MEMORANDUM OF TRANSMITTAL

U.S. Army Research Office
ATTN: AMSRL-RO-BI (TR)
P.O. Box 12211
Research Triangle Park, NC 27709-2211

This report was submitted only
electronically to *reports@arl.aro.army.mil*

__ Reprint (Orig + 2 copies)   __ Technical Report (Orig + 2 copies)

__ Manuscript (1 copy)   _x_ Final Progress Report (PDF file)

                                        __ Related Materials, Abstracts, Theses (1 copy)

CONTRACT/GRANT NUMBER: DAAD 19-99-1-0342

REPORT TITLE: ___ ***Quantum Computing in Solid State, and***

                 Coherent Behavior of Open Quantum Systems

is forwarded for your information.

SUBMITTED FOR PUBLICATION TO (applicable only if report is manuscript):

DO NOT REMOVE LABEL BELOW
FOR IDENTIFICATION PURPOSES

Sincerely,   U. Privman.

Dr. Vladimir Privman   40316-PH-QC
Clarkson University
Dept. of Physics
Potsdam, NY 13699-5720

REPORT DOCUMENTATION PAGE

Public Reporting burden for this collection of information is estimated to average 1 hour per response, including the time for reviewing instructions, searching existing data sources, gathering and maintaining the data needed, and completing and reviewing the collection of information. Send comment regarding this burden estimates or any other aspect of this collection of information, including suggestions for reducing this burden, to Washington Headquarters Services, Directorate for information Operations and Reports, 1215 Jefferson Davis Highway, Suite 1204, Arlington, VA 22202-4302, and to the Office of Management and Budget, Paperwork Reduction Project (0704-0188,) Washington, DC 20503.

1. AGENCY USE ONLY (Leave Blank)	2. REPORT DATE **January 2003**	3. REPORT TYPE AND DATES COVERED **Final report, 9/1999 – 10/2002**

4. TITLE AND SUBTITLE
Quantum Computing in Solid State, and
Coherent Behavior of Open Quantum Systems

5. FUNDING NUMBERS
G
DAAD 19-99-1-0342

6. AUTHOR(S)
Vladimir Privman

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Clarkson University
Division of Research, Mail Stop 5630
Potsdam, NY 13699-5630

8. PERFORMING ORGANIZATION REPORT NUMBER

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

U. S. Army Research Office
P.O. Box 12211
Research Triangle Park, NC 27709-2211

10. SPONSORING / MONITORING AGENCY REPORT NUMBER

11. SUPPLEMENTARY NOTES
The views, opinions and/or findings contained in this report are those of the author(s) and should not be construed as an official Department of the Army position, policy or decision, unless so designated by other documentation.

12 a. DISTRIBUTION / AVAILABILITY STATEMENT

Approved for public release; distribution unlimited.

12 b. DISTRIBUTION CODE

13. ABSTRACT (Maximum 200 words)

We have developed and investigated models of realization of quantum computing in solid-state semiconductor heterostructures, and explored decoherence properties of relevance in evaluation of quantum-computing systems. Quantum bits (qubits) are nuclear or outer bound electron spins in donor atoms embedded in the zero-spin host material, which could be an isotope of Si. In order to accomplish control of each qubit and also have controlled qubit-qubit interactions, we consider exchange of electrons, either bound or in two-dimensional electron gas. Our emphasis has been on spin-excitons that form in the electron gas in heterostructures under quantum Hall effect conditions: at low temperatures and in high magnetic fields. Their spectral gap causes slow relaxation and decoherence, while still allowing controlled qubit-qubit interactions at qubit separations of order 100 nm. We have carried detailed many-body perturbative calculations of qubit interactions and decoherence in such systems. We have also obtained results promoting general understanding of quantum decoherence and measurement processes, within the setting appropriate for quantum computing applications.

14. SUBJECT TERMS
Semiconductors, quantum computing, spins, qubits, relaxation, spin interactions, NMR, decoherence, Si, GaAs, quantum Hall effect, low temperatures, high magnetic fields

15. NUMBER OF PAGES
48

16. PRICE CODE

17. SECURITY CLASSIFICATION OR REPORT **UNCLASSIFIED**	18. SECURITY CLASSIFICATION ON THIS PAGE **UNCLASSIFIED**	19. SECURITY CLASSIFICATION OF ABSTRACT **UNCLASSIFIED**	20. LIMITATION OF ABSTRACT **UL**

NSN 7540-01-280-5500

Final Report for the ARO Grant DAAD-19-99-1-0342

Quantum Computing in Solid State, and Coherent Behavior of Open Quantum Systems

(September 1999 — October 2002)

PI: Vladimir Privman

TABLE OF CONTENTS

Appendices:

A.   *Quantum Computing with Spin Qubits in Semiconductor Structures*

B.   *Indirect Interaction of Solid-State Qubits via Two-Dimensional Electron Gas*

C.   *Initial Decoherence of Open Quantum Systems*

SCIENTIFIC ACCOMPLISHMENTS

The goal of this program has been to develop theoretical understanding of processes of decoherence and relaxation, as well as of qubit interactions, in order to evaluate quantum computing designs in solid state, with emphasis on spin-based schemes in low-temperature, high magnetic field, quantum Hall effect regime semiconductor heterostructures. A broader aim has been to contribute to the understanding of spin control and measurement in semiconductor and other materials, to support experimental efforts in quantum information processing and spintronic device development.

For a quantum-computing design based on quantum-Hall semiconductor heterostructures, we have accomplished, in several publications, calculation of all the relevant control and relaxation/decoherence time scales. This has allowed us to combine elements of the 1998 quantum computing designs by Privman, Vagner and Kventsel [1], and by Kane [2], with the new idea [3] 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 [3-5] 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. Two articles are attached detailing these results: Appendix A is an overview-style paper [5], whereas Appendix B is a more technical work [3].

In order to generally gain understanding of decoherence in materials considered for quantum computing realizations, we [6], as well as other groups [7,8], have studied the low-temperature dynamics of a shallow donor ^{31}P impurity or quantum-dot bound-electron spins in silicon. Specifically, we considered its interactions with the bath of nuclear spins of the ^{29}Si isotope. For small applied magnetic fields, the electron spin relaxation is controlled by the steady state distribution of the nuclear spins. We calculated the relaxation times T_1 and T_2 as functions of the external magnetic field, and concluded that nuclear spins play an important role in the donor electron spin decoherence in Si:P at low magnetic fields.

For general evaluation of relaxation processes at short times, of relevance for gate control of qubits and qubit-qubit interactions, we have initiated development of a new approximation scheme [9,10] for evaluation of decoherence. At low temperatures, the approximation is argued to apply at intermediate times as well, up to the thermal time scale $\hbar/kT$. It then provides an approach complementary to Markovian-type approximations, and is appropriate for evaluation of deviations from pure states in quantum computing models. Our work to apply this method to qubits in quantum-computing architectures, is ongoing, continuing under the new ARO grant. In various collaborations, we have also contributed to studies of spin transport, with applications in spintronics and quantum measurement: the full list of publications is provided in a later section. Appendix C is a manuscript [10] detailing our new approach to evaluation of relaxation and decoherence at short times.

REFERENCES

[1]   V. Privman, I. D. Vagner and G. Kventsel, *Phys. Lett.* **A 239**, 141 (1998).

[2]   B. E. Kane, *Nature* **393**, 133 (1998).

[3]   D. Mozyrsky, V. Privman and M. L. Glasser, *Phys. Rev. Lett.* **86**, 5112 (2001)
       — this article is attached as Appendix B.

[4]   D. Mozyrsky and V. Privman, *Mater. Phys. Mech.* **4**, 5 (2001).

[5]   V. Privman, D. Mozyrsky and I. D. Vagner, *Comp. Phys. Commun.* **146**, 331
       (2002) — this article is attached as Appendix A.

[6]   S. Saykin, D. Mozyrsky and V. Privman, Nano Letters **2**, 651 (2002).

[7]   A. V. Khaetskii, D. Loss and L. Glazman, *Electron spin decoherence in quantum
       dots due to interaction with nuclei*, preprint (2002).

[8]   I. A. Merkulov, A. L. Efros and M. Rosen, *Electron spin relaxation by nuclei in
       semiconductor quantum dots*, preprint (2002).

[9]   V. Privman, Modern Phys. Lett. B 16, 459 (2002).

[10]   V. Privman, *Initial Decoherence of Open Quantum Systems*, *J. Stat. Phys.*,
       in print (2003) — this article is attached as Appendix C.

PUBLICATIONS AND TECHNICAL REPORTS

Papers published in peer-reviewed journals

Measurement of a Quantum System Coupled to Independent Heat-Bath and Pointer Modes, D. Mozyrsky and V. Privman, Modern Phys. Lett. B 14, 303-312 (2000).

Nuclear-Spin Qubit Dephasing Time in the Integer Quantum Hall Effect Regime, D. Mozyrsky, V. Privman and I. D. Vagner, Phys. Rev. B 63, 085313, 1-6 (2001).

Indirect Interaction of Solid-State Qubits via Two-Dimensional Electron Gas, D. Mozyrsky, V. Privman and M.L. Glasser, Phys. Rev. Lett. 86, 5112-5115 (2001).
      This article was featured as an important new scientific breakthrough in the *Bulletin on Technology Perspectives*, published by the Ministry of Commerce, Science and Technology of the Russian Federation, Vol. 8, page 7 (July 2001).

Quantum Computing with Spin Qubits in Semiconductor Structures, V. Privman, D. Mozyrsky and I. D. Vagner, Computer Phys. Commun. 146, 331-338 (2002).

Quantum Computing in Semiconductor Structures with 0.1 μm Separation of Nuclear-Spin Qubits, D. Mozyrsky and V. Privman, Mater. Phys. Mech. 4, 5-7 (2001).

Interference Effects in Resonant Magneto-Transport, D. Mozyrsky, L. Fedichkin, S. A. Gurvitz and G. P. Berman, Phys. Rev. B 66, 161313, 1-4 (2002).

Short-Time Decoherence and Deviation from Pure Quantum States, V. Privman, Modern Phys. Lett. B 16, 459-465 (2002).

Relaxation of Shallow Donor Electron Spin due to Interaction with Nuclear Spin Bath, S. Saykin, D. Mozyrsky and V. Privman, Nano Letters 2, 651-655 (2002).

Manuscripts in-process in peer-reviewed journals

Initial Decoherence of Open Quantum Systems, V. Privman, J. Stat. Phys. 110, 957-970 (2003), in print.

Electron States in Nuclear-Spin-Polarization-Induced Quantum Dots, Yu. V. Pershin, submitted to Phys. Rev. B (2002).

Indirect Hyperfine Interaction Between Nuclear-Spin Qubits in Mesoscopic Wires and Rings, Yu. V. Pershyn, I. D. Vagner and P. Wyder, submitted to J. Phys.: Cond. Mat. (2002).

Paper published in conference proceedings

Invited Review *Decoherence and Measurement in Open Quantum Systems*,
V. Privman and D. Mozyrsky, in *Proceedings of the Conference "Quantum Computing III. AeroSense 2000"* (SPIE — The International Society for Optical Engineering), SPIE Proceedings Vol. 4047, 36-47 (2000).

Manuscript in-process in conference proceedings

Nuclear-Spin-Polarization-Induced Low-Dimensional Electron Structures,
Yu. V. Pershin, V. Fleurov, V. A. Ivanov, F. M. Peeters, S. N. Shevchenko, I. D. Vagner and P. Wyder, Proceedings of NATO ARW "Recent Trends in Theory of Physical Phenomena in High Magnetic Field" (Les Houches, 2002), in print.

Paper presented at a meeting, but no conference proceedings were published

Semiconductor Quantum Computer Design with 100 nm Separation of Nuclear-Spin Qubits, V. Privman and D. Mozyrsky, presented at "International Conference on Quantum Information 2001," Rochester, NY, June 12, 2001 (available online at http://arxiv.org/ftp/quant-ph/papers/0103/0103116.pdf).

Technical reports submitted to ARO

Annual Report for 1999 (covering September through December 1999).

Annual Report for 2000.

Brief Progress Report for ARDA, submitted in March 2001.

Annual Report for 2001.

Brief Progress Report for ARDA, submitted in March 2002.

Final Report: this document.

PRESENTATIONS BY THE PRINCIPAL INVESTIGATOR

Lectures and posters that did not involve publication, presented during the grant performance period

Presentation at the ARO Conference "Demonstration of and Algorithmic Development for Quantum Computers," DC area, Sept. 1, 1999.

"Hyperfine Interaction and Quantum Computation in Quantum Hall Effect Systems" — Poster at the Workshop on "Physics of Quantum Dots for Quantum Computing" at Naval Research Laboratory, DC area, Sept. 13, 1999.

"Decoherence of a Nuclear-Spin Qubit in 2D Semiconductor Structures in High Magnetic Fields," by D. Mozyrsky, V. Privman, I. D. Vagner — Contributed Talk at the 82nd Statistical Mechanics Meeting, Rutgers University, Dec. 10, 1999.

"Quantum Computing in Semiconductor Structures" — Presentation and Poster at the DARPA Workshop "Spins in Semiconductors (SPINS)," Santa Barbara, CA, Jan. 6, 2000.

"Quantum Information Processing: An Introduction" — Physics Department Colloquium at University of Central Florida, Orlando, FL, April 20, 2000.

"Quantum Computing with Nuclear Spins in Semiconductor Structures," by D. Mozyrsky and V. Privman — Poster at the CAMP Annual Conference, Lake Placid, NY, May 24, 2000.

"Nanotechnology" — Physics Department Seminar at Lehigh University, Bethlehem, PA, June 20, 2000.

"What is Nanotechnology?" — Invited Talk at the Workshop "Phase Separation Problems in Physics, Chemistry, and Biology" at Eotvos University, Budapest, Hungary, July 8, 2000.

"Quantum Computing with Nuclear Spins in Semiconductor Structures" — Invited Talk at the PIERS 2000 Conference, Cambridge, MA, July 12, 2000.

Presentation at the ARO 2000 Quantum Computing Program Review Conference, DC area, Aug. 30, 2000.

"Solid-State Quantum Computing in Semiconductor Structures" — Invited Presentation at the 2000 Air Force Research Laboratory Workshop "Quantum Computation for Physical Modeling," Boston area, MA, Oct. 18, 2000.

"Quantum Computing with Nuclear Spins in Semiconductor Structures," by D. Mozyrsky and V. Privman — Poster at the CAMP-Industry Symposium, Potsdam, NY, Oct. 19, 2000.

"Time Scales of Solid-State Quantum Computing" — Presentation and Poster at the DARPA Workshop "Quantum Information Science and Technology (QuIST)," Santa Barbara, DC area, Oct. 24, 2000.

"Quantum Computing with Nuclear Spins in Semiconductor Structures," by D. Mozyrsky and V. Privman — Presentation at the Special Poster Session for the Conference "Fine, Ultrafine and Nano Powders 2000", Potsdam, NY, Nov. 1, 2000.

"Solid-State Quantum Computing and Time Scales of Quantum Dynamics," Seminar at JPL, Pasadena, CA, Dec. 11, 2000.

