REPORT DOCUMENTATION PAGE	Form Approved OMB NO. 0704-0188

1. REPORT DATE (DD-MM-YYYY)	2. REPORT TYPE	3. DATES COVERED (From - To)
30-11-2007	Final Report	1-Jun-2001 - 28-Feb-2007

4. TITLE AND SUBTITLE	5a. CONTRACT NUMBER
Closed Loop Quantum Control and Quantum Information Sciences: Concepts and Laboratory Implementations	DAAD19-01-1-0534
	5b. GRANT NUMBER
	5c. PROGRAM ELEMENT NUMBER 5720L7
6. AUTHORS	5d. PROJECT NUMBER
herschel rabitz, ian walmsley, robert kosut	5e. TASK NUMBER
	5f. WORK UNIT NUMBER

7. PERFORMING ORGANIZATION NAMES AND ADDRESSES	8. PERFORMING ORGANIZATION REPORT NUMBER
Princeton University Office Of Research & Project Administration The Trustees of Princeton University Princeton, NJ 08544 -0036	

9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)	10. SPONSOR/MONITOR'S ACRONYM(S)
U.S. Army Research Office P.O. Box 12211 Research Triangle Park, NC 27709-2211	ARO
	11. SPONSOR/MONITOR'S REPORT NUMBER(S) 42674-PH-QC.19

12. DISTRIBUTION AVAILIBILITY STATEMENT

Approved for public release; Federal purpose rights

13. SUPPLEMENTARY NOTES

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

14. ABSTRACT

This is the final report on research concerned with combining control concepts and quantum information systems. Particular emphasis is being given to closed loop laboratory techniques for obtaining the maximum performance from quantum information systems. These studies entail minimization of the influence of environmental decoherence effects, maximum robustness to noise in the system controllers, the creation of robust gate operations, and the means to identify quantum information system Hamiltonians and evolving state behavior. The research includes both theoretical and laboratory components. The research summary is broken out into the accomplishments and findings in a set of interrelated QuIST

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	15. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT	b. ABSTRACT	c. THIS PAGE			Herschel Rabitz
U	U	U	SAR		19b. TELEPHONE NUMBER 609-258-3917

Standard Form 298 (Rev 8/98)
Prescribed by ANSI Std. Z39.18

Report Title

ABSTRACT

This is the final report on research concerned with combining control concepts and quantum information systems. Particular emphasis is being given to closed loop laboratory techniques for obtaining the maximum performance from quantum information systems. These studies entail minimization of the influence of environmental decoherence effects, maximum robustness to noise in the system controllers, the creation of robust gate operations, and the means to identify quantum information system Hamiltonians and evolving state behavior. The research includes both theoretical and laboratory components. The research summary is broken out into the accomplishments and findings in a set of interrelated QuIST projects.

List of papers submitted or published that acknowledge ARO support during this reporting period. List the papers, including journal references, in the following categories:

(a) Papers published in peer-reviewed journals (N/A for none)

Constructing global functional maps between molecular potentials and quantum observables, J.M. Geremia, H. Rabitz, and C. Rosenthal, J. Chem. Phys., 114, 9325-9336 (2001).

Global, nonlinear algorithm for inverting quantum-mechanical observations, J.M. Geremia and H. Rabitz, Phys. Rev. A, 64, 022710-1-13 (2001).

Quantum Optimal Quantum Control Field Design Using Logarithmic Maps, J.S. Biteen, J.M. Geremia, and H. Rabitz, Chem. Phys. Lett., 348, 440-446 (2001).

Quantum Wavefunction Controllability, G. Turinici and H. Rabitz, Chem. Phys., 267, 1-9 (2001).

Algorithms for Closed Loop Ultrafast Control of Quantum Dynamics, H. Rabitz, Springer Ser. Chem. Phys., 66, 14-18 (2001).

Non-iterative optimal design of quantum controls, Z. Murtha and H. Rabitz, Eur. Phys. J. D, 14, 141-145 (2001).

Achieving the Laboratory Control of Quantum Dynamics Phenomena Using Nonlinear Functional Maps, J.M. Geremia, E. Weiss, and H. Rabitz, Chem. Phys., 267, 209-222 (2001).

Rotationally induced collapse and revivals of molecular vibrational wavepackets: model for environment-induced decoherence, S. Wallentowitz, I.A. Walmsley, L.J. Waxer, and Th. Richter, J. Phys. B, 35, 1967-1984 (2002).

Identification of Quantum Systems, R.L. Kosut and H. Rabitz, Proceedings of the 15th IFAC World Congress, (2002).

Control of a coupled two-spin system without hard pulses, V. Ramakrishna, R.J. Ober, K.L. Flores, and H. Rabitz, Phys. Rev. A, 65, 063405-1-9 (2002).

Constructive control of quantum systems using factorization of unitary operators, S.G. Schirmer, A. Greentree, V. Ramakrishna, and H. Rabitz, J. Phys. A, 35, 8315-8330 (2002).

Optimal Identification of Hamiltonian Information by Closed-Loop Laser Control of Quantum Systems, J.M. Geremia and H. Rabitz, Phys. Rev. Lett., 89, 263902-1-4 (2002).

Optimal Control of Quantum Systems: Origins of Inherent Robustness to Control Field Fluctuations, H. Rabitz, Phys. Rev. A, 66, 063405-1-8 (2002).

Closed loop learning control with quantum reduced space dynamics, Y.-S. Kim and H. Rabitz, J. Chem. Phys., 117, 1024-1030 (2002).

Closed loop learning control to suppress the effects of quantum decoherence, W. Zhu and H. Rabitz, J.Chem. Phys., 118, 6751-6757 (2003).

A propagation toolkit to design quantum controls, F. Yip, D. Mazziotti, and H. Rabitz, J. Chem. Phys.,118, 8168-8172 (2003).

Bell trajectories for revealing quantum control mechanisms, E. Dennis and H. Rabitz, Phys. Rev. A, 67, 033401-1-10 (2003).

