GEORGIA INSTITUTE OF TECHNOLOGY — OFFICE OF CONTRACT ADMINISTRATION

PROJECT ADMINISTRATION DATA SHEET

[X] ORIGINAL [ ] REVISION NO. ______

Project No. G-37-604 — GTRI/GIT — DATE 7/21/83

Project Director: E. M. HARRELL — School/Lab MATH

Sponsor: National Science Foundation
Washington, D.C. 20550

Type Agreement: Grant No. MCS-8300551

Award Period: From 7-1-83 To 12-31-85 (Performance) 3-31-86 (Reports)

Sponsor Amount:

	This Change	Total to Date
Estimated:	$	$ 28,100
Funded:	$	$ 28,100

Cost Sharing Amount: $ 414 — Cost Sharing No: G-37-313

Title: Mathematical Sciences: Operator Theory and Mathematical Physics

ADMINISTRATIVE DATA

OCA Contact Don Hasty

1) Sponsor Technical Contact:

Mr Harvey B. Keynes
Program Director
Modern Analysis Program
Division of Mathematical and Computer Sciences
Phone (202) 357-9764

2) Sponsor Admin/Contractual Matters:

Mr Stephen G. Burnisky
Division of Grants and Contracts
(202) 357-9671

Defense Priority Rating: N/A

Military Security Classification: N/A
(or) Company/Industrial Proprietary: N/A

RESTRICTIONS

See Attached NSF Supplemental Information Sheet for Additional Requirements.

Travel: Foreign travel must have prior approval — Contact OCA in each case. Domestic travel requires sponsor approval where total will exceed greater of $500 or 125% of approved proposal budget category.

Equipment: Title vests with Ga Tech, tho none proposed

COMMENTS:

JUL 1983 RECEIVED Research Reports Office

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FORM OCA 4:383

GEORGIA INSTITUTE OF TECHNOLOGY   OFFICE OF CONTRACT ADMINISTRATION

SPONSORED PROJECT TERMINATION/CLOSEOUT SHEET

Date April 14, 1986

Project No. G-37-604 (R5653-0A0)   School/XXX Math

Includes Subproject No.(s)

Project Director(s) E. M. Harrell   GTRC / XXX

Sponsor National Science Foundation

Title Mathematical Sciences: Operator Theory and Mathematical Physics

Effective Completion Date: 12/31/85 (Performance) 3/31/86 (Reports)

Grant/Contract Closeout Actions Remaining:

- [ ] None
- [ ] Final Invoice or Final Fiscal Report
- [ ] Closing Documents
- [X] ~~Final Report of Inventions~~ Patent Questionnaire
- [ ] Govt. Property Inventory & Related Certificate
- [ ] Classified Material Certificate
- [ ] Other

Continues Project No.   Continued by Project No. G-37-629

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Form OCA 60:1028

School of Mathematics
Georgia Institute of Technology
Atlanta GA 30332-0160
404 233 3381
404 894 2715
February 10, 1986

Kenneth Gross, Director
Modern Analysis Program
National Science Foundation
Washington DC 20550

Dear Dr. Gross:

Enclosed please find a final report for my NSF grant MCS 8300551, which expired last December (and has been replaced by DMS 8504354). Please let me know if anything further is required, other than copies of additional reprints, which will be sent when available.

For the technical description of the project, the instructions on NSF form 98A state "The information supplied in proposals for further support, updated as necessary, may be used to fulfill this requirement." I thus provide a copy of the proposal for grant DMS 85043051, submitted in late 1984 and beginning in June 15, 1985, and a copy of the progress report for that grant, submitted in December, 1985. Additional technical information is to be found in the progress report of September, 1984.

Sincerely yours,

Evans M. Harrell II

NATIONAL SCIENCE FOUNDATION
Washington, D.C. 20550

FINAL PROJECT REPORT
NSF FORM 98A

PLEASE READ INSTRUCTIONS ON REVERSE BEFORE COMPLETING

PART I—PROJECT IDENTIFICATION INFORMATION

1. Institution and Address	2. NSF Program	3. NSF Award Number
School of Mathematics Georgia Inst. of Technology Atlanta GA 30332	modern analysis	8300551
	4. Award Period From June 83 To Dec. 85	5. Cumulative Award Amount $28,100

6. Project Title
Operator Theory and Mathematical Physics

PART II—SUMMARY OF COMPLETED PROJECT *(FOR PUBLIC USE)*

Quantum physics benefits from rigorous mathematical analysis in two ways: 1. A general theorem delineates the types of spectra (energy levels) a given model can possibly have, and is thus the starting point for detailed theoretical study; and 2. Quantitative study is frequently a delicate matter, and the mathematical approach is then the only reliable way to make calculations when the usual perturbative expansions are of dubious validity.