"Solid-State Quantum Computing in Semiconductor Structures," Colloquium at CNLS, Los Alamos National Lab, Los Alamos, NM, Jan. 3, 2001.

"The Quantum Future of Information Nano-Technology," Seminar at the Materials Institute of SUNY at Albany, Albany, NY, March 5, 2001.

"Modeling of Coherent Solid-State Quantum Computing Devices," Presentation at the APS National Meeting, Seattle, WA. March 12, 2001.

"Solid-State Quantum Computing in Semiconductor Structures," Colloquium at Old Dominion University, Norfolk, VA, March 23, 2001.

"Solid-State Quantum Computing in Semiconductor Structures," Colloquium at University of Delaware, Newark, DE, April 13, 2001.

"The Quantum Future of Information Nano-Technology," Invited Talk at the Workshop "Quantum Processes and Modern Electronics," Holon, Israel, May 30, 2001.

"Quantum Computing with Spin Qubits in Semiconductor Structures," Seminar at Technion, Haifa, Israel, June 3, 2001.

"Quantum Computing with Spin Qubits in Semiconductor Structures," Poster at the "Advanced Research Workshop on Quantum Transport in Semiconductors," Maratea, Italy, June 21, 2001.

"Quantum Computing with Spin Qubits in Semiconductor Structures," Invited Talk at the "International Workshop on Computational Science and Engineering," National University of Singapore, July 2, 2001.

"Quantum Computing with Spin Qubits in Semiconductor Structures," Contributed Talk at the "International Conference on Materials for Advanced Technologies," Singapore, July 3, 2001.

"Quantum Computing with Spin Qubits in Semiconductor Structures," Colloquium at the Department of Physics, Hong Kong University of Science and Technology, July 9, 2001.

Presentation at the ARO Program Review, Baltimore, MD, Aug. 2001.

"The Quantum Future of Information Nanotechnology," Colloquium at University of South Florida, Tampa, Feb. 2002.

"The Quantum Future of Information Nanotechnology," Invited Talk at the NATO Advanced Research Workshop "Recent Trends in Theory of Physical Phenomena in High Magnetic Fields," February 26, 2002, Les Houches, France.

"Modeling of Coherent Solid-State Quantum Computing Devices," Colloquium at University of Porto, Portugal, April 19, 2002.

"Quantum Hall Semiconductor Quantum Computer Design," Invited Talk at the AFOSR Workshop "Quantum Computing for Physical Modeling" at Matha's Vineyard, MA, May 8, 2002.

"Quantum Information Processing and Spintronics," Invited Talk at CAMP Technical Meeting, Saratoga Springs, NY, May 14, 2002.

"Quantum Point Contact Detector," V. Privman, M.-C. Cheng, L. Fedichkin and D. Mozyrsky, Poster at CAMP Technical Meeting, Saratoga Springs, NY, May 14, 2002.

"Measures of Decoherence of Open Quantum Systems," V. Privman, A. Fedorov and L. Fedichkin, Poster at CAMP Technical Meeting, Saratoga Springs, NY, May 14, 2002.

"Spin Dephasing in Electron Spin-Polarized Transport," V. Privman, M.-C. Cheng and S. Saykin, Poster at CAMP Technical Meeting, Saratoga Springs, NY, May 14, 2002.

"Decoherence of Quantum States," V. Privman and D. Tolkunov, Poster at CAMP Technical Meeting, Saratoga Springs, NY, May 14, 2002.

"Transport of Spin Polarized Electrons in Semiconductors," V. Privman and Y. Pershin, Poster at CAMP Technical Meeting, Saratoga Springs, NY, May 14, 2002.

"Semiconductor Solid State Quantum Computing," Tutorial Talk at the NSF Workshop "Quantum Device Technology" at Clarkson University, Potsdam, NY, May 20, 2002.

"Decoherence of Quantum States," D. Tolkunov and V. Privman, Poster at the NSF Workshop "Quantum Device Technology" at Clarkson University, Potsdam, NY, May 21, 2002.

"Spin Dephasing in Electron Spin-Polarized Transport," S. Saykin, M.-C. Cheng and V. Privman, Poster at the NSF Workshop "Quantum Device Technology" at Clarkson University, Potsdam, NY, May 21, 2002.

"Transport of Spin Polarized Electrons in Semiconductors," Y. Pershin and V. Privman, Poster at the NSF Workshop "Quantum Device Technology" at Clarkson University, Potsdam, NY, May 21, 2002.

"Measures of Decoherence of Open Quantum Systems," A. Fedorov, L. Fedichkin and V. Privman, Poster at the NSF Workshop "Quantum Device Technology" at Clarkson University, Potsdam, NY, May 21, 2002.

"Initial Decoherence of Open Quantum Systems," Invited Talk at the NSF Workshop "Quantum Device Technology" at Clarkson University, Potsdam, NY, May 23, 2002.

"Transport of Spin-Polarized Electrons in Semiconductors," Y. Pershyn and V. Privman, Poster at the NSF Workshop "Computational Materials Theory" at University of Illinois at Urbana-Champagne, June 19, 2002.

"Modeling of Quantum Dynamics, Relaxation and Decoherence in Solid State Physics," Invited Talk at the NSF Workshop "Computational Materials Theory" at University of Illinois at Urbana-Champagne, June 20, 2002.

"Quantum Device Technology," Overview Talk at the Quantum Information Workshop, US Air Force Rome Laboratory, Aug. 6, 2002.

Presentation and Poster at the ARO Program Review, Nashville, TN, Aug. 21, 2002.

"Power Spectrum of Tunnel Current in Devices Candidates for Single Spin Measurement," L. Fedichkin and V. Privman, Poster at the ARO Program Review, Nashville, TN, Aug. 19, 2002.

"Spin Dephasing in Electron Spin Polarized Transport in 2DEG," S. Saykin and V. Privman, Poster at the ARO Program Review, Nashville, TN, Aug. 20, 2002.

 "Nuclear Spintronics," I. D. Vagner and V. Privman, Poster at the ARO Program Review, Nashville, TN, Aug. 22, 2002.

"Short Time Decoherence and Deviation from Pure Quantum States," Invited Talk at Feynman Festival, College Park, MD, Aug. 25, 2002.

"Modeling of Coherent Quantum Computing Devices," Physics Colloquium at University of Missouri, Columbia, MO, Sept. 23, 2002.

"Modeling of Coherent Quantum Computing Devices," Physics Colloquium at RPI, Troy, NY, Sept. 25, 2002.

"Quantum Device Technology," Invited Talk at the 2002 Workshop on Advanced Materials for Nano-Science and Nano-Technology, Montreal, Canada, Oct. 5, 2002.

"Spin Dephasing in Electron Spin Polarized Transport in 2DEG," S. Saykin, M. Shen, M.-C. Cheng and V. Privman, Poster at the 2002 Workshop on Advanced Materials for Nano-Science and Nano-Technology, Montreal, Canada, Oct. 5, 2002.

"Power Spectrum of Devices Candidate for Single Spin Measurement," L. Fedichkin, G. Berman, Sh. Gurvitz, D. Mozyrsky and V. Privman, Poster at the 2002 Workshop on Advanced Materials for Nano-Science and Nano-Technology, Montreal, Canada, Oct. 5, 2002.

"Transport of Spin Polarized Electrons in Semiconductors," Yu. Pershin and V. Privman, Poster at the 2002 Workshop on Advanced Materials for Nano-Science and Nano-Technology, Montreal, Canada, Oct. 5, 2002.

"Decoherence of Localized Electronic Spins In Semiconductors," A. Fedorov, L. Fedichkin and V. Privman, Poster at the 2002 Workshop on Advanced Materials for Nano-Science and Nano-Technology, Montreal, Canada, Oct. 5, 2002.

"Spin Dephasing in Electron Spin Polarized Transport in 2DEG," S. Saykin, M. Shen, M.-C. Cheng and V. Privman, Poster at the CAMP Fall Meeting, Potsdam, NY, Oct. 17, 2002.

"Decoherence of Localized Electronic Spins In Semiconductors," A. Fedorov, L. Fedichkin and V. Privman, Poster at the CAMP Fall Meeting, Potsdam, NY, Oct. 17, 2002.

"Interference Effects in Resonant Magnetotransport," L. Fedichkin, D. Mozyrsky, S. Gurvitz, G. Berman and V. Privman, Poster at the CAMP Fall Meeting, Potsdam, NY, Oct. 17, 2002.

"Solid State Quantum Computing," Solid State and Optics Seminar, Yale University, New Haven, CT, Oct. 23, 2002.

"Modeling of Coherent Solid-State Quantum Computing Devices," ECE Colloquium at University of Connecticut at Storrs, Oct. 24, 2002.

PARTICIPATING SCIENTIFIC PERSONNEL AND COLLABORATIONS

The PI:

Dr. V. Privman holds the rank of Professor of Physics and Professor of Electrical and Computer Engineering at Clarkson University. He is also the Director of the Center for Quantum Device Technology at Clarkson University and Member of the New York State Center for Advanced Materials Processing. He has received the following recognitions during the project performance period: Guest Editor, *Colloids and Surfaces A*; Member, Editorial Board, *Journal of Statistical Physics*; Member, Editorial Advisory Board, *Trends in Statistical Physics*; Member, Editorial Board, *High-Mag Theory Journal*; Scientific Advisory Board, PERI (Physics and Eng. Res. Inst.); Organizer, NSF-sponsored workshop series *Quantum Device Technology*; Program Committee for the symposia series *Quantum Computing* organized by The International Society of Optical Engineering; International Program Committee for the workshop series *Quantum Processes and Modern Electronics*; Program Committee for the symposia series *Experimental Quantum Computation and Quantum Communication*; Member, Technical Committee on *Spintronics, Nanomagnetism and Quantum Computing* of the IEEE Nanotechnology Council.

Researchers:

Theoretical collaborator Dr. I. D. Vagner is the Head of the Theory Group at the joint Max-Planck-Institut (Germany) and CNRS (France) High Magnetic Field Laboratory in Grenoble. In order to facilitate collaboration on this project, he was granted the courtesy rank of Research Professor at Clarkson University and occasionally visited for 1-2 months during the project performance period. Recently, he has moved to the Department of Communication Engineering at Holon Academic Institute of Technology in Israel, where he is full professor and department chairperson.

Theoretical collaborator Dr. D. Mozyrsky holds the rank of Research Assistant Professor at Clarkson University. Early in the project performance period, he was a postdoctoral associate with the PI. During the Summer of 2001, he moved to Los Alamos National Laboratory, but has retained the aforementioned courtesy affiliation with Clarkson in order to facilitate visits and collaborative work.

Postdoctoral associates Drs. L. Fedichkin, Yu. V. Pershyn and S. Saykin, have joined the group relatively recently, partially working on the topics of this project.

Students:

Graduate student A. Macchiavello has completed his M.Sc. thesis on a topic of this project, and Ya. Kievsky completed a non-thesis-option M.Sc. degree. Both degrees were in Physics. Undergraduate student J. Nesteroff, has worked on the topics of this project during 2001, and was awarded the prestigious McNair Scholarship for his undergraduate

research. Recently, he, as well as A. Fedorov, M. Shen and D. Tolkunov have joined the cadre of beginner graduate students who will progress towards Ph.D. in ECE (Nesteroff, Shen) or Physics (Fedorov, Tolkunov), in the general topics of this project.

Experimental collaborations:

During the project, contacts have been developed and maintained with experimental efforts. Communications with Dr. S. E. Barrett at Yale University resulted in useful research interactions and identification of experimental data related to our ongoing calculations of the decoherence times. Contacts with the group of Drs. H.-W. Jiang and E. Yablonovitch at UCLA, has helped us define research directions of importance in studies of spin-decoherence and measurement by transport in P-doped silicone. Collaborative effort has been initiated with the group of Dr. V. Narayanamurti at Harvard University. This group is presently setting up an effort, coordinated by Dr. R. Mani of Harvard, in realizing controlled nuclear spin quantum mechanical dynamics in semiconductor structures in the quantum Hall effect regime. The PI has been their theoretical advisor for this research.

Quantum computing with spin qubits in semiconductor structures

Vladimir Privman [*], Dima Mozyrsky, Israel D. Vagner

Department of Physics and Center for Advanced Materials Processing, Clarkson University, Potsdam, NY 13699-5820, USA

Received 16 February 2001

Abstract

We survey recent work on designing and evaluating quantum computing implementations based on nuclear or bound-electron spins in semiconductor heterostructures at low temperatures and in high magnetic fields. General overview is followed by a summary of results of our theoretical calculations of decoherence time scales and spin–spin interactions. The latter were carried out for systems for which the two-dimensional electron gas provides the dominant carrier for spin dynamics via exchange of spin-excitons in the integer quantum Hall regime. © 2002 Elsevier Science B.V. All rights reserved.

PACS: 73.20.Dx; 71.70.Ej; 03.67.Lx; 76.60.-k

Keywords: Quantum computing; Semiconductor; Decoherence; Spin; Qubit; Electron gas

1. Introduction

The field of quantum computing has seen explosive growth of experimental and theoretical interest. The promise of quantum computing [1–5] has been in exponential speedup of certain calculations via quantum parallelism. In Fig. 1, the top flow chart shows the "classical" computation which starts from binary input states and results in binary output states. The actual dynamics is not really that of Newtonian classical mechanics. Rather the computation involves many-body irreversible "gate" device components, made of semiconductor materials in modern computers, which evolve irreversibly, "thermodynamically" according to the laws of statistical mechanics. As the size of the modern computer components approaches atomic, the many-body quantum behavior will have to be accounted for in any case [6].

The idea of quantum computing, however, is not just to account for, but to actually utilize the quantum-mechanical dynamical behavior. This is not an easy task. Quantum mechanics allows for parallelism in evolution: one can "process" a linear superposition of several input states at once, as illustrated in the lower flow chart in Fig. 1. The price paid is that coherent processing of information, according to the law of quantum mechanics, must be accomplished in systems much larger than atomic-size (or more importantly, with many degrees of freedom). There are numerous conceptual and experimental obstacles to accomplishing this task, that have generated a lot of interest, excitement, and new results in computer science, physics, and engineering.

The functioning of a quantum computer involves initialization of the input state, then the actual dynamical evolution corresponding to computation, and finally reading off the result. Various specific requirements for implementation have been identified

---

[*] Corresponding author.
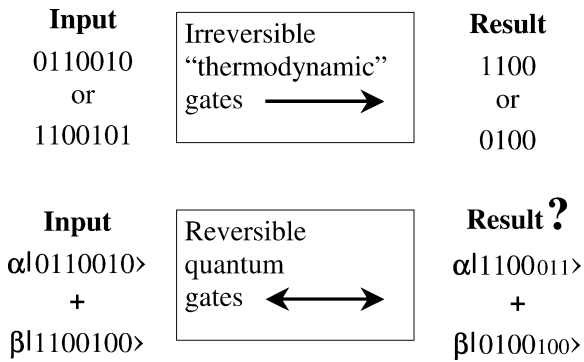*E-mail address:* privman@clarkson.edu (V. Privman).

