

Air Force Research Laboratory

**Quantum Computation for Physical Modeling Workshop
2001/2002
Contributed Talks
May 7 – 9 2002**

Contents

1 Session I: Superconducting Electronics Technologies

- 1.1 Progress in Implementing a Superconductive Type-II Quantum Computer**
- 1.2 Architectures for Superconductive Type-II Quantum Computers**
- 1.3 Superconducting Qubits for Type-II Quantum Computing**

2 Session II: Optical/Solid State Technologies

- 2.1 Simulating Physical Phenomena by Quantum Networks**
- 2.2 Type II Quantum Computing with Optically Addressed Spins in Solids**
- 2.3 Quantum-Hall Semiconductor Quantum Computer Design**

3 Session III: Nuclear Magnetic Resonance Spectroscopic Technologies

- 3.1 Single-Spin Measurement Using Magnetic Resonance Force Microscopy with Cyclic Adiabatic Inversion**
- 3.2 Simulation of the Diffusion Equation on a Type II Quantum Computer**
- 3.3 NMR Perspectives on the Physics of Quantum Information Processing**
- 3.4 Implementation of a Quantum Lattice Gas Algorithm using NMR**
- 3.5 Simulation of Burger Equation on NMR by QLGA**

4 Session IV: Quantum Algorithms

- 4.1 Quantum Algorithm for the Nonlinear Schroedinger Equation**
- 4.2 Quantum Computer Architectures for Physical Simulations**
- 4.3 Efficient Quantum Mechanical Representation of Physical Dynamics**
- 4.4 Quantum-Computational Fluid Dynamics**
- 4.5 Quantum Simulation of Classical Diffusion**

1 Session I: Superconducting Electronics Technologies

TUESDAY THE 7TH OF MAY FROM 10:15AM TO 12:30PM

1.1 Progress in Implementing a Superconductive Type-II Quantum Computer

Karl K. Berggren, J. Sage, P. Cho, E. Macedo, R. Slattery, T. Weir, MIT Lincoln Laboratory, D. Nakada, D. Berns, T. P. Orlando, MIT, Department of Electrical Engineering and Computer Science

Several crucial questions underlying the design of a Type-II quantum computer using superconductive technology are: (1) What is the optimal qubit design? (2) What circuits are ideal for performing two-qubit gate operations? (3) To what extent do unavoidable inaccuracies in qubit properties limit the machine performance? These questions at present have not been answered, but we will discuss the various issues involved in resolving them. There are also practical technical challenges that must be overcome before a prototype machine would be achievable: (1) the limiting sources of noise and dissipation in this system should be identified and eliminated; (2) the sources of fabrication inaccuracy need to be overcome; and (3) a viable packaging technology must be developed that will keep the noise down, while retaining the ability to move heat off the chip. We will present a summary of our results in addressing these issues.

1.2 Architectures for Superconductive Type-II Quantum Computers

Jay Sage, K.K. Berggren, MIT, Lincoln Laboratory, T. P. Orlando, D. Berns, MIT, Department of Electrical Engineering and Computer Science

Our investigations of architectures for type-II quantum computers based on superconductive electronics have led to two promising approaches. The first, which bears an architectural resemblance to the NMR implementation, is a quantum coprocessor for a quantum lattice Boltzmann model (QLBM) computer. It achieves a separation between the quantum elements, which must operate in an electrically quiet and ultra-low-temperature environment, and the classical support circuitry. The superconductive integrated circuit comprises an array of groups of coupled qubits (quantum nodes) that are operated identically in parallel to compute the statistical mechanical collision operator. The second approach implements a quantum lattice-gas cellular automaton (QLGCA) with a probabilistic collision operator.

1.3 Superconducting Qubits for Type-II Quantum Computing.

Terry P. Orlando, MIT, Department of Electrical Engineering and Computer Science, and David Berns, MIT Department of Physics, Karl Berggren and Jay Sage, MIT Lincoln Laboratory.

Recent experiments with superconducting qubits have demonstrated coherent macroscopic states with relaxation times of about 1-10 microseconds and dephasing times of about 0.1 microseconds. Theoretical estimates indicated that these times can be made larger. We will review these developments and their implications for type-II quantum computing.