Controlling the Dephasing of Vibrational Wavepackets in Potassium Dimers, I. Walmsley, P. Londero, M. Fitch, S. Wallentowitz, L. Waxer, and C. Radzewicz, in Ultrafast Phenomena XIII, R.D. Miller, M.M. Murnane, N.F. Scherer, and A.M. Weiner, eds. (Springer, Berlin, 2003).

Closed-loop quantum control utilizing time domain maps, J.S. Biteen, J.M. Geremia, and H. Rabitz, Chem. Phys., 290, 35-45 (2003).

Wavefunction controllability for finite dimensional bilinear quantum systems, G. Turinici and H. Rabitz, J. Phys. A: Math. Gen., 36, 2565-2576 (2003).

Quantum optimal control of wave packet dynamics under the influence of dissipation, Y. Ohtsuki, K. Nakagami, W. Zhu, and H. Rabitz, Chem. Phys., 287, 197-216 (2003).

Quantum Control via Adaptive Tracking, W. Zhu and H. Rabitz, J. Chem. Phys., 2003, 119, 3619-3625 (2003).

Revealing Quantum Control Mechanisms through Hamiltonian Encoding in Different Representations, A. Mitra, I. Solá, and H. Rabitz, Phys. Rev. A, 67,043409-1-9 (2003).

Quantum System Optimal Control Landscapes, H. Rabitz, M. Hsieh, and C. Rosenthal, Science, 303, 998 (2004).

Coherent Control (aka: Theoretical Considerations for Laser Control of Quantum Systems), H. Rabitz, in Encyclopedia of Modern Optics, B. D. Guenther, Ed., Elsevier, New York, pp. 123-134 (2004).

Optimal Discrimination of Multiple Quantum Systems: Controllability Analysis, G. Turinici, V. Ramakrishna, B. Li, and H. Rabitz, J. Phys. A, 37, 273-282 (2004).

The Landscape for Optimal Control of Quantum Mechanical Unitary Transformations, H. Rabitz, M. Hsieh, and C. Rosenthal, Phys. Rev. A, 72, 052337, (2005).

Perturbative and Non-perturbative master equations for open quantum systems, W. Zhu and H. Rabitz, , J. Math. Phys., 46, 022105 (2005).

Encoding a qubit into multilevel subspaces, M. Grace, C. Brif, H. Rabitz, I. Walmsley, R. Kosut, and D. Lidar, New J. Phys., 8, 35 (2006).

Laboratory observation of quantum control level sets, J. Roslund, M. Roth, H. Rabitz, Phys. Rev. A, 74, 043414 (2006). DARPA, ARO-MURI, NSF

Topology of optimally controlled quantum mechanical transition probability landscapes, H. Rabitz, T.-S. Ho, M. Hsieh, R. Kosut, M. Demiralp, Phys Rev A, 74, 012721 (2006).

Why do effective quantum controls appear easy to find? T.-S. Ho, H. Rabitz, Special Issue of J. Photo Chem. A, 180, 226-240 (2006).

Quantum control mechanism analysis through field based hamiltonian encoding, A. Mitra, H. Rabitz, J. Chem. Phys, 125, 194107 (2006).

Photonic reagent control of dynamically homologous quantum systems, V. Beltrani, J. Dominy, T.-S. Ho, and H. Rabitz, NSF, DARPA, J. Chem. Phys., 126, 094105 (2007).

Optimal control of quantum gates and suppression of decoherence in a system of interacting two-level particles, M. Grace, C. Brif, H. Rabitz, I. Walmsley, R. Kosut, D. Lidar, J. Phys. B: At. Mol. Opt. Phys., 40, S103 (2007).

Number of Papers published in peer-reviewed journals: 35.00

(b) Papers published in non-peer-reviewed journals or in conference proceedings (N/A for none)

Number of Papers published in non peer-reviewed journals: 0.00

(c) Presentations

Number of Presentations:

Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):

Peer-Reviewed Conference Proceeding publications (other than abstracts):

Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):

(d) Manuscripts

Number of Manuscripts: 0.00

Number of Inventions:

Graduate Students

NAME	PERCENT_SUPPORTED
Manuel Delacruz	0.75
Pablo Londero,	0.75
Matthijs Branderhorst	0.75
Matthew Grace	0.75
FTE Equivalent:	**3.00**
Total Number:	**4**

Names of Post Doctorates

NAME	PERCENT_SUPPORTED
Piotr Wasylczyk	0.75
FTE Equivalent:	**0.75**
Total Number:	**1**

Names of Faculty Supported

NAME	PERCENT_SUPPORTED	National Academy Member
herschel rabitz	0.50	No
Ian Walmsley	0.50	No
FTE Equivalent:	**1.00**	
Total Number:	**2**	

Names of Under Graduate students supported

NAME	PERCENT_SUPPORTED
FTE Equivalent:	
Total Number:	

Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period:	0.00
The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:......	0.00
The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:......	0.00
Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale):	0.00
Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:	0.00
The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense	0.00
The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields:	0.00

Names of Personnel receiving masters degrees

NAME

Total Number:

Names of personnel receiving PHDs

NAME

Total Number:

Names of other research staff

NAME	PERCENT_SUPPORTED	
wusheng Zhu	0.75	No
Robert Kosut - co-PI	0.50	No
Ignacio Sola - RA	0.75	No
Rebing Wu - RA	0.75	No
Marco Dettori, RA	0.75	No
Constantin Brif	0.75	No
FTE Equivalent:	**4.25**	
Total Number:	**6**	

Sub Contractors (DD882)

Inventions (DD882)

REPORT DOCUMENTATION PAGE (SF298)
(Continuation Sheet)

Abstract

This is the final report on research concerned with combining control concepts and quantum information systems. Particular emphasis is being given to closed loop laboratory techniques for obtaining the maximum performance from quantum information systems. These studies entail minimization of the influence of environmental decoherence effects, maximum robustness to noise in the system controllers, the creation of robust gate operations, and the means to identify quantum information system Hamiltonians and evolving state behavior. The research includes both theoretical and laboratory components. The research summary is broken out into the accomplishments and findings in a set of interrelated QuIST projects.