Input		**Result**
0110010	Irreversible "thermodynamic" gates $\longrightarrow$	1100
or		or
1100101		0100

Input		**Result** $?$
$\alpha|0110010\rangle$	Reversible quantum gates $\longleftrightarrow$	$\alpha|1100_{011}\rangle$
$+$		$+$
$\beta|1100100\rangle$		$\beta|0100_{100}\rangle$

Fig. 1. Comparison of the classical and quantum approaches to computing. The upper flow chart schematically represents implementation of a traditional irreversible "classical" computation process, where transformation of the input set of bits into the result is accomplished by a succession of irreversible gates. Owing to their irreversibility, the gates can be connected in space rather than switched on and off at different times. The lower flow chart shows quantum processing of information, where the input and the final result are both in superposition states, yielding quantum parallelism. The dynamics is reversible: there is a one-to-one correspondence between the initial and final states. Therefore, number of the input and output quantum bit (qubits) is the same even though some of the output qubits (set in a smaller font) might not be used in the final extraction of the classical result by measurement. The quantum gates are applied in succession by being switched on and of at different times during the computation. The question mark signifies the difficulty of finding quantum algorithms that retain the power of quantum parallelism after measurement needed to read off the final result as classical information.

[2–5]; here we provide only a limited introductory overview.

Let us begin by considering the reading off of the final result. The reason for the question mark in the lower chart in Fig. 1 is that quantum measurement of the final superposition state can erase the gain of the parallel dynamics, by collapsing the wave function. Therefore, a key issue in quantum computing has been to find those algorithms for which the readout of the final state, by way of projecting out a certain average property, still retains the power of the quantum parallelism. To date, only few such examples are known [1,3,4,7], the most celebrated being the Shor algorithm [1] for factoring of integers, the invention of which boosted quantum computing from an obscure theoretical field to a mainstream research topic.

The preparation of the initial state does not seem to present a problem for most quantum computing realizations [2–5], except perhaps the ensemble liq-

uid state NMR approach [8,9] which relies on the initial thermal distribution to produce deviation of the density matrix from the equal-probability mixture state. In most other approaches, the initial state can be produced by first fully polarizing the quantum bits (qubits), i.e. putting them in one of the two quantum levels. Note that we consider two-state qubits here, realized, for instance, by spins 1/2 of nuclei or gate- or impurity-bound electrons, in applied magnetic field. The fully polarized state is then subject to gate operations to form the desired input state. Part of a quantum-computing algorithm should be the prescription on how to choose the initial state to represent the classical information of the input, like the input integer in the factoring. In most cases, this prescription is easily accomplished by single-qubit and two-qubit gates.

The actual dynamical evolution (the process of computation) in quantum computing is fully reversible and nondissipative, unlike classical computing. Much progress has been made in resolving both the conceptual and computer-engineering "design" issues for quantum computation. Specifically, the computation can be carried out [2–5,10–13] by a universal set of gates: single-qubit rotations and nearly any two-qubit gate. The gates are not connected in space like in classical computers but are activated in succession in time, to control single-spin dynamics and also switch on and off two-spin interactions (we use "spin" and "qubit" interchangeably).

Many interesting matters have been resolved, which are not reviewed here. These include the understanding of how the finiteness of the state space (i.e. two states for spin 1/2) replaces the "classical" digitalization in quantum computing. Also, the "classical" copying (fan-out) function is not possible in quantum mechanics. It is replaced by entanglement with ancillary qubits to accomplish redundancy needed for error correction [14–20]. Sources of errors due to interactions with environment in quantum mechanics involve not only the usual relaxation (thermalization) but also loss of coherence [21–28]. This quantum decoherence (dephasing) can be faster than relaxation because it does not require energy exchange.

A conceptually important issue has been the scalability of quantum computing: can one process macroscopically large amounts of information by utilizing quantum error correction based on redundancy via entanglement with ancillary qubits? The affirmative an-

swer to this question has been one of the triumphs of the theory [14–20]. It provided a new paradigm for emergence of controlled/organized macroscopic behavior from microscopic dynamics, on par with the conceptual possibility of living organisms, which we observe but cannot yet "manufacture", and million-gate classical computers which are man-made.

With all these theoretical advances at hand, the next step is to ask whether a man-made quantum computer can be realized? There have been several experimental directions of exploration, most presently are still at the level of one or two qubits, or, for ensemble liquid-state NMR, which emulates quantum dynamics by evolution of the density matrix of a large collection of molecules, 5–7 qubits.

In this introductory survey, we summarize results of our work on two-spin interactions and spin decoherence in semiconductor heterostructures. In Section 2, we consider the spin-based quantum computing proposals in such systems. Time scales of relaxation and decoherence are addressed in Section 3. Finally, Section 4 reports results for models with nuclear spins as qubits.

2. Spin-based quantum computing in semiconductor heterostructures

The general layout of a solid-state quantum computer is shown in Fig. 2. Qubits are positioned with precision of few nanometers in a heterostructure. One must propose how to effect and control single-qubit interactions, two-qubit interactions, and explore how the controlled dynamics owing to these interactions compares to decoherence and relaxation. The proposal must include ideas for implementation of initialization, readout, and gate functions.

The first proposal including all these components was for qubits realized in an array of quantum dots [29] coupled by electron tunneling. The first spin-based proposal [30] utilized nuclear spins coupled by the two-dimensional electron gas, the latter in the dissipationless integer quantum Hall state [31] that requires low temperatures and high magnetic fields. An important advancement was the work of Kane [32] where gate control of nuclear-spins of donor impurities, separated less than 10 nm and coupled via the outer impurity electrons which are bound at low tem-
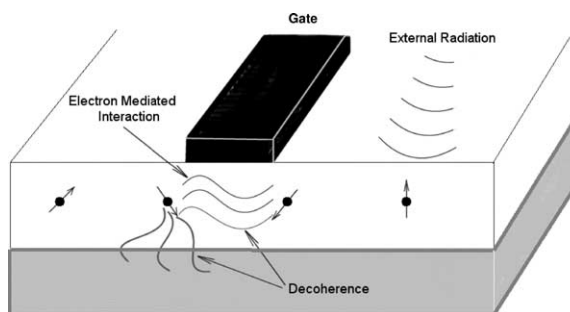

Fig. 2. Schematic illustration of a semiconductor heterostructure quantum information processor. The qubits, represented by the arrows overlaying heavy dots, are spins 1/2 of nuclei or localized electrons. Individual control of the temporal evolution of the spins can be achieved with the use of external electromagnetic radiation, i.e. NMR or ESR pulses. The spins are also coupled with each other via interaction mediated by the two-dimensional electron gas in the heterostructure, or by other means. The external and internal interactions can be controlled by gates formed on top of the heterostructure. The external environment, that includes crystal lattice, electron gas, defects, impurity potentials, causes relaxation and decoherence of the qubits.

peratures, was proposed. Most of these ideas also apply to electron-spin qubits, bound at impurities, in quantum dots, or directly by gates. Several elaborate solid-state heterostructure quantum computing schemes have been proposed in the literature recently [28,33–41]. There are also other promising proposals involving surface geometries: superconducting electronics [42–46] and electrons on the surface of liquid helium [47].

There have been several planned and ongoing experimental efforts [32–36,43–45,48–54] ultimately aimed at solid-state quantum computing and other quantum information processing realizations. The final geometry is expected to be most sensitive to the implementation of readout, because it involves quantum measurement, i.e. supposedly interaction with or transfer of information to a macroscopic device. Therefore, much of the experimental effort presently has been focused on single-qubit (single-spin) measurement approaches.

The theoretical efforts can be divided into two majors tasks. The process of single-spin measurement must be understood for the readout stage of quantum computing. Several conceptual and calculational advancements have been made in understanding quantum measurement [26,32–36,46,50,55,56] as it applies

to atomic-size qubit systems interacting with environment and typically "measured" directly by the effect of the spin-qubit state on transport, or first transferring the spin state to a charge state that is easier to measure, e.g., in single-electron transistors and similar devices.

In this survey, we outline results of the second evaluation task: that of understanding the processes and times scales involved in the dynamics of the actual computation. As summarized in Fig. 3, this main stage of the quantum computation process involves control of spins and their interactions. It also involves processes that we do not control and are trying to minimize: relaxation and decoherence.

Control of individual qubits is usually accomplished externally. For nuclear spins, NMR radio-frequency radiation can be used, see Fig. 2. For electron spins, the ESR microwave frequencies are suitable. Such radiation cannot be focused on the scale of 10–100 nm. Instead, selectivity must be accomplished by independent means. Several proposals exist, the most promising being control by gates. The applied gate voltage modifies the electronic wave function changing interactions and therefore resonant frequencies. We will denote the time scale of the external single-qubit control by T_{ext}. This can be the Rabi time of a spin flip.

The qubit–qubit interactions are typically assumed to be mediated by electrons that "visit" both qubit environments. For instance, in liquid-state ensemble NMR [8,9] with complex molecules, or in the original model [32] of phosphorous impurity donors in silicon, the wave functions of the valence, outer electrons of nearby qubits overlap. Specifically, in the P donor case, the single outer electron of the donor atom remains bound at low temperatures but has orbital radius of order 2 nm owing to the large dielectric constant of the silicon host. Therefore, it is hoped that these electrons, in nearby donors positioned as in Fig. 2, will mediate nuclear-spin qubit interactions.

Our approach [27,28] allows for larger qubit separation, up to order 100 nm, by relying on the two-dimensional electron gas in the heterostructure to mediate qubit–qubit interactions. This two-dimensional electron gas is usually obtained by spontaneous or gate-induced transfer of electrons from impurities to the two-dimensional interface layer in which the qubits are positioned. The source impurities are located at some separation from this layer or in the bulk. The two-dimensional electron gas can be made nondissipative in certain ranges of large applied magnetic fields at low temperatures, when these conduction electrons in the layer are in the integer quantum Hall effect state. Owing to this property and also larger qubit separation allowed, we consider this the most promising approach and focus our present review on such systems.

The time scale of the qubit–qubit interactions will be denoted by T_{int}. This is the time it takes to accomplish a two-qubit quantum gate, such as CNOT [2–5,57]. Typically for semiconductor quantum computing proposals, $T_{\text{int}} < T_{\text{ext}}$, and in fact the case with $T_{\text{int}} \ll T_{\text{ext}}$ has some advantages because one can use several fast single-spin flips to effectively switch interactions of some qubits off over the gate cycle. Another approach to controlling (on/off) of the two-qubit interactions is by gates, see Fig. 2, which affect the two-dimensional electron gas and the localized electron wavefunctions.

However, the same conduction electrons that provide the qubit–qubit interactions, also expose the qubits to the environment, causing relaxation and decoherence. Other interactions will also be present, that play no role in the useful quantum-computing dynamics but contribute to these undesirable processes. Relaxation and decoherence, and their associated time scales, are addressed in the next section.

3. Time scales of relaxation and decoherence

The processes of relaxation and decoherence considered here [21–28] are associated with the dynamics of a small, few-qubit quantum system as it interacts with the environment. Ultimately, for a large, multi-qubit system, many-body quantum chaos-like behavior must also be accounted for, and some advances in model system studies have been reported recently [5, 58]. Our discussion here will be for the few-qubit case mostly because it allows more system-specific investigations for actual quantum-computing proposals.

Dynamical processes that are unwanted in quantum computing, because they result from the environmental influences rather than from the controlled radiation pulses and gate potentials, can proceed on various time scales. In fact, it is not guaranteed that processes of various types, relaxation/thermalization vs. decoher-

ence/dephasing, can even be unambiguously distinctly identified.

At low temperatures, it is generally hoped that thermalization, which requires transfer of energy, slows down. If the fastest such processes proceed on time scales of order T_1, then this time increases at low temperatures because there are less excitations (phonons, electron gas modes, etc.) to couple the small quantum system to the rest of the solid-state host material.

On the other hand, processes that do not require flow of energy to or from the environment, can still effect the phase of the quantum-superposition amplitudes and cause decoherence. These processes can thus proceed faster, on the time scale T_2. While these comments seem to suggest that $T_2 \leqslant T_1$, there is no obvious reason to have generally $T_2 \ll T_1$ at low temperatures.

However, if the spectrum of the dominant excitations mediating the qubit coupling (both to each other and to the host material) has a gap, then we expect that all the relaxation and decoherence processes will be suppressed. Furthermore, the suppression of the relaxation will be exponential, with the Boltzmann factor for that energy gap. Then, $T_2 \ll T_1$ will be satisfied but also, more importantly, the actual values of both time scales will be inordinately large. This was found, theoretically and experimentally, to be the case for the integer-quantum-Hall-state two-dimensional electron gas as mediator of the localized-spin (nuclear, electronic) coupling in semiconductor heterostructures [27,28,59–63].

It is important to emphasize that relaxation and decoherence are really many-body properties of the system plus environment. Entanglement with the environment owing to the unwanted couplings results in the small quantum system having no pure wavefunction even if initially it was prepared in a pure state. Instead, it can be described by a statistical mixture represented by a density matrix, once the environment is traced over.

This reduced density matrix of the system is expected to evolve to the thermal one at large times. The approach to the thermal density matrix, which is diagonal in the system-energy basis, defines the time scale T_1. If the temperature is low enough, then there is the expectation, see [25,26] and references therein, that for some intermediate time scales, of order T_2, the density matrix becomes nearly-diagonal in a basis

Initialize

$$
\begin{array}{l}
\textbf{Control and} \\
\textbf{evolve in time} \\
T_{ext}, T_{int} \ll T_2, T_1
\end{array}
\left\{
\begin{array}{ll}
\textbf{Control qubits:} & T_{ext} \\
\textbf{\& interactions:} & T_{int} \;\; (> T_{ext}) \\
\\
\textbf{Avoid relaxation:} & T_1 \\
\textbf{\& decoherence:} & T_2 \;\; (\leq T_1)
\end{array}
\right.
$$

Measure

Fig. 3. Evaluation of quantum computing models. One of the criteria for feasibility of quantum computing in a given physical system is the possibility of initialization of the qubits in the desired superposition state. Another important design consideration is control of qubit states and of their interactions. In order to implement quantum computing effectively, the time scales for realization of single and two-qubit logic gates, T_{ext} and T_{int}, respectively, should be several orders of magnitude smaller than the time scales of relaxation and decoherence, T_1 and T_2. The relationships between these time scales are further explained in the text. Finally, efficient and reliable measurement of the output state of the qubits is required for reading off the result of the computation and presently represents a formidable experimental challenge.

which is determined not by the systems Hamiltonian (energy), but by the interaction operator with the environment. This latter process corresponds to loss of quantum coherence.

As emphasized in Fig. 3, evaluation of a quantum-computing proposal requires, among other things, establishing the relation $T_{ext}, T_{int} \ll T_2, T_1$. Owing to calculational difficulties, the single-qubit times $T_{1,2}$ will usually be used, though, as mentioned earlier, some study of the multi-qubit "quantum chaos" effects may be required. For spin-qubit quantum computing in semiconductor heterostructures, the relation is typically $T_{ext} \ll T_{int} \leqslant T_2 \ll T_1$, so the issue is usually how small is the quality ratio $Q = T_{int}/T_2$.