The major accomplishments of this project have to do with tunneling effects and the semiclassical limit, in which quantum mechanics often manifests itself through effects which are exponentially small functions of some physical parameter. Notable examples are the decay of atomic resonances and the eigenvalue splitting of diatomic molecules - the "double-well problem." Perturbation theory is both too insensitive to understand these phenomena and, generally, divergent. The articles written with support from this NSF grant provide both general and quantitative analysis of the spectra and wave-functions in these and similar problems. In addition, they provide some new foundational study of the nature of the semiclassical limit in one dimension.

PART III—TECHNICAL INFORMATION *(FOR PROGRAM MANAGEMENT USES)*

1. ITEM *(Check appropriate blocks)*	NONE	ATTACHED	PREVIOUSLY FURNISHED	TO BE FURNISHED SEPARATELY TO PROGRAM: Check (√)	TO BE FURNISHED SEPARATELY TO PROGRAM: Approx. Date
a. Abstracts of Theses	x				
b. Publication Citations		x			
c. Data on Scientific Collaborators	x				
d. Information on Inventions	x				
e. Technical Description of Project and Results		x			
f. Other *(specify)*					

2. Principal Investigator/Project Director Name *(Typed)*	3. Principal Investigator/Project Director Signature	4. Date
Evans M. Harrell II		Feb. 6, 1986

NSF Form 98A (5-78) Supersedes All Previous Editions

Form Approved OMB No. 99R0013

List of publications of Evans M. Harrell II supported by NSF grant MCS 8300551

1/R Expansion for H_2^+: Analyticity, Summability, Asymptotics, and Calculation of Exponentially Small Terms, Phys. Rev. Lett. 52(1984)1112-1115. (With R.J. Damburg, R. Kh. Propin, S. Graffi, V. Grecchi, J. Cizek, J. Paldus, and H.J. Silverstone)

Potentials Producing Maximally Sharp Resonances, Trans. Amer. Math. Soc., to appear. (With R. Svirsky)

Potentials Producing Extremal Eigenvalues Subject to p-Norm Constraints, in: Proceedings of the 1984 Conference on Ordinary Differential Equations, Argonne National Laboratories Report 84-73 (1984) 19-29.

The 1/R Expansion for H_2^+: Analyticity, Summability, and Asymptotics, Ann. Phys. (N.Y.), to appear. (With S. Graffi, V. Grecchi, and H.J. Silverstone)

The 1/R Expansion for H_2^+: Calculation of Exponentially Small Terms and Asymptttics, Phys. Rev. A, to appear. (With H.J. Silverstone, R.J. Damburg, R. Kh. Propin, S. Graffi, V. Grecchi, J. Cizek, J. Paldus, S. Nakai, and J. Harris)

Les Potentiels les Plus Résonnants, in: Comptes-Rendus du Colloque sur les Méthodes Semiclassiques en Mécanique Quantique, Univ. de Nantes, 1984.

On the Extension of Ambarzumian's Inverse Spectral Theorem to Compact Symmetric Spaces, Am. J. Math. to appear.

Maximal and Minimal Eigenvalues and Their Associated Nonlinear Equations, 1985 preprint. (With M.S. Ashbaugh)

L^2 Estimates for Galerkin Methods for Semilinear Elliptic Equations, 1985 preprint. (With W. Layton)

Conformal Riemannian Metrics, Schrödinger Operators, and Semiclassical Approximation, J. Diff. Eq., to appear. (With E.B. Davies)

Evans M. Harrell II
MCS 8300551
Technical Description

PROPOSAL

OPERATOR THEORY AND MATHEMATICAL PHYSICS

Submitted to

National Science Foundation
Washington, DC

Submitted by

Evans M. Harrell II
Georgia Institute of Technology
School of Mathematics
Atlanta, GA 30332

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NOTICE OF RESEARCH PROJECT
SCIENCE INFORMATION EXCHANGE
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PROJECT SUMMARY

SIE PROJECT NO	NSF AWARD NO.