REPORT DOCUMENTATION PAGE (SF298)
(Continuation Sheet)

(1) List of papers published under ARO sponsorship:

1. Constructing global functional maps between molecular potentials and quantum observables, J.M. Geremia, H. Rabitz, and C. Rosenthal, *J. Chem. Phys.*, **114**, 9325-9336 (2001).

2. Global, nonlinear algorithm for inverting quantum-mechanical observations, J.M. Geremia and H. Rabitz, *Phys. Rev. A*, **64**, 022710-1-13 (2001).

3. Quantum Optimal Quantum Control Field Design Using Logarithmic Maps, J.S. Biteen, J.M. Geremia, and H. Rabitz, *Chem. Phys. Lett.*, **348**, 440-446 (2001).

4. Quantum Wavefunction Controllability, G. Turinici and H. Rabitz, *Chem. Phys.,* **267**, 1-9 (2001).

5. Algorithms for Closed Loop Ultrafast Control of Quantum Dynamics, H. Rabitz, *Springer Ser. Chem. Phys.*, **66**, 14-18 (2001).

6. Non-iterative optimal design of quantum controls, Z. Murtha and H. Rabitz, *Eur. Phys. J. D*, **14**, 141-145 (2001).

7. Achieving the Laboratory Control of Quantum Dynamics Phenomena Using Nonlinear Functional Maps, J.M. Geremia, E. Weiss, and H. Rabitz, *Chem. Phys.*, **267**, 209-222 (2001).

8. Rotationally induced collapse and revivals of molecular vibrational wavepackets: model for environment-induced decoherence, S. Wallentowitz, I.A. Walmsley, L.J. Waxer, and Th. Richter, J. Phys. B, 35, 1967-1984 (2002).

9. Identification of Quantum Systems, R.L. Kosut and H. Rabitz, Proceedings of the 15th IFAC World Congress, (2002).

10. Control of a coupled two-spin system without hard pulses, V. Ramakrishna, R.J. Ober, K.L. Flores, and H. Rabitz, Phys. Rev. A, 65, 063405-1-9 (2002).

11. Constructive control of quantum systems using factorization of unitary operators, S.G. Schirmer, A. Greentree, V. Ramakrishna, and H. Rabitz, J. Phys. A, 35, 8315-8330 (2002).

12. Optimal Identification of Hamiltonian Information by Closed-Loop Laser Control of Quantum Systems, J.M. Geremia and H. Rabitz, Phys. Rev. Lett., 89, 263902-1-4 (2002).

13. Optimal Control of Quantum Systems: Origins of Inherent Robustness to Control Field

Fluctuations, H. Rabitz, Phys. Rev. A, 66, 063405-1-8 (2002).

14. Closed loop learning control with quantum reduced space dynamics, Y.-S. Kim and H. Rabitz, *J. Chem. Phys.*, **117**, 1024-1030 (2002).

15. Closed loop learning control to suppress the effects of quantum decoherence, W. Zhu and H. Rabitz, J.Chem. Phys., 118, 6751-6757 (2003).

16. A propagation toolkit to design quantum controls, F. Yip, D. Mazziotti, and H. Rabitz, J. Chem. Phys.,118, 8168-8172 (2003).

17. Bell trajectories for revealing quantum control mechanisms, E. Dennis and H. Rabitz, Phys. Rev. A, 67, 033401-1-10 (2003).

18. Controlling the Dephasing of Vibrational Wavepackets in Potassium Dimers, I. Walmsley, P. Londero, M. Fitch, S. Wallentowitz, L. Waxer, and C. Radzewicz, in Ultrafast Phenomena XIII, R.D. Miller, M.M. Murnane, N.F. Scherer, and A.M. Weiner, eds. (Springer, Berlin, 2003).

19. Closed-loop quantum control utilizing time domain maps, J.S. Biteen, J.M. Geremia, and H. Rabitz, Chem. Phys., 290, 35-45 (2003).

20. Wavefunction controllability for finite dimensional bilinear quantum systems, G. Turinici and H. Rabitz, J. Phys. A: Math. Gen., 36, 2565-2576 (2003).

21. Quantum optimal control of wave packet dynamics under the influence of dissipation, Y. Ohtsuki, K. Nakagami, W. Zhu, and H. Rabitz, Chem. Phys., 287, 197-216 (2003).

22. Quantum Control via Adaptive Tracking, W. Zhu and H. Rabitz, J. Chem. Phys., 2003, **119**, 3619-3625 (2003).

23. Revealing Quantum Control Mechanisms through Hamiltonian Encoding in Different Representations, A. Mitra, I. Solá, and H. Rabitz, Phys. Rev. A, 67,043409-1-9 (2003).

24. Quantum System Optimal Control Landscapes, H. Rabitz, M. Hsieh, and C. Rosenthal, Science, **303**, 998 (2004).

25. Coherent Control (aka: Theoretical Considerations for Laser Control of Quantum Systems), H. Rabitz, in *Encyclopedia of Modern Optics*, B. D. Guenther, Ed., Elsevier, New York, pp. 123-134 (2004).

26. Optimal Discrimination of Multiple Quantum Systems: Controllability Analysis, G. Turinici, V. Ramakrishna, B. Li, and H. Rabitz, *J. Phys. A*, 37, 273-282 (2004).

REPORT DOCUMENTATION PAGE (SF298)
(Continuation Sheet)

27. The Landscape for Optimal Control of Quantum Mechanical Unitary Transformations, H. Rabitz, M. Hsieh, and C. Rosenthal, *Phys. Rev. A*, **72**, 052337, (2005).

28. Perturbative and Non-perturbative master equations for open quantum systems, W. Zhu and H. Rabitz, , *J. Math. Phys.,* **46**, 022105 (2005).