The required value of Q, needed for fault-tolerant quantum error correction, depends on the physical model of error sources and can be as small as $Q = 10^{-6}$–10^{-4}, see [15,18–20], or as large as $Q = 1/2$, see [64]. For the systems of interest to us here, spin qubits in semiconductor structures, the value of $Q = 10^{-5}$ is a reasonable working estimate. Thus, we seek systems/conditions with $T_{int}/T_2 \leqslant 10^{-5}$.

4. Results for nuclear-spin qubits

In this section we outline results for models of quantum computing with nuclear spins as qubits, and with coupling mediated by the two-dimensional elec-

Appendix A

tron gas in the integer quantum Hall effect state [27, 28,30]. In strong magnetic fields, the spatial states of the electrons confined in the two-dimensional layer in which the qubits are placed, see Fig. 2, are quantized by the field to resemble free-space Landau levels. The lattice potential and the impurities actually cause formation of narrow bands instead of the sharp levels, separated by localized states. As a result, for ranges of magnetic field, the localized states fill up while the extended states resemble completely filled integer number of Landau levels. These states are further Zeeman split owing to the electron spin. At low temperatures, one can find field values such that only one Zeeman sublevel is completely filled in the ground state.

The electronic state in such systems, that show the quantum Hall effect [31] in conductivity, are highly correlated and nondissipative. If nuclear spins are used as qubits, i.e. atoms with nuclear spin $1/2$ are sparsely positioned in the zero-nuclear spin host, such as the zero-nuclear-spin isotope 28 of Si, which constitutes 92% of natural silicone, then their zero-temperature relaxation will be significantly slowed down: experimentally, $T_1 \simeq 10^3$ sec [62].

Localized spins, both nuclear and electronic, interact by exchanges of spin excitons—spin waves consisting of a superposition of bound electron–hole pair states. The spectrum of these excitations [65,66], observed experimentally in [67], has a gap corresponding to the Zeeman splitting. This gap is the cause of slow relaxation and decoherence. The exchange of virtual spin excitons mediates the qubit–qubit interaction and also, via scattering of virtual excitons from impurity potentials, relaxation and decoherence of single qubits.

The original proposal to use nuclear spin qubits directly coupled by the two-dimensional electron gas [30], required positioning the qubits at distances comparable to several magnetic lengths. The latter is of order 10 nm for magnetic fields of several Tesla. The qubit–qubit interaction decays exponentially on this length scale. Recently, we proposed a new improved model [28] in which the qubit interactions are mediated via coupling of the two-dimensional electron gas to the outer impurity electrons. This applies if the atoms, whose nuclear spins are the qubits, are single-electron donors such as the isotope 31 of P. These phosphorous impurities were originally utilized in the model of Kane [32] where they must be actually positioned at separations of about 4 nm for the wavefunctions of the outer electrons, which are bound at low temperatures, to overlap significantly.

In our new improved model [28], with nuclear spins coupling to the outer bound electrons which, in turn, interact via the two-dimensional electron gas, the interaction turned out to be of a much longer range as compared to the model of [32]: the qubit separation can be of order 100 nm. Another advantage is that gate control of the individual qubits and of qubit–qubit interactions is possible. We have carried out extensive perturbative many-body calculations [27,28, 30,68] allowing estimation of T_{int} and T_2 for both the original quantum-computing proposal [30] and its improved version [28], where the main improvement is in the possibility of the gate control along the lines of [32]. The "clock speed" of the improved model is also faster by about two orders of magnitude. The technical details of these rather cumbersome calculations are available in the literature and will not be reviewed here.

The results are summarized in Table 1. We show estimates of all four relevant time scales for the two models introduced earlier. The "original" model [30] corresponds to nuclear spins $1/2$ introduced at qubits in atoms without an outer loosely bound electron. The "improved" model corresponds to the case when the outer electron is present and its interaction with the nuclear spin and the two-dimensional electron gas dominates the dynamics.

The data shown in Table 1 were obtained assuming typical parameters for the standard heterojunctions utilized in quantum-Hall-effect experiments today, and qubit separation of 65 nm. Thus, the parameter values taken [28,30] were more appropriate for the GaAs system than for Si, even though the main isotopes of gallium and arsenic have nuclear spin $3/2$ and cannot serve as spin-zero hosts. The reason

Table 1

Time scales of the qubit dynamics for the original [30] and improved [28] versions of the nuclear spin quantum computer with interactions mediated by the two-dimensional electron gas

	The original model	The improved model
T_{ext}	$O(10^{-5})$ sec	$O(10^{-5})$ sec
T_{int}	$O(1)$ sec	$O(10^{-2})$ sec
T_1	$O(10^3)$ sec	$O(10)$ sec
T_2	$O(10)$ sec	$O(10^{-1})$ sec

Appendix A

for using these values has been that experimental verification of some of the numbers might be possible in the available materials before cleaner and different composition materials needed for quantum computing are produced.

Our estimates, see Table 1, indicate that the quality factor $Q = 10^{-5}$ is not obtained for the present system. Actually, no quantum computing proposal to date, scalable by other criteria, satisfies the 10^{-5} quality-factor criterion. The values range from 10^{-1} to 10^{-2}. The resolution could come from development of better error-correction algorithms or from improving the physical system to obtain a better quality factor. In our estimation of the decoherence time scale, we used parameters typical of a standard, "dirty" heterostructure with large spatial fluctuations of the impurity potential. These heterostructures have been suitable for standard experiments because they provide wider quantum-Hall plateaus, i.e. ranges of magnetic field for which all the extended states of a Zeeman sublevel are filled. Much cleaner, ultra-high mobility structures can be obtained by placing the ionized impurity layer at a larger distance from the two-dimensional gas or by injecting conduction electrons into the heterostructure by other means. Thus, our quantum-computing proposals [28,30] are unique not only in the large qubit separation allowed but also in that there is a clear direction of exploration to allow physical, rather than algorithmic, resolution of the quality factor problem. This possibility should be further explored both experimentally and theoretically.

Acknowledgements

References

[1] P.W. Shor, in: Proc. 35th Annual Symposium on the Foundations of Computer Science, IEEE Computer Science Society Press, Los Alamitos, CA, 1994, p. 124.

[2] D.P. DiVincenzo, Science 270 (1995) 255.

[3] A. Ekert, R. Jozsa, Rev. Mod. Phys. 68 (1996) 733.

[4] A.M. Steane, Rept. Prog. Phys. 61 (1998) 117.

[5] G.P. Berman, G.D. Doolen, R. Mainieri, V.I. Tsifrinovich, Introduction to Quantum Computers, World Scientific, Singapore, 1998.

[6] S. Datta, Electronic Transport in Mesoscopic Systems, Cambridge University Press, 1997.

[7] L.K. Grover, Phys. Rev. A 79 (1997) 4709.

[8] N.A. Gershenfeld, I.L. Chuang, Science 275 (1997) 350.

[9] D.G. Cory, A.F. Fahmy, T.F. Havel, Proc. Natl. Acad. Sci. USA 94 (1997) 1634.

[10] A. Barenco, Proc. Roy. Soc. London A 449 (1995) 679.

[11] A. Barenco, C.H. Bennett, R. Cleve, D.P. DiVincenzo, N. Margolus, P. Shor, T. Sleator, J.A. Smolin, H. Weinfurter, Phys. Rev. A 52 (1995) 3457.

[12] D.P. DiVincenzo, Phys. Rev. A 51 (1995) 1015.

[13] S. Lloyd, Phys. Rev. Lett. 75 (1995) 346.

[14] P.W. Shor, in: Proc. 37th Annual Symposium on the Foundations of Computer Science, IEEE Computer Science Society Press, Los Alamitos, CA, 1996, p. 56.

[15] D. Aharonov, M. Ben-Or, Fault-tolerant quantum computation with constant error, Preprint, available at http://arxiv.org/abs/quant-ph/9611025, extended version at http://arxiv.org/abs/quant-ph/9906129.

[16] A. Steane, Phys. Rev. Lett. 78 (1997) 2252.

[17] D.P. DiVincenzo, in: L. Kowenhoven, G. Schoen, L. Sohn (Eds.), Mesoscopic Electron Transport, NATO Adv. Study Inst. Series E, Kluwer, Dordrecht, 1997.

[18] E. Knill, R. Laflamme, Phys. Rev. A 55 (1997) 900.

[19] D. Gottesman, Phys. Rev. A 57 (1998) 127.

[20] J. Preskill, Proc. Roy. Soc. London A 454 (1998) 385.

[21] A. Garg, Phys. Rev. Lett. 77 (1996) 764.

[22] G.M. Palma, K.A. Suominen, A.K. Ekert, Proc. Roy. Soc. London A 452 (1996) 567.

[23] I.S. Tupitsyn, N.V. Prokof'ev, P.C.E. Stamp, Int. J. Modern Phys. B 11 (1997) 2901.

[24] T. Maniv, Yu.A. Bychkov, I.D. Vagner, P. Wyder, Fast incomplete decoherence of nuclear spins in quantum hall ferromagnet, Preprint, available at http://arxiv.org/abs/cond-mat/0011361.

[25] D. Mozyrsky, V. Privman, J. Stat. Phys. 91 (1998) 787.

[26] D. Mozyrsky, V. Privman, Modern Phys. Lett. B 14 (2000) 303.

[27] D. Mozyrsky, V. Privman, I.D. Vagner, Phys. Rev. B 63 (2001) 085313.

[28] D. Mozyrsky, V. Privman, M.L. Glasser, Indirect interaction of solid-state qubits via two-dimensional electron gas, Preprint, available at http://arxiv.org/abs/cond-mat/0012470.

[29] D. Loss, D.P. DiVincenzo, Phys. Rev. A 57 (1998) 120.

[30] V. Privman, I.D. Vagner, G. Kventsel, Phys. Lett. A 239 (1998) 141.

[31] R.E. Prange, S.M. Girvin (Eds.), The Quantum Hall Effect, Springer-Verlag, New York, 1987.

[32] B.E. Kane, Nature 393 (1998) 133.

[33] A. Imamoglu, D.D. Awschalom, G. Burkard, D.P. DiVincenzo, D. Loss, M. Sherwin, A. Small, Phys. Rev. Lett. 83 (1999) 4204.

Appendix A

[34] R. Vrijen, E. Yablonovitch, K. Wang, H.W. Jiang, A. Balandin, V. Roychowdhury, T. Mor, D.P. DiVincenzo, Phys. Rev. A 62 (2000) 012306.

[35] G.P. Berman, G.D. Doolen, P.C. Hammel, V.I. Tsifrinovich, Solid-state nuclear spin quantum computer based on magnetic resonance force microscopy, Preprint, available at http://arxiv.org/abs/quant-ph/9909033.

[36] S. Bandyopadhyay, Phys. Rev. B 61 (2000) 13 813.

[37] J.H. Reina, L. Quiroga, N.F. Johnson, Quantum information processing in semiconductor nanostructures, Preprint, available at http://arxiv.org/abs/quant-ph/0009035.

[38] R. Ionicioiu, G. Amaratunga, F. Udrea, Quantum computation with ballistic electrons, Preprint, available at http://arxiv.org/abs/quant-ph/0011051.

[39] J. Levy, Quantum information processing with ferroelectrically coupled quantum dots, Preprint, available at http://arxiv.org/abs/quant-ph/0101026.

[40] X. Hu, S. Das Sarma, Solid state quantum computation with spin qubits: Can it be done in multielectron dots?, Preprint, available at http://arxiv.org/abs/cond-mat/0101102.

[41] X. Hu, S. Das Sarma, Theoretical issues in spin-based quantum dot quantum computation, Preprint, available at http://arxiv.org/abs/cond-mat/0102019.

[42] Yu. Makhlin, G. Schoen, A. Shnirman, Nature 398 (1999) 305.

[43] J. Mooij, T. Orlando, L. Levitov, L. Tian, V. van der Wal, S. Lloyd, Science 285 (1999) 1036.

[44] Y. Nakamura, Yu.A. Pashkin, J.S. Tsai, Nature 398 (1999) 786.

[45] J.R. Friedman, V. Patel, W. Chen, S.K. Tolpygo, J.E. Lukens, Detection of a Schröedinger's cat state in an rf-SQUID, Preprint, available at http://arxiv.org/abs/cond-mat/0004293.

[46] D.V. Averin, Quantum computing and quantum measurement with mesoscopic Josephson junctions, Preprint, available at http://arxiv.org/abs/quant-ph/0008114.

[47] P.M. Platzman, M.I. Dykman, Science 284 (1999) 1967.

[48] J.A. Jones, M. Mosca, J. Chem. Phys. 109 (1998) 1648.

[49] J.R. Tucker, T.-C. Shen, Solid State Electron. 42 (1998) 1061.

[50] B.E. Kane, N.S. McAlpine, A.S. Dzurak, R.G. Clark, G.J. Milburn, H.B. Sun, H. Wiseman, Phys. Rev. B 61 (2000) 2961.

[51] R.G. Clark, unpublished results presented at a quantum-computing conference held in Baltimore, MD, August 2000.

[52] R. Vrijen, E. Yablonovitch, A spin-coherent semiconductor photo-detector for quantum communication, Preprint, available at http://arxiv.org/abs/quant-ph/0004078.

[53] H.W. Jiang, E. Yablonovitch, Gate-controlled electron spin resonance in a GaAs/AlGaAs heterostructure, Preprint, available at http://arxiv.org/abs/quant-ph/0102044.

[54] H. Kosaka, A.A. Kiselev, F.A. Baron, K.W. Kim, E. Yablonovitch, Electron g-factor engineering in III–V semiconductors for quantum communications, Preprint, available at http://arxiv.org/abs/quant-ph/0102056.

[55] A.N. Korotkov, D.V. Averin, Continuous weak measurement of quantum coherent oscillations, Preprint, available at http://arxiv.org/abs/cond-mat/0002203.

[56] A.N. Korotkov, Selective quantum evolution of a qubit state due to continuous measurement, Preprint, available at http://arxiv.org/abs/cond-mat/0008461.

[57] V. Privman, D. Mozyrsky, S.P. Hotaling, in: Proc. Conf. Photonic Quantum Computing. AeroSense 97, SPIE Proc., Vol. 3076, SPIE—The International Society for Optical Engineering, 1997, p. 84.

[58] G.P. Berman, F. Borgonovi, F.M. Izrailev, V.I. Tsifrinovich, Avoiding quantum chaos in quantum computation, Preprint, available at http://arxiv.org/abs/quant-ph/0012106.

[59] I.D. Vagner, T. Maniv, Phys. Rev. Lett. 61 (1988) 1400.

[60] R. Tycko, S.E. Barrett, G. Dabbagh, L.N. Pfeiffer, K.W. West, Science 268 (1995) 1460.

[61] S.E. Barrett, G. Dabbagh, L.N. Pfeiffer, K.W. West, R. Tycko, Phys. Rev. Lett. 74 (1995) 5112.

