LA-UR-97- 3252

Approved for public release; distribution is unlimited

Title:

Numerical Simulations of Disordered Superconductors

RECEIVED
DEC 01 1997
OSTI

Authors:

K. S. Bedell, MST-CMS
J. E. Gubernatis, T-11
R. T. Scalettar, U.C.-Davis
G. T. Zimanyi, U.C.-Davis

Submitted to:

DOE Office of Scientific and Technical Information (OSTI)

DISTRIBUTION OF THIS DOCUMENT IS UNLIMITED

MASTER

Los Alamos
NATIONAL LABORATORY

Numerical Simulations of Disordered Superconductors

Kevin S. Bedell[*] and James E. Gubernatis
Los Alamos National Laboratory

Richard T. Scalettar and Gergely T. Zimanyi
University of California-Davis

Abstract

This is the final report of a three-year, Laboratory Directed Research and Development (LDRD) project at Los Alamos National Laboratory (LANL). We carried out Monte Carlo studies of the critical behavior of superfluid ^{4}He in aerogel. We found the superfluid density exponent increases in the presence of fractal disorder with a value roughly consistent with experimental results. We also addresssed the localization of flux lines caused by splayed columnar pins. Using a Sine-Gordon-type of renormalization group study we obtained an analytic form for the critical temperature. We also determined the critical temperature from I-V characteristics obtained from a molecular dynamics simulation. The combined studies enabled us to construct the phase diagram as a function of interaction strength, temperature, and disorder. We also employed the recently developed mapping between boson world-lines and the flux motion to use quantum Monte Carlo simulations to analyze localization in the presence of disorder. From measurements of the transverse flux line wandering, we determined the critical ratio of columnar to point disorder strength needed to localize the bosons.

Background and Research Objectives

Quantum Monte Carlo (QMC) and Molecular Dynamics (MD) are powerful and general techniques for studying the properties of systems of ions and electrons in a solid. They have important applications to condensed matter physics, chemistry, and materials science, where they are now able to simulate the properties of sizable clusters of interacting particles. QMC and MD have made great strides recently, both due to improved algorithms and to the availability of more powerful computers. They are nearly always a "large scale" project because of the complexity associated with incorporating interactions into systems of large numbers of degrees of freedom and with ensuring the correct symmetry of the many-body wave function. Despite their recent achievements, further developments are

---

[*] Principal Investigator, Phone: 505-665-0478

necessary before they can address some of the most interesting problems in solid state systems.

Computational scientists have long known the basic ways of increasing the throughput of a given application: 1) devise a more efficient algorithm for the problem at hand or 2) run the application on a faster computer. In fact, 1) can be further decomposed into the case of simple code changes, e.g., reorganization of the program to eliminate repeated or unneeded work and the case of radical redesign of the algorithm. In either case, as computing power is becoming increasingly tied to hardware architecture, the speedup methods 1) and 2) cannot be treated independently: a proposed new algorithm may not be suitable for a given architecture, so that added efficiency may be negated by poorer performance on the hardware platform. This problem is especially true for redesigned or accelerated algorithms for parallelism. Yet, it is increasingly important to be able to parallelize new algorithms in order to take full advantage of the hardware that computational scientists will be using in the future. We explored these issues within the context of specific physical applications—the strongly correlated boson problem.

a) The Physics of Disordered Superconductors

Over the last forty years a rather complete understanding of the basic physical processes of noninteracting systems has been developed and experimentally verified. Therefore, the primary focus of research in more recent times turned increasingly towards the study of interacting problems. The use of newly introduced many body techniques proved highly successful in developing a concise physical picture and achieving consistency with the experimental data.

This progress has set the stage for exploring new directions of research. One of the central questions, raised by experiments and technical applications, is connected with that omnipresent problem: the influence of the material imperfections or disorder. In the case of electronic materials, the central phenomenon of interest is the metal-insulator transition. On one hand, by increasing the repulsion between particles, interactions can constrain the possible motion so much that the particles eventually lock up in a frozen nonconducting, insulating state. Similarly, disorder can reduce mobility by selecting out special low energy sites where the electrons then become localized. Both of these transitions are exhaustively documented experimentally.