A prototypical design using superconducting persistent-current qubits will be discussed for a type-II quantum computer. In particular, the factorized quantum lattice-gas algorithm for one-dimensional diffusion equation will be used as an example which incorporates two qubits per node. The qubits are initialized by a mapping of the occupation numbers to the bias flux for each

qubit. We will also show how we will apply unitary transformations to nodes in different product states as well as discuss current technological advantages and limitations of the design.

2 Session II: Optical/Solid State Technologies

TUESDAY THE 7TH OF MAY FROM 2:00PM TO 4:30PM

2.1 Simulating Physical Phenomena by Quantum Networks

James E. Gubernatis, E. Knill, R. Laflamme, G. Ortiz, and R. Somma Los Alamos National Laboratory

Physical quantum systems, characterized by an ensemble of interacting elementary constituents, can be represented and studied by different algebras of observables (Hermitian operators). Recently, we noted [Phys. Rev. A 64, 22319 (2001)] that a general class of one-to-one mappings between these algebras exists and enables one to represent any physical system in a quantum computer. For example, a fully polarized electronic system can be investigated by means of the algebra generated by the usual fermionic creation and annihilation operators, or by using the algebra of Pauli (spin-1/2) operators, the algebra of the universal model of quantum computation. The correspondence between these two algebras is given by the well known Jordan-Wigner isomorphism. Here, we evolve and exploit this fundamental concept in quantum information processing to simulate generic physical phenomena by quantum networks. We give quantum circuits useful for the efficient evaluation of many physical properties (e.g. spectrum of observables or relevant correlation functions) of an arbitrary system with Hamiltonian \hat{H} . From these circuits we illustrate how to implement a quantum network simulator based on the Jordan-Wigner isomorphism on a classical computer. More recently, the steps in this simulator were implemented in a 3 qubit liquid state quantum computer [Somma et al., unpublished]. Excellent agreement between theory and experiment was found.

2.2 Type II Quantum Computing with Optically Addressed Spins in Solids

Philip Hemmer, Department of Electrical Engineering, Texas A&M University

Optically addressed spins in solids have a number of potential advantages for the development of scalable quantum computers. For type II quantum computers, the capability for 2D optical addressing is especially useful. Current and planned experiments with nitrogen-vacancy color centers in diamond, as well as other potential material systems, will be described.

2.3 Quantum-Hall Semiconductor Quantum Computer Design

Vladimir Privman, Center for Quantum Device Technology, Clarkson University

We survey recent advances in semiconductor spin-qubit quantum computing, both theoretical and experimental. We then outline our recent work that combined elements of the 1998 quantum computing proposals by Privman, Vagner and Kventsel, and by Kane, with the new idea of nuclear-spin qubit interactions mediated indirectly via the bound outer electrons of impurity atoms whose nuclear spins 1/2 are the qubits. These electrons, in turn, interact via the two-dimensional electron gas in the quantum Hall effect regime. The resulting quantum computing scheme retains all the gate-control and measurement aspects of the proposal by Kane, but allows qubit spacing at distances of order 100 nm, attainable with the present-day semiconductor-heterostructure device technologies.

3 Session III: Nuclear Magnetic Resonance Spectroscopic Technologies

WEDNESDAY THE 8TH OF MAY FROM 9:00AM TO 1:00PM

3.1 Single-Spin Measurement Using Magnetic Resonance Force Microscopy with Cyclic Adiabatic Inversion

Gennady P. Berman, P.C. Hammel, D.V. Pelekhov, Los Alamos National Laboratory, F. Borgonovi Dipartimento di Matematica e Fisica, Universita Cattolica, via Trieste 17, 25121 Brescia, Italy and I.N.F.N., Sezione di Pavia, and I.N.F.M., Unita di Brescia, Italy)
G. Chapline, Lawrence Livermore National Laboratory, Livermore, CA), S.A. Gurvitz, Department of Particle Physics, Weizmann Institute of Sciences, Israel), V.I. Tsifrinovich. IDS Department, Polytechnic University, Six Metrotech Center, Brooklyn NY)

We consider the process of a single-spin measurement using magnetic resonance force microscopy (MRFM) with a cyclic adiabatic inversion (CAI). This technique is also important for different applications, including a measurement of a qubit state in quantum computation. The measurement takes place through the interaction of a single spin with a cantilever modeled by a quantum oscillator in a coherent state in a quasi-classical range of parameters. The entire system is treated rigorously within the framework of the Schroedinger equation, without any artificial assumptions.