[62] A. Berg, M. Dobers, R.R. Gerhards, K.V. Klitzing, Phys. Rev. Lett. 64 (1990) 2563.

[63] S.V. Iordanskii, S.V. Meshkov, I.D. Vagner, Phys. Rev. B 44 (1991) 6554.

[64] E. Knill, R. Laflamme, G. Milburn, Thresholds for linear optics quantum computation, Preprint, available at http://arxiv.org/abs/quant-ph/0006120.

[65] Yu.A. Bychkov, S.V. Iordanskii, G.M. Eliashberg, JETP Lett. 33 (1981) 143.

[66] C. Kallin, B.I. Halperin, Phys. Rev. B 30 (1984) 5655.

[67] A. Pinczuk, B.S. Dennis, D. Heiman, C. Kallin, L. Brey, C. Tejedor, S. Schmitt-Rink, L.N. Pfeiffer, K.W. West, Phys. Rev. Lett. 68 (1992) 3623.

[68] Yu.A. Bychkov, T. Maniv, I.D. Vagner, Solid State Commun. 94 (1995) 61.

Indirect Interaction of Solid-State Qubits via Two-Dimensional Electron Gas

Dima Mozyrsky, Vladimir Privman, and M. Lawrence Glasser

Department of Physics, Clarkson University, Potsdam, New York 13699-5820
(Received 2 January 2001)

We propose a mechanism of long-range coherent coupling between nuclear spin qubits in semiconductor-heterojunction quantum information processing devices. The coupling is via localized donor electrons which interact with the two-dimensional electron gas. An effective interaction Hamiltonian is derived and the coupling strength is evaluated. We also discuss mechanisms of decoherence and consider gate control of the interaction between qubits. The resulting quantum computing scheme retains all the control and measurement aspects of earlier approaches, but allows qubit spacing at distances of the order of 100 nm, attainable with the present-day semiconductor device technologies.

Recent technological advances in electronics related to spin polarization [1,2] have boosted experimental and theoretical interest in quantum information science in condensed matter systems, specifically, in semiconductor heterostructures at low temperatures and in high magnetic fields. The solid-state implementations of quantum information devices seem to be among the most promising ones, due to possible scalability of the elementary logic gates into more complicated integrated circuits. Several designs for solid state and related spin-based quantum information processors have been suggested [3–8]. Preliminary experiments, involving several quantum bits (qubits), have been carried out or are being contemplated [9,10].

Our work stems from the proposals that utilize nuclear or electronic spins as qubits for information processing [3–7]. These are natural choices for qubits because at low temperatures spin states in semiconductors have relatively long decoherence times, sometimes milliseconds or even longer for electronic spins, and seconds for nuclear spins [11–14]. We propose a new mechanism for coupling between two nuclear-spin qubits, combining aspects of two models of quantum information processors, one based on nuclear spins in quantum-Hall effect systems [4], and another utilizing the nuclear spins of phosphorous donors in a silicon heterostructure [5].

An appealing aspect of Kane's model [5] is a possibly experimentally feasible scheme for reading out the state of the quantum register, i.e., measurement of a nuclear spin, achieved by transferring the nuclear-spin polarization to the electronic state, while the latter is measured with the use of a single electron transistor. The model proposed in [4] has a different advantage: Unlike [5], the interaction between the nuclear spins is mediated by the two-dimensional (2D) electron gas, and thus is longer ranged due to the highly correlated state of the 2D electron gas in the quantum-Hall regime. This opens up possibilities for experimental realization of such quantum information processors, because large separation between spin qubits means greater lithographic dimensions in manufacturing the device. The price paid is that the coupling is weak,

and therefore the time scales of the "gate function" can be as large as 1 s.

In this work we combine the two proposals, thus retaining the measurement and control scheme proposed in [5,7,9] and at the same time allowing larger separations, of the order of 100 nm, between interacting qubits. The resulting system is thus realizable with the present-day semiconductor technologies. We propose a model where sparsely positioned phosphorous donors are imbedded in a 2D electron gas in the quantum-Hall regime. The localized donor electrons interact via the delocalized 2D electrons and thus indirectly mediate nuclear-spin interactions. In 3D, spin coupling mechanisms via conduction electrons have been well studied [15]. Here, we estimate the range of this induced nuclear-spin interaction for the 2D case and find it to be of the order of 100 nm. This is large compared to atomic dimensions, donor-electron bound state radii, and even the electronic magnetic length which is typically of the order of 10 nm. We find that this interaction is also stronger, thus corresponding to faster gate function times, than in [4].

We assume that the coupling between the electronic and the nuclear donor spins is given by the Fermi contact interaction, $H_{e-n} = A\sigma_n \cdot \sigma_e$. Here, $A = (8\pi/3)\mu_B g_n \mu_n |\Psi_0(0)|^2$, where μ_n and g_n are the nuclear magnetron and nuclear g factor, respectively, $|\Psi_0(0)|^2$ is the donor-electron probability density at the nucleus, μ_B denotes the Bohr magnetron, and σ's are Pauli matrices. Coupling of the delocalized electrons to the nuclear spin is considerably weaker than that of the localized donor electron. Therefore, we assume that the nuclear spin interacts with conduction electrons indirectly via the donor electron.

As a prototype system, we consider ^{31}P donors positioned in Si, so all the spins involved are $\frac{1}{2}$. The donor electronic and nuclear spins form a four-level system. The spectrum of this two-spin system can be obtained to $O(A)$ with H_{e-n} treated as perturbation. The energy levels are $E_0 = -(\gamma_n + \Delta)/2 + A$, $E_1 = (\gamma_n - \Delta)/2 - A$, $E_2 = (-\gamma_n + \Delta)/2 - A$, and $E_3 = (\gamma_n + \Delta)/2 + A$, where $\gamma_n = g_n \mu_n H$ is the nuclear-spin splitting. Here, H is the

magnetic field, and the expression for Δ, the electronic Zeeman gap, will be given shortly. The eigenstates associated with these energy levels are $|0\rangle = |\downarrow e \downarrow n\rangle$, $|1\rangle = |\downarrow e \uparrow n\rangle + (2A/\Delta)|\uparrow e \downarrow n\rangle$, $|2\rangle = |\uparrow e \downarrow n\rangle + (2A/\Delta)|\downarrow e \uparrow n\rangle$, and $|3\rangle = |\uparrow e \uparrow n\rangle$, where $|\downarrow e \downarrow n\rangle$ represents the electronic and nuclear-spin down state, etc. Here we propose to consider the states $|0\rangle$ and $|1\rangle$ as qubit states of a quantum computer. By altering the hyperfine coupling constant A by distorting the spatial state Ψ_0 of the donor electron with an electrostatic gate [5,7], one can selectively control the state of an individual qubit by means of the NMR technique.

In order to calculate the interaction Hamiltonian between two qubits, we first consider the coupling between the donor electron and conduction electrons. The ground state of the donor electron is bound (localized) and will typically lie in the energy gap, several meV below the conduction band edge. For temperatures of order mK, electronic transitions from this localized state to the conduction band are highly improbable. The dominant interaction between the localized electron and conduction electrons is their Coulomb interaction. We are interested only in the exchange part of this interaction, i.e., the spin-dependent part. The spin-independent part causes screening, but it is weak in 2D [16] and, especially in the presence of the magnetic field, cannot ionize the donor.

In a large magnetic field, the delocalized 2D electrons occupy highly degenerate Landau energy levels [16]. It is convenient to introduce electron bound state creation and annihilation operators $b_{ns}^{\dagger}$ and b_{ns}, where n represents the donor spatial state, and s is the spin z component, $\uparrow$ or $\downarrow$. Let $a_{mk_x s}^{\dagger}$, $a_{mk_x s}$ denote the creation and annihilation operators for the delocalized 2D electrons, where m labels the Landau level, while $\hbar k_x$ is the x momentum (we use the asymmetric gauge). Then the exchange coupling between the bound and delocalized electrons can be written as

$$H_{\text{ex}} = \frac{1}{2} \sum G_{m,m',k_x,k_x'}^{n,n'} b_{ns}^{\dagger} a_{mk_x s'}^{\dagger} b_{n's'} a_{m'k_x' s}, \quad (1)$$

where the sum is over all the indices. Here, we have neglected the spin-orbit interaction. In what follows, we will retain only the lowest donor-electron spatial state, i.e., account only for the transitions between the two Zeeman levels of the ground state.

The 2D electrons are assumed to be in a nondissipative quantum-Hall state with filling factor $\nu = 1$; i.e., the lower Zeeman sublevel of the Landau ground state is completely filled [4]. This choice ensures reduced decoherence and relaxation effects [14], owing to the energy gap in the spectrum of the lowest-energy spin-wave excitations which are well studied [17,18]; their spectrum is given

by $\mathcal{E}_{\mathbf{k}} = \Delta + E_c[1 - I_0(\ell^2 k^2/4) \exp(-\ell^2 k^2/4)]$, where I_0 is the modified Bessel function. Here, $\Delta = g\mu_B H$ is the Zeeman gap, $E_c = (\pi/2)^{1/2}(e^2/\epsilon\ell)$ is the characteristic Coulomb energy, and g is the effective g factor in the potential well that holds the 2D electron gas, while ϵ is the dielectric constant of the material, and $\ell = (\hbar c/eH)^{1/2}$ is the magnetic length. Extension to larger integer filling factors is possible [14,17,18]. One can also introduce [18] normalized creation and annihilation operators for the spin waves, quadratic in electronic operators,

$$S_{\mathbf{k}}^{\dagger} = \left(\frac{2\pi\ell^2}{L_x L_y}\right)^{1/2} \sum_p e^{i\ell^2 k_y p} a_{p+(k_x/2),\downarrow}^{\dagger} a_{p-(k_x/2),\uparrow}, \quad (2)$$

Here, $L_{x,y}$ are the transverse dimensions, taken to infinity in the final calculation. The summation over p is taken in such a way [18] that the wave number subscripts are quantized in multiples of $2\pi/L_x$. The spectrum of these spin waves has been experimentally verified in GaAs heterostructures [19].

We will include only these lowest excitations in the sum (1); our goal is to rewrite (1) in terms of the spin-wave operators (2). The exchange coupling is thus truncated to $G_{m,m',k_x,k_x'}^{n,n'} = G_{k_x,k_x'} \delta_{n,0} \delta_{n',0} \delta_{m,0} \delta_{m',0}$, where

$$G_{k_x,k_x'} = \int d^3\mathbf{R}_1 \, d^3\mathbf{R}_2 \, \Psi_0^*(\mathbf{R}_1)\Psi_0(\mathbf{R}_2)$$
$$\times U(\mathbf{R}_1 - \mathbf{R}_2)\Phi_{0,k_x}^*(\mathbf{R}_2)\Phi_{0,k_x'}(\mathbf{R}_1), \quad (3)$$

$U(\mathbf{R}_1 - \mathbf{R}_2) = e^2/\epsilon|\mathbf{R}_1 - \mathbf{R}_2|$ is the Coulomb interaction, and $\Psi_0(\mathbf{R})$ is the donor-electron ground state. The states of the conduction electrons confined in the 2D well are $\Phi_{0,k_x'}(\mathbf{R}) = \phi_{0,k_x'}(\mathbf{r})\chi(z)$, where $\phi_{0,k_x'}(\mathbf{r})$ are the standard 2D Landau states [16]; $\chi(z)$ describes the confinement of the conduction electron wave function in the z direction and depends on the nature of the confinement potential. Here and in the following $\mathbf{R} = (\mathbf{r}, z)$, with $\mathbf{R}$ and $\mathbf{r} = (x, y)$ being 3D and 2D coordinates, respectively, while z is the direction perpendicular to the heterostructure, in which the applied magnetic field is pointing.

With the use of the expressions for Landau ground state wave functions, $\phi_{0,k_x'}(\mathbf{r}) = \ell^{-1}(\pi L_x)^{-1/2} e^{ik_x x} \times \exp[-(y - \ell^2 k_x)^2/2\ell^2]$, and (2), after a lengthy calculation, we get

$$H_{\text{ex}} = \frac{1}{2} \sum_{\mathbf{k}} [W_{\mathbf{k}}|\uparrow_e\rangle\langle\downarrow_e|S_{\mathbf{k}} + W_{\mathbf{k}}^*|\downarrow_e\rangle\langle\uparrow_e|S_{\mathbf{k}}^{\dagger}], \quad (4)$$

where $|\uparrow_e\rangle\langle\downarrow_e| = b_{\uparrow}^{\dagger} b_{\downarrow}$ in the appropriate subspace, and

$$W_{\mathbf{k}} = \frac{1}{\ell(2\pi L_x L_y)^{1/2}} \int d^3\mathbf{R}_1 \, d^3\mathbf{R}_2 \, \Psi_0^*(\mathbf{R}_1)\Psi_0(\mathbf{R}_2)$$
$$\times U(\mathbf{R}_1 - \mathbf{R}_2)\chi^*(z_2)\chi(z_1)C_{\mathbf{k}}(\mathbf{r}_1, \mathbf{r}_2), \quad (5)$$

$$C_{\mathbf{k}}(\mathbf{r}_1, \mathbf{r}_2) \equiv \exp\left\{-\frac{1}{4\ell^2}[(x_1 - x_2)^2 + (y_1 - y_2)^2 - 2i(x_1 - x_2)(y_1 + y_2)]\right\}$$
$$\times \exp\left[-\frac{\ell^2}{4}(k_x^2 + k_y^2) - \frac{k_y}{2}(iy_1 + iy_2 - x_1 + x_2) - \frac{k_x}{2}(ix_1 + ix_2 + y_1 - y_2)\right]. \quad (6)$$

Note that since all the position vectors $\mathbf{R}$, $\mathbf{r}$ are measured from the origin at the donor atom, the quantity $W_{\mathbf{k}}$ depends also on the donor coordinates. To the leading order, (4) gives the interaction of the donor electron spin with excitations of the 2D electron gas in the $\nu = 1$ integer quantum-Hall state.

One can rewrite the interaction (4)–(6), with (4) multiplied by the unit operator in the nuclear-spin Hilbert space, in terms of the eigenstates of the electron-nucleus system. With the use of the expressions derived earlier for these eigenstates in terms of direct products of electronic and nuclear spin states, we obtain

$$H_{\text{ex}} = \frac{1}{2} \sum_{\mathbf{k}} W_{\mathbf{k}} \left(\frac{2A}{\Delta} |1\rangle\langle 0| + |2\rangle\langle 0| \right.$$
$$\left. + |3\rangle\langle 1| - \frac{2A}{\Delta} |3\rangle\langle 2| \right) S_{\mathbf{k}} + \text{H.c.} \qquad (7)$$

Now one can calculate an effective Hamiltonian for the interaction of two qubits. Since the electronic Zeeman gap is much larger than the nuclear one, we can truncate the Hilbert space of the combined electron-nucleus spins to the two lowest lying states. Thus, we retain only the $|0\rangle\langle 1|$ and conjugate transitions in the exchange interaction (7).

