the field of quantum chemistry to advance dramatically. However, the lack of computationally efficient methods for the exact simulation of quantum systems on classical computers presents a limitation of current computational approaches. We report, in detail, how a set of pre-computed molecular integrals can be used to explicitly create a quantum circuit, i.e. a sequence of elementary quantum operations, that, when run on a quantum computer, obtains the energy of a molecular system with fixed nuclear geometry using the quantum phase estimation algorithm. We extend several known results related to this idea and discuss the adiabatic state preparation procedure for preparing the input states used in the algorithm. With current and near future quantum devices in mind, we provide a complete example using the hydrogen molecule of how a chemical Hamiltonian can be simulated using a quantum computer.

Article title: Modified Scaled Hierarchical Equation of Motion Approach for the Study of Quantum Coherence in Photosynthetic Complexes

Authors: J. Zhu, **S. Kais**, P. Rebentrost and **A. Aspuru-Guzik**

Journal: J. Phys. Chem. B, 2011, 115 (6), pp 1531–1537

Publication date: Jan. 26, 2011 (see reprints)

Abstract: We present a detailed theoretical study of the transfer of electronic excitation energy through the Fenna−Matthews−Olson (FMO) pigment−protein complex, using the newly developed modified scaled hierarchical approach (Shi, Q.; et al. J. Chem. Phys.2009, 130, 084105). We show that this approach is computationally more efficient than the original hierarchical approach. The modified

approach reduces the truncation levels of the auxiliary density operators and the correlation function. We provide a systematic study of how the number of auxiliary density operators and the higher-order correlation functions affect the exciton dynamics. The time scales of the coherent beating are consistent with experimental observations. Furthermore, our theoretical results exhibit population beating at physiological temperature. Additionally, the method does not require a low-temperature correction to obtain the correct thermal equilibrium at long times.

Article title: Dynamics of Entanglement in one and two-dimensional spin systems

Authors: Gehad Sadiek, Qing Xu, **Sabre Kais**

Journal: APS Physics Vol. 83

Publication date: Jan. 2011

Abstract: We consider the time evolution of entanglement in a finite two-dimensional transverse Ising model. The model consists of a set of seven localized spin-1/2 particles in a two-dimensional triangular lattice coupled through nearest-neighbor exchange interaction in the presence of an external time-dependent magnetic field. The magnetic field is applied in different function forms: step, exponential, hyperbolic, and periodic. We found that the time evolution of the entanglement shows an ergodic behavior under the effect of the time-dependent magnetic fields. Also, we found that while the step magnetic field causes great disturbance to the system, creating rapid oscillations, the system shows great controllability under the effects of the other magnetic fields where the entanglement profile follows closely the shape of the applied field even with the same frequency for periodic fields. This follow-up trend breaks down as the strength of the field, the transition constant for the exponential and hyperbolic forms, or the frequency for periodic field increase leading to rapid oscillations. We observed that the entanglement is very sensitive to the initial value of the applied periodic field: the smaller the initial value is, the less distorted the entanglement profile is. Furthermore, the effect of thermal fluctuations is very devastating to the entanglement, which decays very rapidly as the temperature increases. Interestingly, although a large value of the magnetic field strength may yield a small entanglement, the magnetic field strength was found to be more persistent against thermal fluctuations than the small field strengths.

Article title: A Quantum Post “Lock and Key” Model of Neuroreceptor Activation

Authors: Ross Hoehn, David Nichols, Hartmut Neven and **Sabre Kais**

Source: Submitted to Scientific Reports

Publication date: Dec 1, 2014

Abstract: Predicting behaviors of an agonist confined within a protein's active site is of interest in the fields of pharmaceuticals. Quantum behavior within biological systems has been shown to be important in such systems as photosynthetic energy transfer, avian magnetic compass, and tunneling

reactions within organisms; herein a possible quantum mechanism for the activation of proteins by bound agonists is explored. Inelastic Electron Tunneling Spectroscopy has been proposed as a method by which olfactory G-Protein Coupled Receptors are activated by an encapsulated agonist; we have applied this approach to GPCRs within the Central Nervous System. Herein it was noted that nonendogenous agonists for the 5-HT receptor share IET spectral aspects both amongst each other and with the serotonin; this peak roughly scales in intensity with the known activities of the agonists. We conclude with a proposed experiential validation by utilizing Lysergic Acid Dimethylamide or Lysergic Acid Diet! Hylamide and their isotopic analogues.