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AME OF INSTITUTION (INCLUDE BRANCH/CAMPUS AND SCHOOL OR DIVISION)

Georgia Tech Research Corporation
Georgia Institute of Technology
College of Sciences and Liberal Studies
School of Mathematics

DDRESS (INCLUDE DEPARTMENT)

Georgia Institute of Technology
School of Mathematics
225 North Avenue
Atlanta, GA 30332

RINCIPAL INVESTIGATOR(S)

E. Harrell II

ITLE OF PROJECT

Operator Theory and Mathematical Physics

ECHNICAL ABSTRACT (LIMIT TO 22 PICA OR 18 ELITE TYPEWRITTEN LINES)

This research will continue a program of spectral analysis and related topics in mathematical physics. It is both pure and applied mathematics; applied in that one of the goals is the derivation of formulae that a physicist can actually use, and pure in that it consists of proving rigorous theorems.

Mathematics and physics have both often benefited from research in areas where they meet. Two such areas connected with quantum physics are semiclassical tunneling phenomena and inverse spectral theory. Quantum theory describes nature with well-defined linear operators, but nature has a perverse fondness for singularities and extreme limits, for which the usual perturbative methods do not work well. Professor Harrell's work on tunneling phenomena (shape resonances, symmetry breaking in double-well Hamiltonians) will remedy the problem by combining elements of abstract functional analysis with the theory of differential equations (ordinary, partial, linear, and nonlinear).

Inverse spectral theory, on the other hand, is the attempt to determine a potential from the spectrum. Since there is usually not enough spectral information to solve the problem completely, Professor Harrell will also systematically explore inequalities for the potential obtainable from incomplete spectral information.

1. Proposal Folder
2. Program Suspense
3. Division of Grants & Contracts
4. Science Information Exchange
5. Principal Investigator
6. Off. of Govt. & Pub. Progs.

F FORM 4 (8-80)

Preface

This proposal is for a renewal of NSF grant MCS 8300551. The research will be undertaken by Professor Harrell probably partially with the assistance of one or more graduate students at Georgia Tech. (Graduate student support is not being requested at this time.) AMS classification numbers that apply include 35J10, 35P15, 35J60, 47A55, and related subdivisions of areas 34 and 81.

Progress Report of Supported Research

July, 1983 - September, 1984

This report is identical to the progress report already mailed to the Foundation.

The proposal for this grant mentioned a selection of problems in mathematical physics, most of which are concerned with the spectral theory of linear operators such as Schrödinger operators. Schrödinger operators arise in quantum mechanics, where they are the fundamental mathematical objects controlling the time-evolution. Their spectra are important both because they help understand and solve the Schrödinger equation and because they often have direct physical significance. Many of the important problems in quantum physics fall under the categories of direct spectral theory, inverse spectral theory, and perturbation theory, frequently under more than one such category. The grant proposal filed about two years described several problems in these categories in some detail.

Once again, I am pleased to report substantial progress on most of the topics mentioned in the grant application. The funds in the grant, of which little remains, supported many professional activities connected with my research, especially the preparation and publication of papers and travel to conferences and colloquia. Some reprints are enclosed for your records.

Travel

Travel supported by the Foundation included: the Congress of the International Association of Mathematical Physicists at Boulder, Colorado, in August, 1983; The Southeastern Atlantic Conference on Differential Equations in Knoxville, Tennessee, November, 1983; The American Mathematical Society meeting in Louisville, Kentucky, January, 1984; and the Southeastern Atlantic Conference on Differential Equations in Winston-Salem, North Carolina, October, 1984. In addition, during 1984 I reported on research supported by the Foundation at Tulane University, the University of Missouri, King's College in London, and at international symposia at Como, Italy, and Marseille, France, without requiring travel funds from the grant.

Publications

The following publications supported by the Foundation through this and the preceding grant have appeared in the last year and a half:

On the Double-Well Problem for Dirac Operators, Ann. de l'Institut H. Poincaré 38 (1983), 151-170, with M. Klaus.

Schrödinger Operator Methods in the Study of a Certain Nonlinear PDE, Proc. Amer. Math. Soc. 88 (1983), 376-377, with B. Simon.

The Mathematical Theory of Resonances whose Widths are Exponentially Small, II, J. Math. Anal. Appl. 9 (1984), 447-457, with N. Corngold and B. Simon.

Hamiltonian Operators with Maximal Eigenvalues, J. Math. Phys. 25 (1984), 48-51.

Book Review of M. S. P. Eastham and H. Kalf, Schrödinger-type Operators with Continuous Spectra, Bull. Amer. Math. Soc. 10 (1984), 311-315.