An effective interaction between two qubits can be obtained within the standard framework of second order perturbation theory by tracing out the states of the spin waves; see [15,20,21] for similar calculations. The result can be written as

$$H_{1,2} = J|0_1 1_2\rangle\langle 1_1 0_2| + J^*|1_1 0_2\rangle\langle 0_1 1_2|. \qquad (8)$$

Here, the coupling constant between the two qubits is

$$J = \left(\frac{A}{\Delta} \right)^2 \sum_{\mathbf{k} \neq 0} \frac{W_{\mathbf{k},1} W_{\mathbf{k},2}^*}{\mathcal{E}_{\mathbf{k}} + E_1 - E_0}. \qquad (9)$$

The subscripts 1 and 2 in (8) and (9) label the two donor qubits, while $W_{\mathbf{k},1}$ and $W_{\mathbf{k},2}$ are the coupling constants of each donor electron spin to spin waves, given by (5), and $\mathcal{E}_{\mathbf{k}}$ is the spin-wave energy.

The nuclear-spin energy gap is much smaller than the electronic spin-wave excitation energies. Therefore, we can ignore $E_1 - E_0$ in the denominator in (9). Furthermore, due to the large value of the spin-wave spectral gap at $\mathbf{k} = 0$, $\mathcal{E}_0 = \Delta$, we do not have the "small denominator" problem encountered in other calculations of this sort, e.g., [20]. Physically, this means that the spin excitations in the 2D electron gas mediating the effective qubit-qubit interaction are virtual, and so this interaction does not cause appreciable relaxation or decoherence on the gate function time scale $\hbar/J$.

It is important to note that one can construct a universal CNOT logic gate from the controlled dynamics governed by Hamiltonians of the form of $H_{1,2}$ and single qubit rotations [6]. The coupling strength J between the qubits can be externally controlled by the electrostatic gates built above the 2D inversion layer. By applying gate voltages, one can locally vary the density of the 2D electrons, thus changing coupling between the delocalized and donor electrons.

This results in control over the effective coupling constant J in (9). The precise effect of gates on interactions between the qubits, as well as on decoherence of their states, should be further studied in order to establish the feasibility of the quantum-computing approach proposed here. Most other semiconductor solid-state quantum-computing approaches [3–7] utilize gates.

Let us explicitly calculate the coupling constant J in (8) and (9). Because the spatial ground state of the donor is localized on a scale smaller than the magnetic length ℓ, the overlap integrand in (5) is vanishingly small for $|\mathbf{r}_1 - \mathbf{r}_2| > \ell$. At the same time, for $|\mathbf{k}| > 1/\ell$, the value of $C_{\mathbf{k}}$ decreases exponentially. Thus, $C_{\mathbf{k}}$ can be simplified by neglecting the $x_1 - x_2$ and $y_1 - y_2$ terms in (6). Moreover, for two donors at separation larger than ℓ, we can put $(\mathbf{r}_1 + \mathbf{r}_2)/2 \simeq \mathbf{r}_j$, with $\mathbf{r}_j$ being the location of either one of them. Then (5) can be approximated by $W_{\mathbf{k},j} = Z(L_x L_y)^{-1/2} \exp(-\frac{\ell^2 k^2}{4} - i\mathbf{k} \cdot \mathbf{r}_j)$, with $Z = (1/2\pi\ell^2)^{1/2} \int d^3\mathbf{R}_1 d^3\mathbf{R}_2 \Psi_0^*(\mathbf{R}_1)\Psi_0(\mathbf{R}_2)U(\mathbf{R}_1 - \mathbf{R}_2) \times \chi^*(z_2)\chi(z_1)$.

Finally, the coupling constant J of the effective interaction (8) can be obtained by transforming the summation in (9) to integration in the limit $L_{x,y} \to \infty$,

$$J = \left(\frac{A}{\Delta} \right)^2 \frac{|Z|^2}{(2\pi)^{1/2} E_c \ell^2} \left(\frac{d}{r} \right)^{1/2} \exp\left(-\frac{r}{d} \right),$$
$$(r > \ell), \qquad (10)$$

where $d = (E_c/2\Delta)^{1/2}\ell$. A similar dependence of the coupling on the donor separation r was obtained in a study of nuclear polarization diffusion in the quantum-Hall regime [21]. Interaction (8) between the spins has finite range d, which, however, is very large compared to the effective Bohr radius of the donor ground state. Thus, the indirect exchange at large distances dominates the direct exchange interaction resulting from the overlap of the two atomic wave functions. For magnetic field $H = 6$ T and $\epsilon = 12$, we get $d \simeq 65$ nm, which is indeed much greater than the characteristic Bohr radius for a donor electron in silicon.

In order to estimate J, we have to evaluate the overlap integral Z. For an order-of-magnitude estimate, we will assume that $\chi(z)$ is constant inside the well and zero outside. Then $Z \simeq (2\pi)^{-1/2}(\delta\ell)^{-1} \int d^3\mathbf{R}_1 d^3\mathbf{R}_2 \times \Psi_0^*(\mathbf{R}_1)\Psi_0(\mathbf{R}_2)U(\mathbf{R}_1 - \mathbf{R}_2)$, where δ is the width of the well. We put $\delta \simeq 4$ nm. For $\Psi_0(\mathbf{R})$, the donor ground state, we choose a spherically symmetric hydrogenlike ground state with the effective Bohr radius $a_B \simeq 2$ nm. This is, of course, not the case in a realistic situation [22]. The ground state of the donor will be influenced by the band structure, by the magnetic field, and by the confining 2D well potential, while the states of the conducting electrons will be distorted by the impurity potentials. We are not aware of a thorough study of these effects for our system. For the purposes of an order of magnitude estimate, however, a spherical state should be sufficient.

Evaluating the integral for the Coulomb potential U, we obtain $Z \simeq (5a_B^2/16\delta)E_c$. Assuming that the two donors are separated by the distance $r = 100$ nm and using the value $2A/h = 58$ MHz from [4], we obtain the estimate $J/\hbar \sim 10^2$ s^{-1}.

The clock speed of the information processor just described appears to be a fraction of kHz and should be compared with the time scales for relaxation and decoherence. The leading mechanism for these at low temperatures is through interaction with impurities. It has been found theoretically [12,23] and confirmed experimentally [2] that nuclear-spin relaxation in the quantum-Hall regime is slow and strongly dependent on the impurity potentials; typically, the relaxation time T_1 is of order 10^3 s. In our case, the interaction of a qubit with the 2D gas is stronger, and, as a result, the relaxation is expected to be faster. An estimate from formulas in [12,23] gives $T_1 \simeq 1$ s. There is, however, another important issue—decoherence, on time scales T_2. Recently, this quantity has been calculated in the same framework, that is, when the interaction of the conduction electrons with impurities is taken into account [14]. The results of [14] can be adjusted for the present case and yield the estimate $T_2 \simeq 10^{-1}$ s.

The existing quantum error correction protocols require the quality factor, equal the ratio of the gate-function clock time to decoherence time, not to exceed 10^{-5} [24]. Our estimates indicate that this is not the case for the present system. Actually, no quantum-computing proposal to date, scalable by other criteria, satisfies this 10^{-5} quality-factor criterion. The values range from 10^{-1} to 10^{-3}. The resolution could come from development of better error-correction algorithms or from improving the physical system to obtain a better quality factor. In our estimate of the decoherence time scale, we used parameters typical of a standard, "dirty" heterostructure with large spatial fluctuations of the impurity potential. These heterostructures have been suitable for standard experiments because they provide wider quantum-Hall plateaus. Much cleaner, ultrahigh mobility structures can be obtained by placing the ionized impurity layer at a larger distance from the 2D gas or by injecting conduction electrons into the heterostructure by other means.

Thus, our present quantum-computing proposal offers a clear direction for exploring a physical, rather than algorithmic, resolution to the quality-factor problem. This possibility should be further examined both experimentally and theoretically. Our new quantum-computing paradigm suggests several interesting avenues for research. The effect of gates on the switching of qubit interactions and on decoherence requires further investigation. The first experimental realizations will probably involve only a few qubits. The interactions of these may be significantly affected by the geometry, specifically, the edges, of the heterostructure.

[1] R. Tycko, S. E. Barrett, G. Dabbagh, L. N. Pfeiffer, and K. W. West, Science **268**, 1460 (1995); S. E. Barrett, G. Dabbagh, L. N. Pfeiffer, K. W. West, and R. Tycko, Phys. Rev. Lett. **74**, 5112 (1995).

[2] A. Berg, M. Dobers, R. R. Gerhards, and K. v. Klitzing, Phys. Rev. Lett. **64**, 2563 (1990).

[3] D. Loss and D. P. DiVincenzo, Phys. Rev. A **57**, 120 (1998).

[4] V. Privman, I. D. Vagner, and G. Kventsel, Phys. Lett. A **239**, 141 (1998).

[5] B. E. Kane, Nature (London) **393**, 133 (1998).

[6] A. Imamoglu, D. D. Awschalom, G. Burkard, D. P. DiVincenzo, D. Loss, M. Sherwin, and A. Small, Phys. Rev. Lett. **83**, 4204 (1999).

[7] R. Vrijen, E. Yablonovitch, K. Wang, H. W. Jiang, A. Balandin, V. Roychowdhury, T. Mor, and D. P. DiVincenzo, Phys. Rev. A **62**, 012306 (2000).

[8] Yu. Makhlin, G. Schoen, and A. Shnirman, Nature (London) **398**, 305 (1999); P. M. Platzman and M. I. Dykman, Science **284**, 1967 (1999); N. A. Gershenfeld and I. L. Chuang, Science **275**, 350 (1997).

[9] B. E. Kane, N. S. McAlpine, A. S. Dzurak, R. G. Clark, G. J. Milburn, H. B. Sun, and H. Wiseman, Phys. Rev. B **61**, 2961 (2000).

[10] D. G. Cory, A. F. Fahmy, and T. F. Havel, Proc. Natl. Acad. Sci. U.S.A. **94**, 1634 (1997); J. A. Jones and M. Mosca, J. Chem. Phys. **109**, 1648 (1998); J. R. Tucker and T. C. Shen, Solid State Electron. **42**, 1061 (1998); R. G. Clark, unpublished results presented at a quantum-computing conference held in Baltimore, MD, 2000.

[11] D. P. DiVincenzo, Science **270**, 255 (1995).

[12] I. D. Vagner and T. Maniv, Phys. Rev. Lett. **61**, 1400 (1988).

[13] Y. Yaffet, in *Solid State Physics,* edited by F. Seitz and D. Turnbull (Academic, New York, 1963), Vol. 14; H. Hasegawa, Phys. Rev. **118**, 1523 (1960); L. M. Roth, Phys. Rev. **118**, 1534 (1960).

[14] D. Mozyrsky, V. Privman, and I. D. Vagner, Phys. Rev. B **63**, 085313 (2001).

[15] T. Kasuya, in *Magnetism,* edited by G. T. Rado and H. Suhl (Academic, New York, 1966), Vol. 2B.

[16] *The Quantum Hall Effect,* edited by R. E. Prange and S. M. Girvin (Springer-Verlag, New York, 1987).

[17] Yu. A. Bychkov, S. V. Iordanskii, and G. M. Eliashberg, JETP Lett. **33**, 143 (1981).

[18] C. Kallin and B. I. Halperin, Phys. Rev. B **30**, 5655 (1984).

[19] A. Pinczuk, B. S. Dennis, D. Heiman, C. Kallin, L. Brey, C. Tejedor, S. Schmitt-Rink, L. N. Pfeiffer, and K. W. West, Phys. Rev. Lett. **68**, 3623 (1992).

[20] M. A. Ruderman and C. Kittel, Phys. Rev. **96**, 99 (1954).

[21] Yu. A. Bychkov, T. Maniv, and I. D. Vagner, Solid State Commun. **94**, 61 (1995).

[22] W. Kohn, in *Solid State Physics,* edited by F. Seitz and D. Turnbull (Academic, New York, 1957), Vol. 5.

[23] S. V. Iordanskii, S. V. Meshkov, and I. D. Vagner, Phys. Rev. B **44**, 6554 (1991).

[24] J. Preskill, Proc. R. Soc. London A **454**, 385 (1998).

Initial Decoherence of Open Quantum Systems

Vladimir Privman

Center for Quantum Device Technology, Clarkson University

Potsdam, New York 13699–5820, USA

Abstract

We present a new short-time approximation scheme for evaluation of decoherence. At low temperatures, the approximation is argued to apply at intermediate times as well. It then provides a tractable approach complementary to Markovian-type approximations, and appropriate for evaluation of deviations from pure states in quantum computing models.

Key Words: decoherence, thermalization, relaxation, open quantum systems

1. Introduction

Consider a microscopic quantum system with the Hamiltonian H_S. We will refer to the quantum-computing single quantum bit (qubit) or multi-qubit paradigm to help define the questions and set up the challenges, in describing how the system, S, interacts with the surrounding macroscopic world. However, in principle S can be any quantum system.

Interactions with the surroundings can be quite different depending on the setting. For example, in quantum measurement, which is presently not fully understood, the wavefunction of the system is probed, so part of the process would involve a strong interaction with the measuring device, such that the system's own Hamiltonian plays no role in the process. However, in most applications, the external interactions are actually quite weak. Furthermore, the aim is to minimize their effect, especially in quantum computing.

Traditionally, interactions with the surrounding world have been modeled by the modes of a bath, B, with each mode described by its Hamiltonian M_K, so that the bath of modes is represented by

$$H_B = \sum_K M_K \ . \tag{1.1}$$

The interaction, I, of the bath modes with the system S, will be modeled by

$$H_I = \Lambda_S P_B = \Lambda_S \sum_K J_K \ , \tag{1.2}$$

where Λ_S is some Hermitean operator of S, coupled to the operator P_B of the bath.

The bath, or "heat bath", can be a collection of modes, such as photons, phonons, spins, excitons, etc. For a bosonic bath of oscillators, [1-6], which we use for derivation

of specific results, we take

$$M_K = \omega_K a_K^\dagger a_K \,, \tag{1.3}$$

$$J_K = g_K^* a_K + g_K a_K^\dagger \,. \tag{1.4}$$

Here we have assumed that the energy of the ground state is shifted to zero for each oscillator, and we work in units such that $\hbar = 1$.

The total Hamiltonian of the system and bath is

$$H = H_S + H_B + H_I \,. \tag{1.5}$$

More generally, the interaction, (1.2), can involve several system operators, each coupling differently to the bath modes, or even to different baths. The bath modes, in turn, can be coupled to specified external objects, such as impurities.

Let $\rho(t)$ represent the reduced density matrix of the system at time $t \geq 0$, after the bath modes have been traced over. For large times, the effect of the environment on a quantum system that is not otherwise externally controlled, is expected to be thermalization: the density matrix should approach

$$\rho(t \to \infty) = \frac{\exp\left(-\beta H_S\right)}{\text{Tr}_S\left[\exp\left(-\beta H_S\right)\right]} \,, \tag{1.6}$$

where $\beta \equiv 1/kT$. At all times, we can consider the degree to which the system has departed from coherent pure-quantum-state evolution. This departure is due to the interactions and entanglement with the bath. We also expect that the temperature, T, and other external parameters that might be needed to characterize the system's density

matrix, are determined by the properties of the bath, which in turn might interact with the rest of the universe.