29. Encoding a qubit into multilevel subspaces, M. Grace, C. Brif, H. Rabitz, I. Walmsley, R. Kosut, and D. Lidar, *New J. Phys.,* **8**, 35 (2006).

30. Laboratory observation of quantum control level sets, J. Roslund, M. Roth, H. Rabitz, *Phys. Rev. A*, **74**, 043414 (2006). DARPA, ARO-MURI, NSF

31. Topology of optimally controlled quantum mechanical transition probability landscapes, H. Rabitz, T.-S. Ho, M. Hsieh, R. Kosut, M. Demiralp, *Phys Rev A*, **74**, 012721 (2006).

32. Why do effective quantum controls appear easy to find? T.-S. Ho, H. Rabitz, Special Issue of *J. Photo Chem. A*, **180**, 226-240 (2006).

33. Quantum control mechanism analysis through field based hamiltonian encoding, A. Mitra, H. Rabitz, *J. Chem. Phys*, **125**, 194107 (2006).

34. Photonic reagent control of dynamically homologous quantum systems, V. Beltrani, J. Dominy, T.-S. Ho, and H. Rabitz, NSF, DARPA, J. Chem. Phys., 126, 094105 (2007).

35. Optimal control of quantum gates and suppression of decoherence in a system of interacting two-level particles, M. Grace, C. Brif, H. Rabitz, I. Walmsley, R. Kosut, D. Lidar, *J. Phys. B: At. Mol. Opt. Phys.*, **40**, S103 (2007).

(2) Scientific personnel supported by this project, and honors/awards received:

Princeton University
Herschel Rabitz, Principal Investigator
Wusheng Zhu, Research Associate
Constantin Brif, Research Associate
Ignacio Sola, Research Associate
Rebing Wu, Research Associate
Matthew Grace, Graduate Student

Oxford University
Ian Walmsley, Co-Principal Investigator
Piotr Wasylczyk, Post Doc

REPORT DOCUMENTATION PAGE (SF298)
(Continuation Sheet)

Pablo Londero, Graduate Student
Matthijs Branderhorst, Graduate Student
Manuel Delacruz, Graduate Student

SC Solutions
Robert Kosut, Co-Principal Investigator
Dr. Marco Dettori, Researcher

(3) Report of inventions (by title only): None

(4) Scientific progress and accomplishments:

The creation and management of quantum information systems faces a number of challenges, but three stand out most prominently: (1) the management of deleterious decoherence effects, (2) the creation of robust quantum gate operations, and (3) optimal performance of experiments for control and observations. The research in this program is specifically concerned with these topics, and the overall goal of extracting the maximum performance from a variety of proposed realizations of quantum information device. In order to address these key issues, a variety of theoretical techniques, algorithms, and laboratory experiments are under way. In addition, these activities are also correlated with those of other QuIST programs. A summary of the research directions is given below.

1. **Constructing global functional maps between molecular potentials and quantum observables.** The relationships that connect potential energy surfaces to quantum observables can be complex and nonlinear. In this paper, an approach toward globally representing and exploring potential-observable relationships using a functional mapping procedure is developed. Based on selected solutions of the Schrödinger equation, it is demonstrated that an observables behavior can be learned as a function of the potential and any other variables needed to specify the quantum system. Once such a map for the observable is in hand, it is available for use in a host of future applications without further need for solving the Schrödinger equation. As formulated here, maps provide explicit information about the global response of the observable to the potential. In this paper, we develop the mapping concept, estimate its scaling behavior ~measured as the number of times the Schrödinger equation must be solved during the learning process!, and numerically illustrate the technique's globality and nonlinearity using well-understood systems that demonstrate its capabilities. For atom–atom scattering, we construct a single map capable of learning elastic cross sections ~i.e., differential cross sections at 2° intervals over angle, as well as integral, diffusion, and viscosity cross sections for scattering energies between 50 meV and 2 eV! Involving collisions between any pair of atoms from the Periodic Table. The map for each class of cross sections over the Periodic Table is quantitative with prediction errors shown to be !1%. We also consider *a* 3S*u* 1 Na2 and create a rovibrational spectral map that encompasses all of the currently proposed potentials for that system. The Na2 map is highly accurate with the

ability to predict rovibrational spectra with errors less than 131023 cm21 over variations in the potential that exceed130 cm21.

2. **Global, nonlinear algorithm for inverting quantum-mechanical observations.** Inverting laboratory measurements of quantum-mechanical observables to recover the underlying molecular potential typically produces non unique solutions. Without quantifying the full family of potentials consistent with the measurements, it is impossible to fully determine how experimental error and limited data affect the inversion, or to assess the quality of the recovered potential. Here, we present a global, nonlinear algorithm for extracting molecular potentials from measurements of quantum-mechanical observables. The method utilizes a mapping technique to learn the relationship between a broad domain of potentials and their resulting observables to facilitate the inversion. Once constructed, the maps reduce the arduous task of repeatedly solving the Schrödinger equation for each trial potential tested during the inversion and permit the use of normally expensive, global optimization procedures to thoroughly explore the distribution of potentials consistent with the data. As a demonstration, the new algorithm is applied to quantum collision cross sections to illustrate the effect of experimental error and finite resolution of the scattering observables on the recovered potential. A series of simulated inversions were performed to examine these issues along with the inversion of laboratory differential cross-section data for He1Ne scattering. These illustrations show that laboratory errors can have a nonlinear effect on the family of extracted potentials. Furthermore, the examples provide a benchmark for the capabilities of the proposed algorithm to stably reveal the full distribution of potentials consistent with the data. The algorithm may be applied to other observables and molecular systems with more spatial coordinates.

3. **Quantum Optimal Control Field Design Using Logarithmic Maps**. A mapping technique is introduced to expand the capabilities of current control field design procedures. The maps relate the control field to the logarithm of the time evolution operator. Over the dynamic range of the maps, which begins at the sudden limit and extends beyond, they are found to be more accurate than field ->observable maps. The maps may be used as part of an iterative computational algorithm for field design. This process is illustrated for the design of a field to meet a population transfer objective.