1/R Expansion for H_2^+: Analyticity, Summability, Asymptotics, and Calculation of Exponentially Small Terms, Phys. Rev. Lett. 52 (1984), 1112-1115, with R. J. Damburg, R. Propin, S. Graffi, V. Grecchi, J. Čížek, J. Paldus, and H. J. Silverstone.

Moreover, the following manuscripts have been written but have not yet appeared:

Coerciveness and Galerkin Methods for Elliptic Equations at Resonance, with W. Layton.

On the Extension of Ambarzumian's Inverse Spectral Theorem to Compact Symmetric Spaces.

Potentials Producing Maximally Sharp Resonances, with R. Svirsky.

Potentials having Extremal Eigenvalues Subject to p-Norm Constraints, with M. S. Ashbaugh.

Theory of Quantum Resonance. This was the first topic mentioned in the grant application, and has been dealt with in the context of two different projects. Quantum resonances can be interpreted as nonreal eigenvalues of certain complexified, formally symmetric differential operators. A graduate student at Johns Hopkins, R. Svirsky, is doing a thesis on this subject under my informal guidance. We have written one paper together (see above) and he should finish his thesis in June. The general idea is to perform a variational analysis using the perturbation theory of linear operators in order to determine the functional form of potentials giving rise to sharp quantum resonances. Resonances are said to be sharp if the eigenvalues lie near the real axis. We obtain generic lower bounds on the imaginary parts of the eigenvalues in terms of the real parts, bounds on the potential V, the size and shape of its support, and Lp norms of V. The second project connects a double-well problem, described below, to the perturbation theory of a resonance problem.

Double-Well Potentials and Their Bender-Wu Theory. This refers to quantum-mechanical Hamiltonians with wells, or minima, which are separated by a large distance or a large barrier. There is a tendency for the eigenvalues of operators of this form to cluster in pairs, and over the last several years in a series of papers I have developed perturbation theory for the eigenvalues and particularly for the splitting between them, which is a delicate "tunneling" phenomenon. The eigenvalue gaps can be expressed in terms of the eigenfunctions in a way that allows evaluation by semiclassical expansions. It has been gratifying to see these papers attract attention recently, particularly from specialists in pseudodifferential operators, who have extended them to a wide class of operators (see, e.g., B. Helffer and J. Sjöstrand, Multiple Wells in the Semiclassical Limit, I - V, the first of which appeared in Commun. PDE 9 (1984), 337-408). My own research in the period covered by the grant has centered on a particular model of some importance in quantum chemistry, the hydrogen molecular ion. It has been a collaborative, interdisciplinary effort with S. Graffi, V. Grecchi, H. J. Silverstone, and others. The Hamiltonian for this molecule separates, making detailed calculations possible, and we have uncovered an intricate analytic structure. The perturbation series for the eigenvalues (as a function of the internuclear distance in the Born Oppenheimer approximation) can be calculated to very high order, and are asymptotic but diverge. They can be summed by a generalized Borel technique, but the sums of the series are not the eigenvalues. Ideas going back to work of Bender and Wu lead one to expect that perturbation series at very high order often become regular in ways that can be related to tunneling calculations. In this case we have discovered how to relate the series coefficients at high order to my earlier estimates of the gaps between the eigenvalues, by first identifying a resonance problem associated with the ion and then analyzing the relationship between the resonance and the gaps on the one hand and the perturbation series on the other.

Nonlinear Elliptic PDEs and Inequalities for Eigenvalues. These two distinct topics have turned out to be related. In attempting to create new bounds on eigenvalues by determining the operator, within a certain class, that maximizes or minimizes a given eigenvalue, I found that what is in effect the Euler equation for the problem is a semilinear partial differential equation (J. Math. Phys. 25 (1984), 48-51). Existence of extremal operators follows from linear functional analysis, so in the above-listed paper with Ashbaugh and another manuscript in preparation, he and I obtain not only eigenvalue bounds but also existence theorems for solutions of these nonlinear equations. Other sorts of eigenvalue bounds, for example lower bounds on the fundamental eigenvalue of $-\Delta + V$ on a sphere in terms of the spectral asymptotics of that operator, have been obtained from inverse methods in my recent manuscript, On the Extension of Ambarzumian's Inverse Spectral Theorem to Compact Symmetric Spaces.

The least successful topic of those listed in the grant application has been that of inverse problems in nuclear magnetic resonance. This was a joint project with Michael Silver, a graduate student at Johns Hopkins, when I was on the faculty there, and although it is still interesting and potentially important, it has not progressed much since my departure. I determined that the equations of interest can be transformed into a version of the Zakharov-Shabat equations, for which an inverse theory already exists, but am unaware of whether Mr. Silver has managed to make use of that observation.