Let us introduce the eigenstates of H_S,

$$H_S|n\rangle = E_n|n\rangle \ , \tag{1.7}$$

and have ΔE denote the characteristic energy gap values of S. We also consider the matrix elements of $\rho(t)$,

$$\rho_{mn}(t) = \langle m|\rho(t)|n\rangle \ . \tag{1.8}$$

For large times, we expect the diagonal elements ρ_{nn} to approach values proportional to $e^{-\beta E_n}$, while the off-diagonal elements, $\rho_{m\neq n}$, to vanish. These properties are referred to as thermalization and decoherence in the energy basis.

To establish these thermalization and decoherence properties, several assumptions are made regarding the system and bath dynamics [1-11]. At time $t = 0$, it is usually assumed that the bath modes, K, are thermalized, i.e., have density matrices

$$\theta_K = e^{-\beta M_K} \Big/ \operatorname{Tr}_K \left(e^{-\beta M_K}\right) \ . \tag{1.9}$$

The density matrix R of the system plus bath at time $t = 0$ is then the direct product

$$R(0) = \rho(0) \prod_K \theta_K \ , \tag{1.10}$$

and the system and bath modes are not entangled with each other.

Now, a series of assumptions are made, e.g., the Markovian and secular approximations. The most important is the Markovian approximation, which, even though it

can be stated and introduced in various ways, essentially assumes that the density matrices of the bath modes are reset externally to the thermal ones, on time scales shorter than any dynamical times of the system interacting with the bath. This is a natural assumption, because each bath mode is coupled only weakly to the system, whereas it is "monitored" by the rest of the universe and kept at temperature T. In its straightforward version, this amounts to using (1.10) for times $t > 0$. Ultimately, such approaches aim at master equations for the evolution of $\rho_{mn}(t)$ at large times, consistent with the Golden Rule and with the expected thermalization and decoherence properties.

In variants of these formalisms, several time scales are identified. One is the inverse of the upper cutoff, Debye frequency of the bath modes, $1/\omega_D$. Another is the thermal time $\hbar/kT = \beta$ (in units of $\hbar = 1$). The system S has its own characteristic time, $1/\Delta E$, as well as the system-bath dynamical times of thermalization and decoherence, etc., $T_{1,2,\ldots}$, corresponding to the "intrinsic" NMR/ESR times T_1, T_2, etc. Heuristically, bath modes of frequencies ω comparable to ΔE are needed to drive thermalization and decoherence. Initial decoherence can be also mediated by the modes near $\omega = 0$. At low temperatures, we can assume that $1/\omega_D < 1/\Delta E < \beta$.

There is evidence [7,11,12] that at low temperatures, the Markovian-type and other approximations used in the derivation of equations for thermalization and decoherence, are only valid for times larger than the thermal time scale β. For quantum computing applications, in solid-state semiconductor-heterostructure architectures [13-19], we expect temperatures of several tens of μK. The thermal time scale then becomes dangerously close to the external single-qubit control, Rabi-flip time even for slower qubits, those based on nuclear spins. We emphasize that not all the approximation schemes have this problem [11].

In Section 2, we offer additional comments on decoherence and quantum computing. Then, in Section 3, we develop a short-time-decoherence approximation. In a

discussion at the end of Section 3, we offer arguments that, at low temperatures, our approximation is actually valid for intermediate times, larger than $1/\omega_D$, hopefully up to times comparable or larger than $1/\Delta E$. Specific results for the bosonic heat bath are presented in Section 4. Section 5 comments on the case of adiabatic decoherence, when the short-time approximation becomes exact.

2. Decoherence and quantum computing

Quantum computing architectures usually emphasize systems, both the qubits and the modes that couple them (and at the same time act as a bath mediating unwanted coupling to the rest of the universe), that have large spectral gaps. It is believed that, especially at low temperatures, spectral gaps slow down relaxation processes. Therefore, quantum computing architectures usually assume [13-19] qubits in quantum dots, or in atoms, or subject to large magnetic fields, and coupled by highly nondissipative quantum media [14,19].

The spectral gaps are expected to slow down exponentially, by the Boltzmann factor, the processes of thermalization, involving energy exchange. Off-shell virtual exchanges, will be also slowed down, but less profoundly. The latter processes contribute to decoherence. Therefore, at low temperatures, we might expect separation of time scales of the initial decoherence vs. later-stage thermalization and further decoherence. The latter two processes are described by the traditional NMR/ESR intrinsic T_1 and T_2, respectively.

Since only thermalization is clearly associated with the energy eigenbasis, one can also ask whether the energy basis is the appropriate one to describe decoherence for short and intermediate times, before the thermalizing processes, that also further drive decoherence, take over. The issue of the appropriate basis for studying decoherence, has also come up in models of quantum measurement. It has been argued [20-24] that the eigenbasis of the interaction operator, Λ_S, may be more appropriate for intermediate times than the energy eigenbasis.

Yet another aspect of decoherence in quantum computing, involves the observation that we really want to retain a *pure state* in the quantum computation process [25-30]. Decay of off-diagonal matrix elements, in whatever basis, might not be the best

measure of deviations from the pure-state density matrix. For instance, the deviation of $\operatorname{Tr}_S \left[\rho^2(t) \right]$ from 1, may be more appropriate. Therefore, it is desirable to have basis-independent expressions for the reduced density operator $\rho(t)$.

Recently, several groups have reported [12,19,24,31-41] results for spin decoherence in solid state systems appropriate for quantum computing architectures. Some of these works have not invoked the full battery of the traditional approximations, Markovian and secular, etc., or have utilized the spectral gap of the bath modes, to achieve better reliability of the short-time results. In [41], interaction of the spin-exciton bath modes with impurities was accounted for, as the main mechanism of decoherence. In the present work, we limit ourselves to the bath modes only interacting with the system. Experimental efforts are picking up momentum, with the first limited results available [42,43] by traditional NMR/ESR techniques, with the quantum-computing emphasis.

An approach, termed adiabatic decoherence, have been developed by us [24], expanding the earlier works [12,31-33], with the goal of avoiding the ambiguity of the basis selection and achieving exact solvability. The price paid was the assumption that H_S is conserved (a particular version of the quantum nondemolition processes), which is equivalent to requiring that

$$[H_S, H] = [H_S, \Lambda_S] = 0 \qquad \text{(adiabatic case)} . \tag{2.1}$$

This makes the eigenbasis of H_S and Λ_S the same, but precludes energy relaxation, thus artificially leaving only energy-conserving relaxation pathways that contribute to decoherence. We will comment on the results of this approach in Section 5.

Most of the results referred to earlier, have involved approximations of one sort or another. The most popular and widely used approximation has been the second-order perturbative expansion in the interaction strength, H_I, though some nonperturbative

results have also been reported. In Section 3, we describe a novel approximation scheme [44] that is valid for short times. It has several advantages, such as becoming exact in the adiabatic case, allowing derivation of several explicit results, and, at least in principle, permitting derivation of higher-order approximations. Certain models of quantum measurement evaluate decoherence by effectively setting $H_S = 0$. Our approximation then becomes exact, and our results are consistent with these studies [45,46].

Our formulation in Section 3, will be quite general, and we will not use the specific bath or thermalization assumptions. However, we do utilize the factorization property (1.10) at time $t = 0$. Thus, we do have to assume that, at least initially, the system and the bath modes are not entangled. In fact, the present formulation also relies on that the Hamiltonians at hand are all time-independent. Therefore, we have excluded the possibility of controlled dynamics, in the quantum computing sense, when gate functions are accomplished by external couplings to individual qubits and by external control of their pairwise interactions. Our formulation, therefore, applies to "idling" qubits or systems of (possibly interacting) qubits. It is reasonable to assume that a lower limit on decoherence rate can be evaluated in such an idling state, even though for quantum error correction, qubits otherwise idling, might be frequently probed (measured) and entangled with ancillary qubits [25-30].

The $t = 0$ factorization assumption (1.10), shared by all the recent spin-decoherence studies, then represents the expectation that external control by short-duration but large externally applied potentials, measurement, etc., will "reset" the qubits, disentangling them from the environment modes to which the affected qubits are only weakly coupled. Thus, we assert that it is the qubit system that gets approximately reset and disentangled from the bath towards time $t = 0$, rather than the bath is thermalized by the rest of the universe, as assumed in Markovian approximation schemes.

3. Short-time decoherence

In addition to the energy basis, (1.7), we also define the eigenstates of the interaction operator Λ_S, by

$$\Lambda_S|\gamma\rangle = \lambda_\gamma|\gamma\rangle \,, \tag{3.1}$$

where the Greek index labels the eigenstates of Λ_S, with eigenvalues λ_γ, while the Roman indices will be used for the energy basis, and, when capitalized, for the bath modes, (1.2)-(1.4).

The time dependence of the density matrix $R(t)$ of the system and bath, is formally given by

$$R(t) = e^{-i(H_S+H_B+H_I)t} R(0) \, e^{i(H_S+H_B+H_I)t} \,. \tag{3.2}$$

We will utilize the following approximate relation for the exponential factors, as our short-time approximation,

$$e^{i(H_S+H_B+H_I)t+O(t^3)} = e^{iH_St/2} \, e^{i(H_B+H_I)t} \, e^{iH_St/2} \,. \tag{3.3}$$

This relation has the following appealing properties. It becomes exact for the adiabatic case, (2.1). Furthermore, if we use the right-hand side and its inverse to replace $e^{\pm iHt}$, then we are imposing three time-evolution-type transformations on $R(0)$. Therefore, the approximate expression for $R(t)$ will have all the desired properties of a density operator. Finally, extensions to higher-order approximations in powers of t are possible, by using relations derived in [47], where various expressions valid to $O(t^4)$ and $O(t^5)$ were considered.

Our goal is to evaluate the resulting approximation to the matrix element,

$$\rho_{mn}(t) = \text{Tr}_B \langle m|e^{-iH_St/2}\, e^{-i(H_B+H_I)t}\, e^{-iH_St/2}R(0)\, e^{iH_St/2}\, e^{i(H_B+H_I)t}\, e^{iH_St/2}|n\rangle\,.$$

(3.4)

First, we apply the operators H_S in the outer exponentials, acting to the left on $\langle m|$, and to the right on $|n\rangle$, replacing H_S by, respectively, E_m and E_n. We then note that the second exponential operator in (3.4) contains Λ_S, see (1.2). Therefore, we insert the decomposition of the unit operator in the system space, in terms of the eigenbasis of Λ_S, before the second exponential, and one in terms of the eigenbasis of H_S after it. This allows us to apply Λ_S in the second exponential and also H_S in the third exponential. The same substitution is carried out on the other side of $R(0)$, with the result

$$\rho_{mn}(t) = \sum_{\gamma\,p\,q\,\delta} \text{Tr}_B\Big[e^{-iE_mt/2}\langle m|\gamma\rangle\langle\gamma|p\rangle e^{-i(H_B+\lambda_\gamma P_B)t}\, e^{-iE_pt/2}\rho_{pq}(0)$$

$$\times\Big(\prod_K \theta_K\Big)e^{iE_qt/2}\, e^{i(H_B+\lambda_\delta P_B)t}\langle q|\delta\rangle\langle\delta|n\rangle e^{iE_nt/2}\Big]\,.$$

(3.5)

The next step is to collect all the terms, and also identify that the trace over the bath can be now carried out for each mode separately. We use (1.1)-(1.2) to write

$$\rho_{mn}(t) = \sum_{\gamma\,p\,q\,\delta} \Big\{ e^{i(E_q+E_n-E_p-E_m)t/2}\langle m|\gamma\rangle\langle\gamma|p\rangle\, \rho_{pq}(0)\, \langle q|\delta\rangle\langle\delta|n\rangle$$

$$\times\prod_K \text{Tr}_K\Big[e^{-i(M_K+\lambda_\gamma J_K)t}\, \theta_K\, e^{i(M_K+\lambda_\delta J_K)t}\Big]\Big\}\,.$$

(3.6)

While this expression looks formidable, it actually allows rather straightforward calculations in some cases. Specifically, the simplest quantum-computing applications involve

two-state systems. Therefore, the sums in (3.6) are over two terms each. The calculations involving the overlap Dirac brackets between the eigenstates of H_S (labeled by m, n, p and q) and of Λ_S (labeled by γ and δ), as well as the energy-basis matrix elements of $\rho(0)$, cf. (1.8), involve at most diagonalization of two-by-two Hermitean matrices. Of course, the approximation (3.6) can be used for evaluation of short-time density matrices for systems more general than two-state.

The challenging part of the calculation involves the trace over each mode of the bath. Since these modes have identical structure, e.g., (1.3)-(1.4) for the bosonic bath case, but with K-dependent coupling constants, the calculation needs only be done once, in the space of *one mode*. Furthermore, results for the bath models ordinarily used, such as the bosonic and spin baths, are either already available in the literature or can be calculated without much difficulty. For the thermalized initial bath-mode density matrix θ_K, we give the exact bosonic-model expression in the next section.

In the remainder of this section, we first further analyze the trace over one bath mode entering (3.6). We then comment on the limits of validity of the present approximation.

In an obvious shorthand notation, we write the single-mode trace in (3.6) as

$$\mathrm{Tr}\left[e^{-i(M+\gamma J)t}\,\theta\,e^{i(M+\delta J)t}\right] = \mathrm{Tr}\left[\theta\,e^{i(M+\delta J)t}\,e^{-i(M+\gamma J)t}\right]. \tag{3.7}$$

Now, to the same order of approximation as used in (3.3), we can write

$$e^{i(M+\delta J)t+O(t^3)} = e^{iMt/2}\,e^{i\delta Jt}\,e^{iMt/2}\,. \tag{3.8}$$

The resulting approximation for the trace (3.7) reads

$$\mathrm{Tr}\left[\left(e^{-iMt/2}\,\theta\,e^{iMt/2}\right)e^{i(\delta-\gamma)Jt}\right],\tag{3.9}$$

which illustrates that, within this approximation, the product of traces in (3.6) is a function of the difference $\lambda_\gamma - \lambda_\delta$. In fact, this product is exactly 1 for $\lambda_\gamma = \lambda_\delta$ and, in most applications, the following form is likely to emerge,

$$\prod_K \mathrm{Tr}_K[\ldots] = e^{-\,\mathrm{const}\,(\lambda_\gamma-\lambda_\delta)^2 t^2 + O(t^3)},\tag{3.10}$$

though we caution the reader that (3.10) is somewhat speculative and suggested by the exact result for the bosonic heat bath, reported in the next section.

Finally, we point out that in most cases of interest, the initial single-mode density matrix θ will commute with the bath-mode energy operator M. In fact, the thermalized θ is a function of M. Therefore, (3.9) can be further simplified to

$$\mathrm{Tr}\left[\theta\,e^{i(\delta-\gamma)Jt}\right].\tag{3.11}$$

However, let us emphasize that the approximate relations (3.9)-(3.11) are likely of value only as far as they help to derive basis-independent (operator) approximations to $\rho(t)$, by a technique illustrated in the next section. Indeed, for most bath models it is advisable to calculate the single-mode trace exactly first, according to (3.6), and then attempt various approximations.