4. **Quantum Wavefunction Controllability**. Theoretical results are presented on the ability to arbitrarily steer about a wavefunction for a quantum system under time-dependent external field control. Criteria on the field free Hamiltonian and the field coupling term in the Hamiltonian are presented that assure full wavefunction controllability. Numerical simulations are given to illustrate the criteria. A discussion on the theoretical and practical relationship between dynamical conservation laws and controllability is also included.

REPORT DOCUMENTATION PAGE (SF298)
(Continuation Sheet)

5. **Algorithms for Closed Loop Ultrafast Control of Quantum Dynamic**s. Learning control techniques have a special role to play in the manipulation of quantum dynamics phenomena. The unique capabilities of quantum systems making them amenable to learning control are (a) the ability to have very large numbers off identical systems for submission to control, (b) the high duty cycle of laboratory laser controls, and (c) the ability to observe the impact of trial controls at ultrafast time scales. Various learning algorithms have been proposed to guide this control process. The present paper will discuss these proposals, as well as some new perspectives.

6. **Non-iterative optimal design of quantum controls**. A non-iterative means for quantum control design is introduced with the aim of ordering practical designs that can later be ne-tuned with laboratory closed-loop techniques. The procedure recognizes that Hamiltonians for realistic system control applications are rarely known accurately. The algorithm takes advantage of this fact by allowing for managed deviations in the equations of motion, thus removing the standard Lagrange multiplier. Suitable time-dependent cost functional weights are introduced that eliminate the traditional final time matching condition, thereby producing non-iterative design equations as an initial value problem. Removal of the final time condition also eliminates the demand that the target state be reached at any imposed time. Tests on a simple molecular system indicate that the algorithm leads to well-behaved designs and that the weight functions are adequately estimated by order of magnitude analysis.

7. **Achieving the Laboratory Control of Quantum Dynamics Phenomena Using Nonlinear Functional Maps**. This research introduces a new algorithm for achieving closed-loop laboratory control of quantum dynamics phenomena. The procedure makes use of the nonlinear functional maps to exploit laboratory control data for revealing the relationship between control fields and their effect on other observables of interest. Control is achieved by (1) constructing the maps by performing laboratory experiments during an initial learning phase and then (2) searching the maps for fields that drive the system to the desired target during a separate, offline optimization stage. Once the map is learned, additional laboratory experiments are not necessarily required if the control target is changed. Maps also help to determine the control mechanism and assess the robustness of the outcome to fluctuations in the field since they explicitly measure the nonlinear response of the observable to field variations. To demonstrate the operation of the proposed map based control algorithm, two illustrations involving simulated population transfer experiments are performed.

8. **Rotationally induced collapse and revivals of molecular vibrational wavepackets: model for environment-induced decoherence**. We present an analytical calculation that predicts the collapse of vibrational wavepackets in molecules due to the coupling of the rotational and vibrational degrees of freedom. At longer times a new class of revivals is predicted in the vibrational degree of freedom, due to the finite size and discrete nature of the rotational reservoir. The interplay of these competing behaviors is studied in the context of current experiments, and conditions for observing the revivals are described.

Furthermore, the conditions for which the molecular vibration and rotation can be regarded as a system and its reservoir-like environment are described, in which case the ro-vibrational coupling can be considered effectively as a mechanism for decoherence of the vibrational motion. Comparison of the dephasing time predicted by this model with that observed in recent experiments is made.

9. **Identification of Quantum Systems.** An observer structure is presented which can be used to reconstruct the state and or parameters of a quantum system using recorded data together with a model Hamiltonian which is assumed to have the same structure as the true Hamiltonian except for the unknown parameters. The parameters are estimated using a gradient algorithm. A numerical simulation of a quantum spin system shows convergence in some but not all cases.

10. **Control of a coupled two-spin system without hard pulses.** Constructive techniques for preparing a specific unitary generator from a coupled two-spin system, via bounded amplitude radio frequency selective single spin pulses, are presented. The frequency of any pulse in the sequence is one of the two Larmor frequencies, while the phase takes one of two values. The fact that the amplitude is bounded implies that the Larmor frequency separation between the two spins need not be large to maintain selectivity. In addition, the contribution of the J coupling term to single spin evolution is not neglected, but instead plays a crucial role. The procedure is based on a certain decomposition of SU(4) Available in the literature. A method for determining the parameters entering this factorization, in terms of the entries of the target unitary generator, is also provided.

11. **Constructive control of quantum systems using factorization of unitary operators**. We demonstrate how structured decompositions of unitary operators can be employed to derive control schemes for finite-level quantum systems that require only sequences of simple control pulses such as square wave pulses with finite rise and decay times or Gaussian wavepackets. To illustrate the technique, it is applied to find control schemes to achieve population transfers for pure-state systems, complete inversions of the ensemble populations for mixed-state systems, create arbitrary superposition states and optimize the ensemble average of dynamic observables

12. **Optimal Identification of Hamiltonian Information by Closed-Loop Laser Control of Quantum Systems.** A closed loop learning control concept is introduced for teaching lasers to manipulate quantum systems for the purpose of optimally identifying Hamiltonian information. The closed loop optimal identification algorithm operates by revealing the distribution of Hamiltonians consistent with the data. The control laser is guided to perform additional experiments, based on minimizing the dispersion of the distribution. Operation of such an apparatus is simulated for two model finite dimensional quantum systems.

REPORT DOCUMENTATION PAGE (SF298)
(Continuation Sheet)

13. **Optimal Control of Quantum Systems: Origins of Inherent Robustness to Control Field Fluctuations.** The impact of control field fluctuations on the optimal manipulation of quantum dynamics phenomena is investigated. The quantum system is driven by an optimal control field, with the physical focus on the evolving expectation value of an observable operator. A relationship is shown to exist between the system dynamics and the control field fluctuations, wherein the process of seeking optimal performance assures an inherent degree of system robustness to such fluctuations. The presence of significant field fluctuations breaks down the evolution of the observable expectation value into a sequence of partially coherent robust steps. Robustness occurs because the optimization process reduces sensitivity to noise-driven quantum system fluctuations by taking advantage of the observable expectation value being bilinear in the evolution operator and its adjoint. The consequences of this inherent robustness are discussed in the light of recent experiments and numerical simulations on the optimal control of quantum phenomena. The analysis in this paper bodes well for the future success of closed-loop quantum optimal control experiments, even in the presence of reasonable levels of field fluctuations.