In the coming budget period my immediate plans include not only rounding out and writing up the projects described above, as well as such engrossing activities as making a renewal application, but also pursuing some new ideas.

In particular, I will focus on finding additional general inequalities for eigenvalues. I can prove, for example, that there are lower bounds to the gap between the first two eigenvalues of some types of Schrödinger operators, in terms of information such as the support and norms of the potential, and will attempt to find the constants in the bounds.

PROPOSED RESEARCH

Operator Theory and Mathematical Physics

The fundamental object in the mathematics of nonrelativistic quantum mechanics is the Schrödinger operator, a linear differential operator of the form

$$-\Delta + V, \tag{1}$$

where Δ is the Laplace operator on Ω, a subset of a space such as R^3, and V represents multiplication by a real-valued potential function V(x). The domain of definition is typically a Sobolev space. Nonrelativistic quantum physics reduces in large measure to the study of the spectrum and eigenfunctions, including generalized eigenfunctions, of (1) with various types of potentials, sometimes equipped with variable parameters. The direct physical relevance of the spectrum and eigenfunctions is to specify the allowed values of a measurement of the energy and the spatial probability distribution of a quantum particle; but, moreover, the spectral theorem allows knowledge of the spectral data to completely determine the dynamical semigroup solving the time-dependent Schrödinger equation. The study of such operators and their relativistic variants is thus quite important in physics. Conversely, they have been a gold mine for mathematics, because, although they have been rigorously understood only in the last couple of decades [30, 36], a number of imperfectly understood techniques have long been used to handle them with fair success in chemical and particle physics. This is good evidence of mathematical structure to uncover.

Since his thesis, Professor Harrell has worked on a range of topics in the spectral theory of Schrödinger operators, primarily by augmenting the theory of perturbations of linear operators with that of differential and integral equations. These topics have included estimates of eigenvalues and eigenfunctions, inverse spectral theory, the nature of spectra of non-self-adjoint realizations of the operators, and existence and properties of solutions to certain semilinear partial differential equations. The physical leitmotiv has been the tunneling effect in the semiclassical limit of quantum mechanics.

Crudely speaking perturbation theory means taking small terms, usually contained in V in (1), into account by making power-series expansions. It can be thought of more abstractly as synonymous with the theory of analytic, operator-valued functions of one or more complex variables. This is well understood when the perturbation is bounded, relatively bounded, or satisfies certain other conditions. Unfortunately for physical theory many of the more important Schrödinger operators contain potential terms that are not small in any very strong sense, and such singular perturbations can cause eigenvalues and eigenfunctions to be nonanalytic or even discontinuous functions of the parameter even when the form of the dependence of the operator on the parameter is apparently quite simple. Although it may not be difficult to write down formal power series for quantities such as eigenvalues and eigenfunctions, the series will then fail to converge or even to have a meaningful, provable relationship to what they putatively represent. In addition, many quantitites of physical interest, particularly those associated with tunneling effects, tend to be exponentially small functions of the perturbation parameter, and as a consequence cannot be calculated perturbatively. Schrödinger operators, however, have additional structure beyond their self-adjointness, which can be exploited to refine the calculation. As a rule of thumb, the crucial properties of the spectrum are reflected somehow in the structure of the eigenfunctions, particularly, for the problems on which Harrell works, in growth properties that can be estimated with semiclassical expansions. There are two steps in the implementation of this idea. The first is to guess the right property of the eigenfunction and to prove a formula showing how the spectrum is related to it. The second is to use the extensive lore about solutions of differential or integral equations to evaluate the functional property.

A subject that benefits in a different way from perturbation theory is the inverse spectral theory of Schrödinger operators, i.e., the study of the extent to which the potential V can be determined the spectrum. Since physical experiments cannot really be expected to measure the entire spectrum of a Hamiltonian operator, Harrell believes in investigating the question of what partial knowledge of the spectrum implies about the potential. This leads to a study of inequalities on eigenvalues in terms of properties of the potential, such as p-norms, which can be derived with perturbative arguments. Some of the inequalities turn out to be connected with the solutions of auxiliary nonlinear differential equations. There are also special cases where partial information (even a single eigenvalue and an asymptotic estimate of the limiting behavior of the eigenvalues) can completely determine the potential.

