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13. ABSTRACT *(Maximum 200 words)*

My staff research on dissipative Hamiltonian systems has evolved from Quantum Optics into three areas over the past three years, exemplifying the type coherent and incoherent processes which when merged lead to dissipative relaxation: 1) High precision scaling and critical exponent relations were derived for the Heisenberg Ferromagnet which show new details that challenge existing theories; 2) Super-enhanced Backscattering of radiation was observed and explained as due to Fabry-Perot type multi-pass multiple scattering from rough thin films where coherency is broken by the spatial stochasticity of the medium leading to photon localization and the ensuing enhancement. Next we need to take higher order correlations into account to include memory effects akin to hysteresis that we studied in Quantum Optics; 3) Showed the necessity of taking the full potential (as opposed to muffin-tin potentials which are partials of the full potential) in the Wigner-Seitz cells of crystalline solids for the calculation of electronic energy levels, including the role of impurities such as sulfur and boron, and therefrom deriving microscopic stress-strain tonsorial relations to study crack propagation -embrittlement problems at the level of details of bonding orbitals. Next Molecular Dynamics will be performed to show effects of temperature on this micromechanical dynamics.

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MONTE CARLO STUDIES OF CONTINUOUS HAMILTONIAN SYSTEMS COUPLED TO DISSIPATIVE MECHANISMS

FINAL REPORT

October 15, 1996

U. S. ARMY RESEARCH OFFICE

DAAH04-93-D-0002 / 31093-PH

DUKE UNIVERSITY

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DISCUSSION OF FINDINGS:

During the term of this completed grant, we advanced our work in three fronts related to the our goal to study how closed Hamiltonian systems that are in nonequilibrium states relax when they are coupled to dissipative mechanisms. Of course the best example is a system that is coupled to a thermal bath, but other intermediate steps usually intervene, such as phonons in spin dynamics, impurities that absorb radiation and thereafter dissipate the energy by nonradiative pathways, and even crack propagation can be looked at as a means of absorbing energy and dissipating it into a multiplicity of pathways.

This staff research on dissipative Hamiltonian systems has evolved from our work in Quantum Optics, specifically into three areas over the past three years, exemplifying the type of coherent and incoherent processes which, when merged, lead to dissipative relaxation: 1) High precision scaling and critical exponent relations were derived for the Heisenberg Ferromagnet which show new details that challenge existing theories; 2) Super-enhanced Backscattering of radiation was observed and explained as due to Fabry-Perot type multi-pass multiple scattering from rough thin films where coherency is broken by the spatial stochasticity of the medium leading to photon localization and the ensuing enhancement. Next we need to take higher order correlations into account to include memory effects akin to hysteresis that we studied in Quantum Optics; 3) Showed the necessity of taking the full potential (as opposed to muffin-tin potentials which are partials of the full potential) in the Wigner-Seitz cells of crystalline solids for the calculation of electronic energy levels, including the role of impurities such as sulfur and boron, and therefrom deriving microscopic stress-strain tonsorial relations to study crack propagation -embrittlement problems at the level of details of bonding orbitals. Next Molecular Dynamics will be performed to show effects of temperature on this micromechanical dynamics.

1)The critical dynamics of the Heisenberg Ferromagnet:

The reason for selecting the Heisenberg ferromagnet was to introduce a time dependent thermal bath in a system with a well studied physical Hamiltonian that is amenable to detailed statistical mechanical analysis both in the classical and quantum mechanical regimes analogous to our Quantum Optics study but with a bath now. Both Monte Carlo simulation and algebraic/analytical studies were carried out. The algebraic results used Grassmann algebra with the derivation of the closed form of the Generating Function of the Heisenberg ferromagnet coupled through phonons to the thermodynamic bath. This work is to be continued to determine if the closed form will give the appropriate scaling relations. The simulational- Monte Carlo work also progressed to a point where we were able to derive extremely accurate values of the critical exponents that satisfy scaling relations in a remarkably universal way. In the process of developing the Monte Carlo methodology, we were forced to conduct further research in Sampling Theory, in order to be sure that our results were reliable. This has also been submitted for publication.

Let us now describe this work in more detail.

After carefully reading the existing literature on this subject, we successfully integrated a thermal bath into a ferromagnetic version of our optical code, extending our simulation techniques to the study of the relaxation of the para/ferromagnetic critical point. In order to fully understand the dynamic critical process, one must first fully understand the static critical process and the (e.g. Finite Size Scaling) methodology used to study it. We spent some time mastering this methodology and advancing a "Heat-bath" Monte Carlo study of the static critical exponents of the 3d Classical Heisenberg Model to the edge of the state of the art. This calculation, which reveals several surprising and puzzling features of the model, was recently published in Physical Review Letters.

This static calculation was completed almost incidental to our primary research effort to understand critical relaxation in this model. This effort was entirely successful; our results significantly advance the understanding of the critical dynamics of relaxation in thermally coupled systems. We completed and are now publishing (in Physical Review B, the most accurate and complete study ever of critical relaxation (critical slowing down) in the 3d Classical Heisenberg Model. (We recall here that our Quantum Optics work also lead to the hysiteresis loop of Optical Bstability wit attendant critical slowing down within that cycle for the first time and without the unphysical branch of the cubic nonlinearity).