Article title: Entanglement creation in cold molecular gases using strong laser pulses

Authors: Felipe Herrera, **Sabre Kais**, and **K. Birgitta Whaley**

Journal: arXiv: 1302.6444

Publication date: Feb. 26, 2013

Abstract: While many-particle entanglement can be found in natural solids and strongly interacting atomic and molecular gases, generating highly entangled states between weakly interacting particles in a controlled and scalable way presents a significant challenge. We describe here a one-step method to generate entanglement in a dilute gas of cold polar molecules. For molecules in optical traps separated by a few micrometers, we show that maximally entangled states can be created using the strong off-resonant pulses that are routinely used in molecular alignment experiments. We show that the resulting alignment-mediated entanglement can be detected by measuring laser-induced fluorescence with single-site resolution and that signatures of this molecular entanglement also appear in the microwave absorption spectra of the molecular ensemble. We analyze the robustness of these entangled molecular states with respect to intensity fluctuations of the trapping laser and discuss possible applications of the system for quantum information processing.

Article title: Persistence of entanglement in thermal states of spin systems

Authors: Gehad Sadiek, and **Sabre Kais**

Journal: J. Phys. B, 46, 245501 (2013).

Publication date: Jan. 1, 2013

Abstract: We study and compare the persistence of bipartite and multipartite entanglement in one and two-dimensional spin XY model in an external transverse magnetic field under the effect of thermal excitations. We compare the threshold temperature at which the entanglement vanishes in both cases. We use the concurrence as a measure of the bipartite entanglement and the geometric measure to evaluate the multipartite entanglement of the system. We have found that for the anisotropic and partially anisotropic systems the nearest neighbor bipartite entanglement vanishes asymptotically at much higher magnetic field compared to both the next to nearest neighbor bipartite

entanglement and the multipartite entanglement which asymptotically coincide. Also the same behavior was observed for the threshold temperatures where the nearest neighbor bipartite one is much higher than both of the next to nearest neighbor bipartite and multipartite where the latter two coincide asymptotically and the three of them increase monotonically with the magnetic field strength. Thus as the temperature increases to certain value, the threshold, the multipartite entanglement and the bipartite entanglement of the far parts of the system may vanish while the nearest neighbor bipartite entanglement may sustain up to much higher temperature. For the isotropic system, all types of entanglement and threshold temperatures vanish at the same exact small value of the magnetic field. We emphasis the major role played by both the properties of the ground state of the system and the energy gap as well. Furthermore, we found that the quantum effects in the system can be maintained at high temperatures, where we have observed that the different types of entanglements in the lattice sustain at high temperatures if we apply sufficiently high magnetic fields.

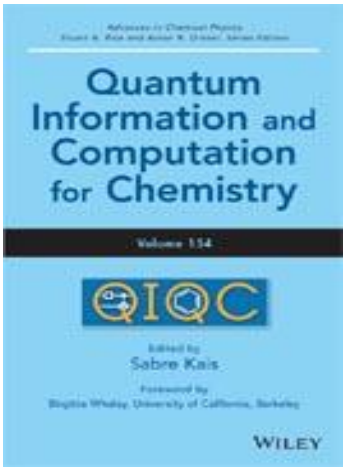
Article title: When is a Quantum Cellular Automaton a quantum Lattice Gas Automation?

Authors: Asif Shakeel and **Peter J. Love**

Source: arXiv:1209.5367

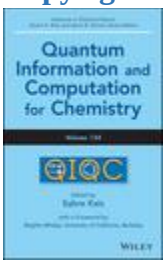
Publication date: Sept. 24, 2012

Abstract: Quantum cellular automata (QCA) are models of quantum computation of particular interest from the point of view of quantum simulation. Quantum lattice gas automata (QLGA - equivalently partitioned quantum cellular automata) represent an interesting subclass of QCA. Prior work on QCA has investigated the relationship between these two classes of models. In the present paper we establish necessary and sufficient conditions for unbounded, finite Quantum Cellular Automata (QCA) (finitely many active cells in a quiescent background) to be Quantum Lattice Gas Automata. We define a local condition that classifies those QCA that are QLGA, and we show that there are QCA that are not QLGA. We use a number of tools from functional analysis of separable Hilbert spaces and representation theory of associative algebras that enable us to treat QCA on finite but unbounded configurations in full detail.



http://onlinelibrary.wiley.com/book/10.1002/9781118742631

Quantum Information and Computation for Chemistry: Advances in Chemical Physics Volume 154



Editor(s): Sabre Kais

Published Online: 21 MAR 2014

Print ISBN: 9781118495667

Online ISBN: 9781118742631

DOI: 10.1002/9781118742631

Book Series: Advances in Chemical Physics

Series Editor(s): Stuart A. Rice, Aaron R. Dinner