Double-Well Potentials

Schrödinger operators with double-well potentials have been a staple of Harrell's research for several years. The distinguishing feature of a double-well potential V is that it consists of two widely separated parts, whose associated Schrödinger operators would have an eigenvalue in common if they were completely decoupled. This is typically due to a reflection symmetry about a central plane, which engenders an approximate, but broken, symmetry in the eigenvalues associated with the symmetric and antisymmetric subspaces. Double-well potentials occur in simplified models for Yang-Mills field theory and in realistic models for diatomic molecules in molecular chemistry. An example is the hydrogen molecular ion H_2^+, the Schrödinger operator for which (in the Born-Oppenheimer approximation) is

$$-\Delta - 1/|x| - 1/|x-Re|, \tag{2}$$

acting on $L^2(R^3)$, where x is the variable in R^3 and e is a fixed unit vector. When the internuclear distance R is large the physical expectation is that H_2^+ should roughly decouple into two independent, hydrogen-like pieces $(-\Delta-1/|x|)$ except for tunneling effects, which are quite small. One of these effects is that the eigenvalues of a double-well operator are paired and separated by gaps $O(\exp(-CR))$ as $R \to \infty$, and it is both the most interesting physical question and the most subtle mathematical question connected with double-wells to understand and estimate the gaps between paired eigenvalues of (2) and similar operators. The general phenomena and techniques for estimating the gaps are fairly well understood as a result of work by Harrell and others exploiting the interplay between the theories of linear operators and partial or ordinary differential equations [8,13,15,16,18,20,27,37]. Harrell proposes to continue these investigations in three directions:

1. Recently, the introduction of refined asymptotic expansions of double-well eigenfunctions by B. Helffer and J. Sjöstrand and by B. Simon [27,28,37,38,39], based on a construction of Agmon [1], has freed some of the earlier gap computations of Harrell from simplifying assumptions, such as that the potentials tend to 0 at large distances from the wells or that the variables in the eigenvalue problem can be separated. While this represents a great technical advance,

there is still room for improvement in the lower bounds for eigenvalue gaps, particularly for excited states. Obtaining better lower bounds might shed light on the nature of the semiclassical limit in quantum mechanics.

2. The perturbation series for the eigenvalues of (2), in powers of 1/R, has been under study by Harrell in collaboration with S. Graffi, V. Grecchi, and H. J. Silverstone, because (2) is one of the simplest realistic double-well operators. A few years ago there was a conjecture, supported by numerical evidence, by the French theoretical physicists E. Brézin and J. Zinn-Justin that the asymptotic behavior of the perturbation series coefficients at large order was related to the eigenvalue gap by a dispersion formula [7]. The study of this sort of relationship is called Bender-Wu theory after the first people to discover a relationship between perturbation series and tunneling quantities in the context of the anharmonic oscillator [5]. In the past the tunneling quantity has always been a resonance width, i.e., the imaginary part of a nonreal eigenvalue of a formally symmetric realization of a Schrödinger operator. In [9,13] the formula of Brézin and Zinn-Justin is made precise and improved exactly by finding a resonance problem, a non-self-adjoint version of (2), which leads to a dispersion reaction in the usual way, and which is also connected in leading order to the eigenvalue gap. The operator (2) is separable, and the Bender-Wu analysis is as a

consequence quite complete. Having succeeded with this model in understanding the connection between the tunneling effects and the large-order perturbation theory in great depth, Harrell and his colleagues would like to see how much of this intricate structure is particular to the model and how much is more widely applicable.

3. There is an inverse problem related to the study of small gaps in the operators described above: To what extent does the presence of a small gap in the spectrum of a Schrödinger operator, especially between the fundamental eigenvalue and the rest of the spectrum, mean that the operator is in some sense of double-well form? This question can be addressed either with the aid of general inequalities (cf., [31]), or, in keeping with the ideas described below in the section on inverse problems and inequalities, by attempting to solve for the potential, within a given class, that minimizes the gap. Harrell has an unpublished proof that if potentials are defined on a finite region and there is a bound on one of their p-norms for sufficiently large p, then there is a potential that minimizes the fundamental eigenvalue gap. The gap-minimizing potential satisfies certain differential equations. Harrell plans to address the question of uniqueness of the gap-minimizing potential, and to determine whether it resembles a double-well potential by, for example, separating the region in which it is supported into two roughly independent pieces. This program

will probably be largely a collaboration with Professor E. B. Davies, who has some related results [10], and who will visit Georgia Tech in 1985. While the two other directions mentioned above continue earlier trends in Harrell's work, this one represents a new development.