For a many-spin system our equations reduce to the classical equations of motion, and we accurately describe conventional MRFM experiments involving CAI of the spin system.

Our computer simulations of the quantum spin-cantilever dynamics show that the cantilever evolves into a Schroedinger-cat (SC) state: the probability distribution for the cantilever position develops two asymmetric peaks with the total relative probabilities mainly dependent on the initial angle between the directions of the average spin and the effective magnetic field, in the rotating frame. The SC state appears and vanishes with the cantilever period. We show that in the "big" (classical) peak the average spin is oriented approximately in the direction of the effective magnetic field, and in the "small" (quantum) peak the average spin is oriented approximately in the direction opposite to the direction of the effective magnetic field. The SC state results in unwanted effect - two possible outcomes (quantum jump) of a single-spin measurement (similar to the Stern-Gerlach effect). We show that turning on adiabatically the amplitude of the rf magnetic field can significantly suppress the probability of the small peak. This will allow one to use MRFM CAI not only for detecting a signal from a single spin, but also for measuring the single-spin state by measuring the phase of the cantilever driving oscillations. Our preliminary numerical simulations show that (similar to the Stern-Gerlach effect) taking into account a thermal bath which interacts with a cantilever, does not change the main conclusions based on the Hamiltonian approach.

3.2 Simulation of the Diffusion Equation on a Type II Quantum Computer

Dmitry I. Kamenev, G.P. Berman, Los Alamos National Laboratory, A.A. Ezhov, Troitsk Institute of Innovation and Fusion Research, Troitsk, Moscow Region, Russia, J. Yezep, Air Force Research Laboratory

A lattice-gas algorithm for the one-dimensional diffusion equation is simulated using radio-frequency pulses in a one-dimensional spin system. The model is a large array of quantum two-qubit nodes interconnected by the nearest-neighbor classical communication channels. We present a quantum protocol for implementation of the quantum collision operator and a method

for initialization and re-initialization of quantum states. Numerical simulations of the quantum-classical dynamics are in good agreement with the analytic solution for the diffusion equation.

3.3 NMR Perspectives on the Physics of Quantum Information Processing

David G. Cory, Department of Nuclear Engineering, Massachusetts Institute of Technology

Quantum information processing aims to harness the complexity of quantum dynamics to overcome the classical barriers to computation, communication, simulation, etc. It is predicated upon the ability to precisely and efficiently control and observe the quantum dynamics of large systems. NMR has a fifty plus year track record of precise coherent spectroscopy. In chemistry, NMR coherent control is commonly used to provide correlated spectroscopic information. For quantum information processing, we can build on this knowledge to improve our ability to control the coherent and decoherent dynamics of spin systems, and to study real-world decoherence processes far more complex than those usually considered.

In this talk we will: Introduce the mapping of quantum information processing on to a nuclear magnetic resonance experiment, Describe the means of obtaining precise coherent control (and the precision so far obtained), Discuss a variety of means for controlling decoherence and the physical limitation of each, Provide a set of examples where NMR implementations of quantum information processing have been used to study entanglement transfers and other metrics of quantum complexity.

3.4 Implementation of a Quantum Lattice Gas Algorithm using NMR

Marco A. Pravia, Department of Nuclear Engineering, Massachusetts Institute of Technology

Recently it has been suggested that an array of small quantum information processors sharing classical information can be used to solve selected computational problems. Quantum lattice-gas algorithms (QLGA) executed on such an architecture have been developed to solve the diffusion equation, the Schrodinger equation, and the Dirac equation. In this presentation, we describe an ensemble NMR implementation of a QLGA for the diffusion equation. This concrete implementation provides a test example from which to probe the strengths and limitations of this new computation paradigm. The NMR experiment consists of encoding a mass density onto an array of 16 two-qubit quantum information processors and then following the computation through 7 time steps of the algorithm. The results show good agreement with the analytic solution for diffusive dynamics, and they demonstrate the application of ensemble NMR techniques to controlling a parallel array of quantum processors.