The latter statement reflects our expectation that the approximation developed here is valid, for low temperatures, not only for short times, defined by $t < 1/\omega_D$, but also for intermediate times, exceeding $1/\omega_D$. This is suggested by the result of an illustrative calculation in the next section, but mainly by the fact that (3.11) only includes the bath-mode energy scales via θ, and, therefore, at low temperatures, is

dominated by the lowest bath-mode excitations, and is not sensitive to frequencies of order ω_D. Thus, we expect our approximation to be applicable complementary to the Markovian-type approximations and definitely break down in the regime of fully developed thermalization, for $t \geq O(\beta)$. Additional supporting observations are offered in Section 5, when we consider the adiabatic case (2.1).

4. The bosonic heat bath

In this section, we consider the bosonic heat bath [6], see (1.3)-(1.4), in the initially thermalized state,

$$\theta_K = e^{-\beta M_K} / \text{Tr}_K \left(e^{-\beta M_K} \right) = \left(1 - e^{-\beta \omega_K} \right) e^{-\beta \omega_K a_K^\dagger a_K} . \tag{4.1}$$

The product of the single-mode traces in (3.6), is then available in the literature [12,24,31],

$$\rho_{mn}(t) = \sum_{\gamma \, p \, q \, \delta} \left\{ e^{i(E_q + E_n - E_p - E_m)t/2} \langle m | \gamma \rangle \langle \gamma | p \rangle \langle q | \delta \rangle \langle \delta | n \rangle \rho_{pq}(0) \right.$$

$$\left. \times \exp \left(-\sum_K \frac{|g_K|^2}{\omega_K^2} \left[2 \left(\lambda_\gamma - \lambda_\delta \right)^2 \sin^2 \frac{\omega_K t}{2} \coth \frac{\beta \omega_K}{2} + i \left(\lambda_\gamma^2 - \lambda_\delta^2 \right) \left(\sin \omega_K t - \omega_K t \right) \right] \right) \right\} . \tag{4.2}$$

The last term in the exponent, linear in t, is usually viewed as "renormalization" of the system energy levels due to its interaction with the bath modes. It can be removed by adding the term,

$$H_R = \Lambda_S^2 \sum_K |g_K|^2 / \omega_K , \tag{4.3}$$

to the total Hamiltonian. However, the usefulness of this identification for short times is not clear, and we will not use it. One can check that, *unmodified*, (4.2) is consistent with the expectation (3.10).

Let us now define two non-negative real spectral sums, $B(t)$ and $C(t)$, over the bath modes,

$$B^2(t) = 8 \sum_K \frac{|g_K|^2}{\omega_K^2} \sin^2 \frac{\omega_K t}{2} \coth \frac{\beta \omega_K}{2} \ , \qquad (4.4)$$

$$C(t) = \sum_K \frac{|g_K|^2}{\omega_K^2} \left(\omega_K t - \sin \omega_K t \right) \ . \qquad (4.5)$$

When converted to integrals over the bath mode frequencies, with the cutoff at ω_D, these sums have been discussed extensively in the literature [6,12,31], for several choices of the bath mode density of states and coupling strength g as functions of the mode frequency.

The final expression is,

$$\rho_{mn}(t) = \sum_{\gamma \, p \, q \, \delta} \left\{ e^{i(E_q + E_n - E_p - E_m)t/2} \langle m | \gamma \rangle \langle \gamma | p \rangle \langle q | \delta \rangle \langle \delta | n \rangle \rho_{pq}(0) \right.$$

$$\left. \times \exp \left[-\frac{1}{4} B^2(t) \left(\lambda_\gamma - \lambda_\delta \right)^2 - iC(t) \left(\lambda_\gamma^2 - \lambda_\delta^2 \right) \right] \right\} \ . \qquad (4.6)$$

When the spectral functions are expanded in powers of t, this result confirms all the conclusions and conjectures discussed in Section 3, in connection with relations (3.9)-(3.11).

Let us now turn to the derivation of the basis-independent representation for $\rho(t)$, by utilizing the integral identity

$$\sqrt{\pi} \exp[-B^2(\Delta\lambda)^2/4] = \int_{-\infty}^{\infty} dy \, e^{-y^2} \exp[iyB(\Delta\lambda)] \ . \qquad (4.7)$$

Exponential factors in (4.6) can then be reproduced by applying operators on the wave-functions entering the overlap Dirac brackets, with the result

$$\sqrt{\pi}\,\rho(t) = \int dy\, e^{-y^2} e^{-iH_S t/2}\, e^{i[yB(t)\Lambda_S - C(t)\Lambda_S^2]}\, e^{-iH_S t/2}\, \rho(0)\, e^{iH_S t/2}\, e^{-i[yB(t)\Lambda_S - C(t)\Lambda_S^2]}\, e^{iH_S t/2}\,.$$

(4.8)

Within the $O(t^2)$ approximation (3.3), given that B and C are of order linear or higher in t, we can combine the exponential operators to get an alternative approximation,

$$\sqrt{\pi}\,\rho(t) = \int dy\, e^{-y^2}\, e^{-i[tH_S - yB(t)\Lambda_S + C(t)\Lambda_S^2]}\, \rho(0)\, e^{i[tH_S - yB(t)\Lambda_S + C(t)\Lambda_S^2]}\,,$$

(4.9)

though (4.6) and (4.8) are in fact easier to handle in actual calculations.

As an application, let us consider the case of H_S proportional to the Pauli matrix σ_z, e.g., a spin-1/2 particle in magnetic field, and $\Lambda_S = \sigma_x$, with the proportionality constant in the latter relation absorbed in the definition of the coupling constants g_K in (1.4). Let us study the deviation of the state of a spin-1/2 qubit, initially in the energy eigenstate $|\uparrow\rangle$ or $|\downarrow\rangle$, from pure state, by calculating $\mathrm{Tr}_S[\rho^2(t)]$ according to (4.8). We note that for a two-by-two density matrix, this trace can vary from 1 for pure quantum states to the lowest value of $1/2$ for maximally mixed states.

A straightforward calculation with $\rho(0) = |\uparrow\rangle\langle\uparrow|$ or $|\downarrow\rangle\langle\downarrow|$, yields

$$\mathrm{Tr}_S[\rho^2(t)] = \frac{1}{2}\left[1 + e^{-2B^2(t)}\right]\,.$$

(4.10)

As the time increases, the function $B^2(t)$ grows monotonically from zero [6,12,24,31]. Specifically, for Ohmic dissipation, $B^2(t)$ increases quadratically for short times $t < O(1/\omega_D)$, then logarithmically for $O(1/\omega_D) < t < O(\hbar/kT)$, and linearly for $t > O(\hbar/kT)$. (For other bath models, it need not diverge to infinity at large times.) This

calculation thus illustrates the fact that the present approximation can yield reasonable results for short and even intermediate times.

Both approximations, (4.8)-(4.9), make the deviation from a pure state $\rho(0) = |\psi_0\rangle\langle\psi_0|$ apparent: $\rho(t > 0)$ is obviously a *mixture* (integral over y) of pure-state projectors $|\psi(y,t)\rangle\langle\psi(y,t)|$, where, for instance for (4.9),

$$\psi(y,t) = e^{-i[tH_S - yB(t)\Lambda_S + C(t)\Lambda_S^2]}\,\psi_0\;, \tag{4.11}$$

with a somewhat different expression for (4.8).

5. The adiabatic case

Relation (2.1) corresponds to the system's energy conservation. Therefore, energy flow in and out of the system is not possible, and normal thermalization mechanisms are blocked. The fact that our approximation becomes exact in this case, provides support to the expectation that, at low temperatures, it is generally valid beyond the cutoff time scale $1/\omega_D$, providing a reasonable evaluation of decoherence and deviation from a pure state, as exemplified by the calculation yielding (4.10), in Section 4.

With (2.1), we can select a common eigenbasis for H_S and Λ_S. Then the distinction between the lower-case Roman and Greek indices in (3.6) becomes irrelevant, and the sums can all be evaluated to yield

$$\rho_{mn}(t) = e^{i(E_n - E_m)t} \, \rho_{mn}(0) \prod_K \text{Tr}_K \left[e^{-i(M_K + \lambda_m J_K)t} \, \theta_K \, e^{i(M_K + \lambda_n J_K)t} \right] . \qquad (5.1)$$

This expression was discussed in detail in our work on adiabatic decoherence [24]. Specifically, for the initially thermalized bosonic heat bath case, we have, for the absolute values of the density matrix elements,

$$\left| \rho_{mn}(t) \right| = \left| \rho_{mn}(0) \right| e^{-B^2(t)(\lambda_m - \lambda_n)^2/4} . \qquad (5.2)$$

The decay of the off-diagonal matrix elements thus depends of the properties of the spectral function $B^2(t)$ as the time increases. Such explicit results [12,24,31-33] illustrate that for true irreversibility, the number of bath modes must be infinite, with the spectral function evaluated in the continuum limit.

In summary, we have derived short-time approximations for the density matrix and its energy-basis matrix elements. Our expressions are quite easy to work with, because

for few-qubit systems they only involve manipulation of finite-dimensional matrices, and they will be useful in estimating decoherence and deviation from pure states in quantum computing models, including results for low temperatures.

References

1. R.P. Feynman and A.R. Hibbs, *Quantum Mechanics and Path Integrals* (McGraw-Hill, NY, 1965).

2. G.W. Ford, M. Kac and P. Mazur, J. Math. Phys. **6**, 504 (1965).

3. A.O. Caldeira and A.J. Leggett, Phys. Rev. Lett. **46**, 211 (1981).

4. A.O. Caldeira and A.J. Leggett, Physica **121A**, 587 (1983)

5. S. Chakravarty and A.J. Leggett, Phys. Rev. Lett. **52**, 5 (1984).

6. A.J. Leggett, S. Chakravarty, A.T. Dorsey, M.P.A. Fisher and W. Zwerger, Rev. Mod. Phys. **59**, 1 (1987) [Erratum *ibid.* **67**, 725 (1995)].

7. N.G. van Kampen, *Stochastic Processes in Physics and Chemistry* (North-Holland, Amsterdam, 2001).

8. W.H. Louisell, *Quantum Statistical Properties of Radiation* (Wiley, NY, 1973).

9. K. Blum, *Density Matrix Theory and Applications* (Plenum, NY, 1996).

10. A. Abragam, *The Principles of Nuclear Magnetism* (Clarendon Press, 1983).

11. H. Grabert, P. Schramm and G.-L. Ingold, Phys. Rep. **168**, 115 (1988).

12. N.G. van Kampen, J. Stat. Phys. **78**, 299 (1995).

13. D. Loss and D.P. DiVincenzo, Phys. Rev. **A57**, 120 (1998).

14. V. Privman, I.D. Vagner and G. Kventsel, Phys. Lett. **A239**, 141 (1998).

15. B.E. Kane, Nature **393**, 133 (1998).

16. A. Imamoglu, D.D. Awschalom, G. Burkard, D.P. DiVincenzo, D. Loss, M. Sherwin and A. Small, Phys. Rev. Lett. **83**, 4204 (1999).

17. R. Vrijen, E. Yablonovitch, K. Wang, H.W. Jiang, A. Balandin, V. Roychowdhury, T. Mor and D.P. DiVincenzo, Phys. Rev. **A62**, 012306 (2000)

18. S. Bandyopadhyay, Phys. Rev. **B61**, 13813 (2000).

19. D. Mozyrsky, V. Privman and M.L. Glasser, Phys. Rev. Lett. **86**, 5112 (2001).

20. W.G. Unruh and W.H. Zurek, Phys. Rev. **D40**, 1071 (1989).

21. W.H. Zurek, S. Habib and J.P. Paz, Phys. Rev. Lett. **70**, 1187 (1993).

22. A.O. Caldeira and A.J. Leggett, Ann. Phys. **149**, 374 (1983).

23. L. Mandel and E. Wolf, *Optical Coherence and Quantum Optics* (Cambridge University Press, 1995).

24. D. Mozyrsky and V. Privman, J. Stat. Phys. **91**, 787 (1998).

25. P.W. Shor, in *Proc. 37th Annual Symp. Found. Comp. Sci.*, p. 56 (IEEE Comp. Sci. Soc. Press, Los Alamitos, CA, 1996).

26. D. Aharonov and M. Ben-Or, *Fault-Tolerant Quantum Computation with Constant Error*, preprints quant-ph/9611025 and quant-ph/9906129.

27. A. Steane, Phys. Rev. Lett. **78**, 2252 (1997).

28. E. Knill and R. Laflamme, Phys. Rev. **A55**, 900 (1997).

29. D. Gottesman, Phys. Rev. **A57**, 127 (1998).

30. J. Preskill, Proc. Royal Soc. London **A454**, 385 (1998).

31. G.M. Palma, K.A. Suominen and A.K. Ekert, Proc. Royal Soc. London **A452**, 567 (1996).

32. J. Shao, M.-L. Ge and H. Cheng, Phys. Rev. **E53**, 1243 (1996).

33. I.S. Tupitsyn, N.V. Prokof'ev, P.C.E. Stamp, Int. J. Mod. Phys. **B11**, 2901 (1997).

34. N.V. Prokof'ev and P.C.E. Stamp, Rep. Prog. Phys. **63**, 669 (2000).

35. J. Ankerhold and H. Grabert, Phys. Rev. **E61**, 3450 (2000).

36. T. Maniv, Y.A. Bychkov, I.D. Vagner and P. Wyder, Phys. Rev. **B64**, 193306 (2001).

37. A.M. Dyugaev, I.D. Vagner and P. Wyder, *On the Electron Scattering and Dephasing by the Nuclear Spins*, preprint cond-mat/0005005.

38. D. Mozyrsky, S. Kogan and G.P. Berman, *Time Scales of Phonon Induced Decoherence of Semiconductor Spin Qubits*, preprint cond-mat/0112135.

39. A.V. Khaetskii, D. Loss and L. Glazman, *Electron Spin Decoherence in Quantum Dots due to Interaction with Nuclei*, preprint cond-mat/0201303.

40. I.A. Merkulov, A.L. Efros and M. Rosen, *Electron Spin Relaxation by Nuclei in Semiconductor Quantum Dots*, preprint cond-mat/0202271.

41. D. Mozyrsky, V. Privman and I.D. Vagner, Phys. Rev. **B63**, 085313 (2001).

42. J. Zhang, Z. Lu, L. Shan and Z. Deng, *Experimental Study of Quantum Decoherence using Nuclear Magnetic Resonance*, preprint quant-ph/0202146.

43. E. Yablonovitch, private communication.

44. V. Privman, *Short-Time Decoherence and Deviation from Pure Quantum States*, preprint cond-mat/0203039.

45. D. Mozyrsky and V. Privman, Mod. Phys. Lett. **B14**, 303 (2000).

46. D. Braun, F. Haake, W.T. Strunz, Phys. Rev. Lett. **86** 2913 (2001).

47. A.T. Sornborger and E.D. Stewart, Phys. Rev. **A60**, 1956 (1999).