In addition to obtaining high precision estimates for the dynamic critical exponents of the model, this work presents a novel algebraic/geometric estimate for the exponent that describes the breaking of symmetry, obtains the first results ever for the exponent that describes the breaking of energy ergodicity, and corrects a number of errors in the literature. Critical slowing down is intimately connected to sample independence in any Monte Carlo methodology, and in this work we demonstrate rigorous and reliable ways for forming error estimates and sample independence times without the need to study system autocorrelation times directly. Preliminary versions of these results were presented (and published) at workshops and informal talks at Duke and the University of North Carolina at Chapel Hill; these presentations allowed us to greatly improve the quality of the final Phys. Rev. publications.

It was necessary for us to master both the heat bath approach and the more modern cluster thermalization methods in order to obtain the desired degree of precision in the static exponent calculations. Incidental to this work, we also measured and optimized the efficiency of "Cluster Methods" in application to this problem. We plan to publish the results as a Brief Report in Physical Review B as a supplement to our recent work.

As might be expected, whenever one significantly increases the resolution of a calculation (our resolution of the specific heat was several orders of magnitude better than any previous calculation) new features are revealed that may challenge accepted results and hence require further examination or explanation. Our results are no exception to this rule. A debate has begun in the literature as to whether the surprising features of our work are in fact statistically significant. In a very recent work (to be published as a Comment in Physical Review Letters) we demonstrate that they are in fact statistically sound. We are preparing a longer publication that examines the problem in a different way that arrives at the same conclusion, but this work will be completed during the term of our current grant.

We also plan to follow through the algebraic/analytical means of deriving the dissipative dynamics of this model system; the results can have a rather significant impact on many-body theory in general.

2) Optics of rough thin films and super-enhanced backscattering:

In reviewing experimental work being conducted at Surface Optics, I noticed that what was being observed as super-enhancement appeared to be insensitive to the type of material that was being examined so long as it had surface roughness. With my intervention we found that we could eliminate a spurious side effect related to the way the aparata were set-up. By eliminating this, we were able to better reveal the more important multi-pass multiple scattering from a thin film on a rough substrate with certain imperfections. Upon analysis of the ring patterns that we observed I calculated the Fabry-Perot type phase relationships that should be taking place between subsequent reflections from the interfaces and the numbers agreed with the film thickness involved. So it turned out that having a properly constructed thin film with surface roughness on the substrate, one would obtain a series of reflections, not just two as is the case for ordinary enhanced backscattering; therefore this series of reflections would bring about a giant enhancement that we recorded and finally published. Here the dissipative mechanism is the spatial stochasticity due to roughness that brings about the rather curious, and counter intuitive, effect of selective enhanced retroreflection, ascribed by some investigators to "photon localization" akin to the Anderson Localization. (Again there is an analogy between this and ou Quantum Opics work where memory plays a special role in controlling the hysteresis ccycle and te associated dissipative relaxation processes.) By designing the roughness type (parameters and geometry) it is possible to force enhanced specular reflections and therein observe a variety of results in speckle patterns related to "memory effects". Because there is an analogy between this phenomenon and the so called "Universal Conductance Fluctuations" in solid state physics tied to higher order correlations, this area of study will be continued. The issue is : how does memory fade away in this dissipative system? Can we understand or separate Markovian and non-Markovian memory components?

3) First principles study of crack propagation and embrittlement:

We have demonstrated that one needs to take all of the potential in a unit cell of a crystalline solid into account in order to derive accurate electronic energy levels, the "band structure", of the solid in the first place. Then proceeding from there one can introduce impurities such as sulfur and boron into the solid and recalculate the electronic energy levels. From these results , repeated at different separations between the constituent atoms, one can derive microscopic stress-strain relations, all quantum mechanically. We have found that the "bond orbitals" and the nature of the chemical bond so derived show us why certain impurities enhance and others degrade the cohesive forces involved. A rather dramatic special case we saw with sulfur versus boron, agreeing with experimental results in very pure crystalline solids thus far studied. It was interesting that the directionality / tonsorial nature of the bonds agreed well with the type of stress-strain relations that were operative in Nickel Aluminides. More work will be conducted to relax the system at each configuration, to determine grain boundary dynamics, etc., in order to make contact with more realistic defect configurations. On my part, I will be working towards a better understanding of correlations (beyond Hartree-Fock and not necessarily in the Density Functional formalisms) that will have to be taken into account in these theoretical studies.

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A) Critical Dynamics of the Heisenberg Ferromagnet:

"Statistical microdynamics of extended systems in natural function spaces," (with R. G. Brown), *International Journal of Quantum Chemistry*, Quantum Chemistry Symposium, 27, 363 (1993).

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B) Optics of Giant Enhanced Backscattering:

"Observation of Giant E Backscattering of light from weakly rough dielectric films on reflecting metal substrates," with Zu-Han Gu and Michel Josse, *Opt. Eng.* **35**(2) 370, 1996.

C)First Principles Quantum Mechanical Theory of Microscopic Stress-Strain Relations and the Effect of Impurities in Brittle Fracture:

"Effects of Boron and Sulfur on the Ideal Yield Stress of Ni_3Al - A First Principles Study", with S. Sun, N. Kioussis, and A. Gonis, NATO. ASI Series, **355**, 413 (1996).

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