3.5 Simulation of Burger Equation on NMR by QLGA

Debra Chen, Department of Nuclear Engineering, Massachusetts Institute of Technology

Recently we used a NMR system to implement a quantum lattice-gas algorithm (QLGA) for the diffusion equation. Here we will discuss the next step, the implementation of Burger equation. This provides a test of the strengths and limitations of NMR implementation. A numerical simulation is used to demonstrate the NMR implementation of Burger equation. The results are in good agreement with numerical solution for the few steps of the algorithm. The simulation helps to predict the sources of experimental errors.

4 Session IV: Quantum Algorithms

WEDNESDAY THE 7TH OF MAY FROM 2:00PM TO 4:30PM
THURSDAY THE 8TH OF MAY FROM 9:00AM TO 11:30AM

4.1 Quantum Algorithm for the Nonlinear Schroedinger Equation

George M. Vahala, Department of Physics, College of William & Mary, Linda Vahala, Department of Electrical & Computer Engineering, Old Dominion University, Jeffrey Yepez, Air Force Research Laboratory

Theoretically, for some problems, quantum computers can yield exponential speed-up over classical computers because of quantum entanglement. Quantum lattice gas algorithms are here generated for the solution of the nonlinear Schroedinger equation (NLS), a generalization of the algorithm for the Schroedinger equation with an external potential. For NLS, the external potential is a function of the wave function and this spatial global information must be extracted at each time step. Since this measurement is a non-unitary operation, global quantum entanglement is destroyed. Nevertheless, the quantum algorithm for NLS still exploits local quantum entanglement at each spatial node between measurement. These types of algorithms are termed Type-II [1] since they involve classical communication between an array of quantum computer nodes, but each node requiring short phase coherence times. Soliton collision simulations, using our quantum algorithm, are presented for both the integrable cubic NLS and the nonintegrable quadratic NLS. For the integrable cubic NLS, the solitons' speed, amplitude and shape are excellently preserved, together with the phase shifts induced by the soliton collisions. The L^2 -norm of the wave function and the energy moment constants are well preserved during the time evolution. For the non-integrable quadratic NLS one finds soliton turbulence, with the L^2 -norm being well preserved, while the energy moment is no longer a constant of the motion. Since the quantum lattice gas algorithm is unconditionally stable it is important to discern when simulation results are spurious.

4.2 Quantum Computer Architectures for Physical Simulations

Michael P. Frank, Department of Computer & Information Science & Engineering, University of Florida

We report past work by members of UF's Reversible & Quantum Computing Research group on numerically stable techniques for simulating nonrelativistic wave mechanics, and on techniques for space-efficient simulation of quantum computers. We also discuss some new research directions we are currently pursuing. Based on our earlier work on classical reversible architectures & languages, we are now designing technology-independent architectures for scalable, general-purpose quantum computers and are also planning to develop programming languages and compilers for these machines. An application of our quantum simulation work that is of particular interest in our group is to simulate future nanocomputing technologies to resolve some open theoretical questions about the scalability of both self-timed and globally clocked energy-recycling reversible computing mechanisms, an issue which will greatly impact the ultimate limits of computational performance.

4.3 Efficient Quantum Mechanical Representation of Physical Dynamics

Jeffrey Yepez, Air Force Research Laboratory

On his death bed, the fluid dynamicist Werner Karl Heisenberg, well known as the discoverer of matrix mechanics and the famous uncertainty principle, is reported to have said, "When I meet God, I am going to ask him two questions: Why relativity? And why turbulence? I really believe he will have an answer for the first." In this talk, I'll address the second question by first presenting an efficient and accurate quantum lattice-gas algorithm to numerically predict solutions of the relativistic Dirac equation in three dimensions which in turn can be used to numerically model turbulent fluid dynamics on a type-II quantum computer.

4.4 Quantum-Computational Fluid Dynamics

Bruce M. Boghosian, Department of Mathematics, Tufts University

We give an overview of various strategies for simulating fluid flow on a Type II quantum computer. While a detailed quantum algorithm is not yet available for this problem, there are nevertheless some features that are likely to be common to any such algorithm, and we focus on those. We also present estimates of quantum-computational complexity for the various strategies.

4.5 Quantum Simulation of Classical Diffusion

David A. Meyer, University of California San Diego

In the past decade quantum algorithms have been found which outperform the best classical solutions known for certain classical problems as well as the best classical methods known for simulation of certain quantum systems. This suggests that they may also speed up the simulation of some classical systems. In this talk I'll describe how quantum lattice gas automata can efficiently simulate certain classically diffusing systems.