14. **Closed loop learning control with quantum reduced space dynamics.** This paper investigates the ability of closed loop quantum learning control techniques to meet a posed physical objective while simultaneously steering the dynamics to lie in a specified subspace. Achievement of successful control with reduced space dynamics can have a number of benefits including a more easily understood control mechanism. Judicious choices for the cost functional may be introduced such that the closed loop optimal control experiments can steer the dynamics to lie within a subspace of the system eigenstates without requiring any prior detailed knowledge about the system Hamiltonian. Learning control with reduced space dynamics takes advantage of the expected existence of a multiplicity of fields that can all give acceptable quality control outcomes. The procedure eliminates the hard demands of following a specific dynamical path by only asking that the dynamics reside in a subspace. Additional measurements characterizing the subspace are necessary to monitor the system evolution during the control field learning process. This procedure is simulated for optimally controlled population transfer experiments in systems of one and two degrees of freedom. The results demonstrate that optimal control fields can be found that successfully derive the system to the target state while staying within the desired subspace.

15. **Closed Loop Learning Control to Suppress the Effects of Quantum Decoherence.** This paper explores the use of laboratory closed loop learning control to suppress the effects of decoherence in quantum dynamics. Simulations of the process are performed in multilevel quantum systems strongly interacting with the environment. A genetic algorithm is used to find an optimal control field, which seeks out transition pathways to achieve a minimum influence of, decoherence upon the system at a target time. The simulations suggest that decoherence may be optimally managed in the laboratory through closed loop operations with a suitable cost that is sensitive to the coherence of

the dynamics. The case studies of dimension $N = 4$ and $N = 10$ with strong system–environment coupling indicate that the additional complexity with increasing system dimension can make it more difficult to manage decoherence.

16. **A Propagation Toolkit to Design Quantum Controls.** A toolkit of time-propagation operators, to be stored and recalled as needed, is incorporated into the algorithms for the optimal control of quantum systems. Typically, the control field revisits the same values many times during the full time evolution. This repetition may be utilized to enhance efficiency through a convenient toolkit of propagators where the propagators are computed and stored only at a small number of discrete electric-field values in a finite dynamic range. At each time step of the controlled evolution a specific member of the pre-calculated toolkit is selected as dictated by the local control field value. The toolkit can reduce the cost of control field design by a factor scaling as $\sim N$ for quantum systems described in a basis set of N states. Optimal control with the toolkit is demonstrated for systems up to dimension $N = 30$.

17. **Bell Trajectories for Revealing Quantum Control Mechanisms.** The dynamics induced while controlling quantum systems by optimally shaped laser pulses have often been difficult to understand in detail. A method is presented for quantifying the importance of specific sequences of quantum transitions involved in the control process. The method is based on a "beable" formulation of quantum mechanics due to John Bell that rigorously maps the quantum evolution onto an ensemble of stochastic trajectories over a classical state space. Detailed mechanism identification is illustrated with a model seven-level system. A general procedure is presented to extract mechanism information directly from closed-loop control experiments. Application to simulated experimental data for the model system proves robust with up to 25% noise.

18. **Controlling the Dephasing of Vibrational Wavepackets in Potassium Dimers.** We have manipulated vibrational wave packet dephasing in potassium dimers using adaptively-shaped optical pulses controlled by a learning algorithm. We identify several wave packet shapes that are resistant to decoherence due to coupling to the rotational degree of freedom of the molecule. A system-reservoir model of the rotational–vibrational dynamics is presented, and used to interpret the experimental results.

19. **Closed-loop quantum control utilizing time domain maps.** Closed-loop laser control of quantum dynamics phenomena may be accomplished through frequency domain manipulations in the laboratory guided by a learning algorithm. This paper presents an alternative method based on the use of nonlinear input→output maps generated in the time domain, although the actual experiments and control optimization are carried out in the frequency domain. The procedure first involves the construction of input→output maps relating the field structure to the observed control performance. These maps are utilized as a substitute for actual experiments in the subsequent optimization stage in order to find the field that drives the system to a specified target. This closed-loop learning process is repeated with a sufficient number of maps until a control field is

found that yields the target observable as best as possible. The overall algorithm is simulated with two model quantum systems. It is shown that excellent quality control can be achieved through this sequential learning procedure, even with individual maps that have only modest global accuracy.

20. **Wavefunction Controllability for Finite Dimensional Bilinear Quantum Systems.** We present controllability results for quantum systems interacting with lasers. Exact controllability for the wavefunction in these bilinear systems is proved in the finite-dimensional case under very natural hypotheses.

21. **Quantum Optimal Control of Wave Packet Dynamics under the Influence of Dissipation.** Optimal control within the density matrix formalism is applied to the production of desired non-equilibrium distributions in condensed phases. The time evolution of a molecular system modeled by a displaced harmonic oscillator is assumed to be described by the Markoffian master equation with phenomenological relaxation parameters. The physical objectives of concern are the creation of a specified vibronic state, population inversion and wave packet shaping. The effects of an initial thermal distribution and dissipation on these targets are examined. In order to transfer a large amount of population (i.e., the strong-field regime) to a target wave packet in an electronic excited state, it is shown that creating a shaped packet in the ground state is often required to achieve high yield. This control pathway cannot be taken into account within the weak-field approximation, and is especially important when the target state includes vibrational states that are weakly accessible from the initial state or that have preferential indirect excitation paths from the initial state. Although relaxation effects usually reduce the control efficiency, under certain conditions, the bath-induced dynamics can help to create an objective state.