Theory of Quantum Resonance

In some physical situations where the tunneling effect arises, such as when a particle is confined within a nucleus by a large potential barrier, the Hamiltonian has a purely continuous spectrum but the dynamical group it generates acts much as if it had discrete eigenvalues. For such resonance problems one can take either a time-dependent or time-independent point of view. The latter, on which Harrell and collaborators have written a series of articles [2,14, 17,18,19,22], partially supported by the grant being renewed, replaces the study of the self-adjoint Hamiltonian with that of a non-self-adjoint operator having discrete but nonreal eigenvalues, related by perturbation theory to the discrete, real eigenvalues of a reference problem. The real and imaginary parts of the complex eigenvalues have different physical interpretations, respectively having to do with the energy level and the decay time of the resonance. The imaginary part of such an eigenvalue will be referred to as the resonance width, and a resonance will be said to be sharp if the width is small. The analysis of resonances may be important for purely mathematical reasons as well, as a step in the construction of a more satisfactory spectral theory for nonnormal operators.

The aspect of resonances that has been predominant in Harrell's previous work has been the asymptotic evaluation of the widths. In the interesting situations the imaginary part is exponentially small in comparison with the real part, and is thus invisible in any usual perturbation expansion. Nevertheless, Harrell and colleagues have succeeded in evaluating the imaginary part asymptotically in several cases by delicate use of estimates of the growth of solutions of differential equations [2,8,13,17,18,19,29]. These analyses have been more complete in one-dimensional and separable cases than in cases without special symmetry. Since a key element is the use of general eigenvalue gap formulae that are independent of symmetry and dimension, Harrell believes he can extend this work by eliminating the reliance on techniques of ordinary differential equations in favor of the new eigenfunction estimates that have been rather useful recently in the study of other tunneling effects mentioned above [27,28,37,38,39].

In a different attempt to understand exactly what makes a resonance sharp, Harrell has come up with some general lower bounds for the imaginary part in terms of properties of the potential, by using comparison techniques and perturbative estimates [22]. More recently, Harrell and a graduate student at Johns Hopkins, R. Svirsky, have gone beyond this to attempt to characterize the potentials, subject to certain bounds on their values and support, that produce maximally sharp resonances within a given energy range [26,40]. Harrell and Svirsky are trying to determine, among other things, whether all very sharp one-body quantum resonances are caused by confinement by a large potential barrier, rather than some other mechanism. Within certain limits, the answer appears to be affirmative.

Finally, the time-independent and time-dependent points of view have not been related in a completely satisfactory way. Professor Harrell hopes to understand the relationship better by comparing his calculations of imaginary parts to time-dependent studies of sojourn times by Lavine [32,33].

Inverse Spectral Theory and Inequalities for Eigenvalues

Inverse spectral theory, the attempt to recover the potential V from the spectrum of a Scrödinger operator, has had some notable successes, particularly in one-dimension, where a complete knowledge of the spectrum (along with norming constants) will completely determine the potential by the Gel'fand-Levitan-Marchenko procedures or more recent alternatives [41]. At least as important, however, are higher-dimensional problems and problems where one has to make do with imperfect information about the spectrum, but much less is known about them. It turns out that the implications of imperfect information are often less tied to one-dimension than are those of perfect information.

On occasion even a limited amount of spectral information can determine the potential. Consider, for instance, a Schrödinger operator $-\Delta + V$ on an n-sphere (or any compact symmetric space of rank 1). The eigenvalues cluster near the (finitely degenerate) eigenvalues λ_k of the Laplace-Beltrami operator $-\Delta$ as the eigenvalue index k tends to infinity. Let η denote the limit of the difference between the average of the k-th cluster for $-\Delta + \bar{V}$ and λ_k. It is easy to see that this limit exists (for, say, bounded, measurable potentials), and it can be shown that the fundamental eigenvalue of $-\Delta + V$ must either lie strictly below η or else $V = \eta$ a.e. (constant function) [24]. This fact curiously ties the top of the spectrum to the bottom. In other words, spectra have to satisfy various not always evident consistency conditions, and if they only marginally satisfy them, then the inverse spectral problem may be overdetermined. It does not appear to be precisely known what sets of real numbers could conceivably be spectra of Schrödinger operators on a given domain or a given manifold. Harrell proposes to study this question on the one hand by investigating other overdetermined inverse problems and on the other by exploring the consequences of general and specific eigenvalue inequalities.