22. **Quantum Control via Adaptive Tracking.** An adaptive tracking algorithm is developed to achieve quantum system control field designs. The adaptive algorithm has the advantage of operating noniteratively to efficiently find desirable controls, and has the feature of high stability by suppressing the influence of disturbances from tracking singularities. The core of the adaptive tracking control algorithm is a self-learning track switch technique, which is triggered by monitoring of the evolving system trajectory. The adaptive tracking algorithm is successfully tested for population transfer.

23. **Revealing Quantum Control Mechanisms through Hamiltonian Encoding in Different Representations.** The Hamiltonian encoding is a means for revealing the mechanism of controlled quantum dynamics. In this context, the mechanism is defined by the dominant quantum pathways starting from the initial state and proceeding through a set of intermediate states to end at the final state. The nature and interpretation of the mechanism depends on the choice of the states to represent the dynamics. Alternative representations may provide distinct insights into the system mechanism, and representations producing fewer pathways are especially interesting. In addition, a

suitable choice of representation may highlight the role of certain couplings in a system that would normally be masked by other, higher magnitude couplings. A simple three-level system is chosen for illustration, where different values for the Rabi frequencies lead to mechanistic analyses that are best described in terms of particular representations. As an examlple, the role of the nonadiabatic terms in stimulated Raman adiabatic passage dynamics is analyzed through the Hamiltonian encoding.

24. **Quantum System Optimal Control Landscapes.** A large number of experimental studies and simulations show that it is surprisingly easy to find excellent quality control over broad classes of quantum systems. We now prove that for controllable quantum systems with no constraints placed on the controls, the only allowed extrema of the transition probability landscape correspond to perfect control or no control. Under these conditions, no suboptimal local extrema exist as traps that would impede the search for an optimal control. The identified landscape structure is universal for all controllable quantum systems of the same dimension when seeking to maximize the same transition probability, regardless of the detailed nature of the system Hamiltonian. The presence of weakcontrol field noise or environmental decoherence is shown to preserve the general structure of the control landscape, but at lower resolution.

25. **Coherent Control.** This paper considers the theoretical issues associated with the optimal manipulation of quantum dynamics phenomena. Shaped laser pulses form the primary tool for manipulating quantum systems, and the article focuses on both the theoretical design of such pulses, as well as their laboratory discovery using closed loop learning algorithms. A variety of conceptual, numerical, and implementational topics are addressed in presenting the state of this field and its promise for the future.

26. **Optimal Discrimination of Multiple Quantum Systems: Controllability Analysis.** A theoretical study is presented concerning the ability to dynamically discriminate between members of a set of different (but possibly similar) quantum systems. This discrimination is analyzed in terms of independently and simultaneously steering about the wavefunction of each component system to a target state of interest using a tailored control (i.e. laser) field. Controllability criteria are revealed and their applicability is demonstrated in simple cases. Discussion is also presented on some uncontrollable cases.

27. **The landscape for optimal control of quantum mechanical unitary transformations.** The optimal creation of a targeted unitary transformation W is considered under the influence of an external control field. The controlled dynamics produces the unitary transformation U and the goal is to seek a control field that minimizes the cost $J = \|W - U\|$. The optimal control landscape is the cost J as a functional of the control field. For a controllable quantum system with N states and without restrictions placed on the controls, the optimal control landscape is shown to have extrema with N + 1 possible distinct values, where the desired transformation at U = W is a minimum and the

maximum value is at U = -W. The other distinct N-1 extrema values of J are saddle points. The results of this analysis have significance for the practical construction of unitary transformations.

28. **Perturbative and nonperturbative master equations for open quantum systems.** Develops perturbative and nonperturbative master equations for open quantum systems based on time-dependent variational functionals. The perturbative equations are more concise and suitable for dealing with cases of weak systemenvironment coupling for short evolution time scales. The nonperturbative equations are valid for all time and appropriate to treat cases of strong systemenvironment coupling. When a system contains an external control field, both the perturbative and nonperturbative master equations reveal the embedded control field dependence upon the system decoherence, which provides a basis for decoherence management.

29. **Encoding a qubit into multilevel subspaces.** This research presents a formalism for encoding the logical basis of a qubit Into subspaces of multiple physical levels. The need for this multilevel encoding (MLE) arises naturally in situations where the speed of quantum operations exceeds the limits imposed by the address ability of individual energy levels of the qubit physical system. A basic feature of the MLE formalism is the logical equivalence of different physical states and correspondingly, of different physical transformations. This logical equivalence is a source of a significant flexibility in designing logical operations, while the multilevel structure inherently accommodates fast and intense broadband controls thereby facilitating faster quantum operations. Another important practical advantage of MLE is the ability to maintain full quantum-computational fidelity in the presence of mixing and decoherence within encoding subspaces. The formalism is developed in detail for single-qubit operations and generalized for multiple qubits. As an illustrative example, we perform a simulation of closed-loop optimal control of single-qubit operations for a model multilevel system, and subsequently apply these operations at finite temperatures to investigate the effect of decoherence on operational fidelity.

30. **Laboratory observation of quantum control level sets.** In controlled quantum dynamics, a level set is defined as the collection of control fields that produce a specific value for a particular observable. We explored the relationship between individual solutions to a control problem, and present the first experimentally observed quantum control level sets, which are found to be continuous submanifolds. Level sets are observed for two photon transitions where the control is the spectral phase function, which is expressed as a fourth-order polynomial. For the systems studied here, the level sets are shown to be closed surfaces in the spectral phase control space. A perturbation analysis provides insight into the observed topology of the level set, which is shown to be preserved by the low-order polynomial phase representation. Each of the multiple control fields forming a level set preserves the observable value by its own distinct manipulation of constructive and destructive quantum interferences. Thus, the richness of quantum

control fields meeting a particular observable value is accompanied by an equally diverse family of control mechanisms.