Not only can inequalities contribute to inverse problems, they can also be derived from constrained inverse problems.

In a paper published earlier this year [23], Harrell solved the following problem: Let an operator $-\Delta + V$ act on a reasonable, bounded domain in an n-dimensional Euclidean space, and constrain the potential only by bounding its 1-norm. Find the maximal possible value of the fundamental (or the n-th) eigenvalue and give conditions under which it is attained. Characterize the maximizing potential and determine when it is unique. Since then Harrell and M. S. Ashbaugh [3,4] have extended these ideas and combined them with ideas of V. Glaser, H. Grosse, E. H. Lieb, A. Martin, and W. Thirring [12,34], to incorporate p-norm constraints and to characterize potentials which either maximize or minimize eigenvalues. The result, from the standpoint of inverse theory, is that the value of any one eigenvalue produces lower bounds on the p-norms of the potential. The techniques are quite general, combining straight-forward functional analysis with formulae from perturbation theory, and thus also apply to other sorts of operators as well as $-\Delta + V$, e.g., self-adjoint elliptic partial differential operators of certain forms. In the near future Harrell proposes to pursue analogous optimizing problems for other spectral properties, including gaps between eigenvalues as mentioned above, and for eigenvalues of non-self-adjoint differential operators.

Nonlinear Partial Differential Equations

It has been known for some time that the theory of certain kinds of nonlinear differential equations is connected with the spectral theory of linear differential operators (cf. [11]). Such connections have shown up in several ways in Harrell's work as well, ranging from the usual phenomenon of nonlinear evolution equations arising in inverse scattering [14] to the need for eigenvalue estimates to prove convergence of numerical schemes [25]. A more unusual connection was the discovery of Harrell and B. Simon [21] that eigenvalue counting could be used to produce an efficient proof of the nonexistence of positive solutions of certain semilinear differential equations of the form

$$\Delta u = -h(x)u^{\alpha}.$$

In addition, M. S. Ashbaugh and Harrell have work in progress, partly described above under "Inequalities for Eigenvalues," which likewise connects linear spectral theory with certain auxiliary nonlinear differential equations. More specifically, the maximizing or minimizing potentials for an eigenvalue of an operator $-\Delta + V$, with V constrained by

$$\|V\|_p \leq M,$$

have been found to be characterized by $V^{p-1} = cu^2$, where u (the associated eigenfunction) satisfies

$$-\Delta u \pm \operatorname{sgn}(u)|u|^{\alpha} = \Lambda u$$

(with $\alpha = (p+1)/(p-1)$). Analogous equations hold for optimizing potentials with other leading linear elliptic operators. The point is that existence theorems for optimizing potentials, which are fairly easy, imply existence theorems of solutions of the associated nonlinear equations. (Some related ideas have been noted in [6,12,34,35] and elsewhere.)

The ideas for proving existence or nonexistence of solutions to nonlinear partial differential equations seem to be rather efficient tools that have by no means been exploited to their fullest. Harrell plans to continue the investigation of the nonlinear equations that arise in the context of inverse problems, and to attempt to discover whether similarities among the apparently independent relationships between spectral theory and nonlinear equations mentioned above are merely accidental or indicative of deeper matters.

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Foreign-Travel

Professor Harrell has extensive European contacts (he has several foreign coauthors and formerly held a position at the University of Vienna), occasioning frequent foreign travel. He has specific plans to visit Marseille, France for two weeks in 1986 for the Congress of the International Association of Mathematical Physicists, the major international mathematical physics meeting held at various sites every two or three years. He will probably combine or supplement that trip with a visit to one of the European universities at which he has standing offers to visit.

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Although this grant has been in effect for only a few months, there has been good progress, especially in the areas of a) semiclassical estimates of solutions of the Schrödinger equation, b) eigenvalue bounds, and c) connections between Schrödinger operators and the Laplace-Beltrami operators of differential geometry. The first two areas are essentially described in the grant proposal, while the third is a related new development. The third area has also used the nonlinear differential equations mentioned in the grant proposal. The concrete embodiment of this progress has been a joint paper with E.B. Davies [1], which was written over the summer and recently accepted for publication.

Travel. Professor Harrell attended two conferences where he spoke about grant-supported research. This grant paid the transportation to one of them, a meeting of the American Mathematical Society in Columbia, Missouri.

Other articles written during the previous grant progressed towards publication, either by getting proofread [2,3] or receiving final revision and getting submitted to journals [4,5].

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