31. **Topology of optimally controlled quantum mechanical transition probability landscapes.** An optimally controlled quantum system possesses a search landscape defined by the physical objective as a functional of the control field. This research particularly explores the topological structure of quantum mechanical transition probability landscapes. The quantum system is assumed to be controllable and the analysis is based on the Euler-Lagrange variational equations derived from a cost function only requiring extremizing the transition probability. It is shown that the latter variational equations are automatically satisfied as a mathematical identity for control fields that either produce transition probabilities of zero or unit value. Similarly, the variational equations are shown to be inconsistent for any control field that produces a transition probability different from either of these two extreme values. An upper bound is shown to exist on the norm of the functional derivative of the transition probability with respect to the control field anywhere over the landscape. The trace of the Hessian, evaluated for a control field producing a transition probability of a unit value, is shown to be bounded from below. Furthermore, the Hessian at a transition probability of unit value is shown to have an extensive null space and only a finite number of negative eigenvalues. Collectively, these findings show that the transition probability landscape extrema consists of values corresponding to no control or full control, approaching full control involves climbing a gentle slope with no false traps in the control space and an inherent degree of robustness exists around any full control solution. Although full controllability may not exist in some applications, the analysis provides a basis to understand the evident ease of finding controls that produce excellent yields in simulations and in the laboratory.

32. **Why do effective quantum controls appear easy to find?** Experimental evidence shows that effective quantum controls in diverse applications appear surprisingly easy to find. The underlying reasons for this attractive behavior are explored in this work through an examination of the quantum control landscape directly in terms of the physically relevant control field and the density matrix at the target time, including an elaboration of the topology around the critical points of an arbitrary physical observable. It is found that for controllable quantum systems the critical points of the landscape correspond to the global maximum and minimum and intermediate saddle points of found is shown to exist on the norm of the slope anywhere over the landscape, implying that the control landscape has gentle slopes permitting stable searches for optimal controls. Moreover, the Hessian at the global maximum (minimum) only possesses a finite number of negative (positive) non-zero eigenvalues and the sum of the corresponding eigenvalues is bounded from below (above). The number of negative eigenvalues of the Hessians evaluated at the saddle points drops as the critical point value becomes smaller and finally converts to all positive non-zero eigenvalues at the global minimum. Collectively, these findings reveal that (a) there are no false traps at the sub-optimal extrema in the landscape, (b) the

searches for optimal controls should generally be stable, and (c) an inherent degree of robustness to noise exists around the global optimal control solutions. As a result, it is anticipated that effective control over quantum dynamics may be expected even in highly complex systems provided that the control fields are sufficiently flexible to traverse the associated landscape.

33. **Quantum control mechanism analysis through field based Hamiltonian encoding.** Optimal control of quantum dynamics in the laboratory is proving to be increasingly successful. The control fields can be complex, and the mechanisms by which they operate have often remained obscure. Hamiltonian encoding has been proposed as a method for understanding mechanisms in quantum dynamics. In this context mechanism is defined in terms of the dominant quantum pathways leading to the final state of the controlled system. HE operates by encoding a special modulation into the Hamiltonian and decoding its signature in the dynamics to determine the dominant pathway amplitudes. Earlier work encoded the modulation directly into the Hamiltonian operators. This present work introduces the alternative scheme of field based HE, where the modulation is encoded into the control field and not directly into the Hamiltonian operators. This distinct form of modulation yields a new perspective on mechanism and is computationally faster than the earlier approach. Field based encoding is also an important step towards a laboratory based algorithm for HE as it is the only form of encoding that may be experimentally executed. HE is also extended to cover systems with noise and uncertainty and finally, a hierarchical algorithm is introduced to reveal mechanism in a stepwise fashion of ever increasing detail as desired. This new hierarchical algorithm is an improvement over earlier approaches to HE where the entire mechanism was determined in one stroke. The improvement comes from the use of less complex modulation schemes, which leads to fewer evaluations of Schrödinger 's equation. A number of simulations are presented on simple systems to illustrate the new field based encoding technique for mechanism assessment.

34. **Photonic reagent control of dynamically homologous quantum systems.** The general objective of quantum control is the manipulation of atomic scale physical and chemical phenomena through the application of external control fields. These tailored fields, or photonic reagents, exhibit systematic properties analogous to those of ordinary laboratory reagents. This analogous behavior is explored further here by considering the controlled response of a family of homologous quantum systems to a single common photonic reagent. A level set of dynamically homologous quantum systems is defined as the family that produces the same value for a target physical observable when controlled by a common photonic reagent. This paper investigates the scope of homologous quantum system control using the level set exploration technique L-SET enables the identification of continuous families of dynamically homologous quantum systems. Each quantum system is specified by a point in a hypercube whose edges are labeled by Hamiltonian matrix elements. Numerical examples are presented with simple finite level systems to illustrate the L-SET concepts. Both connected and disconnected families of dynamically

homologous systems are shown to exist.

35. **Optimal control of quantum gates and suppression of decoherence in a system of interacting two-level particles.** Methods of optimal control are applied to a model system of interacting two level particles (e.g., spin-half atomic nuclei or electrons or two-level atoms) to produce high-fidelity quantum gates while simultaneously negating the detrimental effect of decoherence. One set of particles functions as the quantum information processor, whose evolution is controlled by a time-dependent external field. The other particles are not directly controlled and serve as an effective environment, coupling to which is the source of decoherence. The control objective is to generate target one- and two-qubit unitary gates in the presence of strong environmentally-induced decoherence and under physically motivated restrictions on the control field. The quantum-gate fidelity, expressed in terms of a novel state-independent distance measure, is maximized with respect to the control field using combined genetic and gradient algorithms. The resulting high-fidelity gates demonstrate the feasibility of precisely guiding the quantum evolution via optimal control, even when the system complexity is exacerbated by environmental coupling. It is found that the gate duration has an important effect on the control mechanism and resulting fidelity. An analysis of the sensitivity of the gate performance to random variations in the system parameters reveals a significant degree of robustness attained by the optimal control solutions.

(5) Technology transfer: None

cc: T.R. Govindan
G. Hicks
R. Kosut
I. Walmsley