Our understanding of the corresponding bosonic materials is much less developed in spite of its experimental relevance. The disordered interacting boson model grasps the essential physics of such different phenomena as ^{4}He absorbed in porous media, homogeneously disordered superconducting wires, thin films, granular superconductors (where the Cooper pairs can be approximated as bosons), and many types of disordered quantum magnets. Finally, and maybe most importantly, this model also describes the disordered vortex states of high temperature superconductors, a problem of primary importance for technological applications. Beyond this generic interest and importance for applications, what makes these materials theoretically fascinating as well is the occurrence of quantum phase transitions, i.e., the onset of a phase transition when a parameter of the Hamiltonian is changed.

On the theoretical side, application of the renormalization group approach to quantum phase transitions has been successful in determining critical exponents for ordered models. Early work on the disordered problem identified the onset of superfluidity with bosons starting to occupy the extended states, which are well separated from the localized ones by a so-called mobility edge. Related studies of disordered superconductors determined the phase diagram at special fillings and showed that a "localized superconducting" phase may exist in the presence of stronger randomness. Finally, a new scaling theory for the quantum phase transition at $T = 0$ introduced a new universality class, the so-called "bose-glass," with exponents different from the previous two theories. Experiments on ordered Josephson junction arrays, thin disordered films, and ^{4}He in Vycor clearly demonstrated the existence of the quantum phase transition, i.e., the onset of superconductivity or superfluidity as the density or disorder was changed.

In parallel with this progress, however, experiments supplied new challenges which revealed significant remaining gaps in our understanding of the boson systems:

- The density driven localization transition in ^{4}He has exponents that contradict earlier theories and constitute a new universality class. The values of the exponents are not predicted by newer theories.

- A "universal" resistivity was reported at the superconductor-insulator transition of disordered films. This is highly unusual, as exponents and amplitude ratios are expected to be universal in the standard picture, but not the amplitudes of response functions themselves. Later measurements also revealed that for different materials the "universal resistivity" is different; and instead of metallic behavior in the critical regime, its temperature dependence often indicates insulating tendencies.

These experimental developments have raised several new theoretical issues:

- The calculations of the critical exponents have yet to be carried out for the disordered case. Actually, the phase diagram itself is controversial; several groups reported markedly different results.

- A universal conductivity was predicted in granular films but given the notoriety of two dimensions for localizing tendencies, this suggestion needs to be thoroughly investigated.

Much of our progress in understanding correlation effects in fermion systems has been developed by studying simple model Hamiltonians with coordinated numerical and analytical techniques. Therefore, we focused on the disordered interacting lattice boson Hamiltonian. It is widely thought that this Hamiltonian represents an essential paradigm for many of the above phenomena.

b) The Physics of Transport in High Magnetic Fields

There has been a great deal of interest generated lately concerning the creation of a deliberately disordered environment as a method to pin flux lines to create a true superconductor with a vanishing linear resistivity. Two types of disorder have been employed to achieve this end: point disorder which is uncorrelated in space and columnar disorder produced by heavy ion irradiation which is correlated in a preferred direction. While much theoretical attention has been lavished on the behavior of flux lines in the presence of either point or columnar disorder and their respective pinned glassy phases, the interplay of the two types of disorder is still an open topic. Flux line pinning in the vortex glass and the bose glass differs in the geometrical nature of the flux line—a meandering path in the case of point-disorder-dominated vortex glass phase and a straight path where the flux line remains locked to the columnar pins in the bose glass phase.

The next issue is the current-voltage (I-V) characteristics of these phases. This is the experimentally most accessible quantity to study, and hence a vast amount of data is available on all high Tc materials. The I-V curves display strong nonlinear tendencies, with power-law exponents up to three. Also, several regions can be observed as the voltage is raised. Finally, for stronger disorder a well-developed depinning feature develops, where the vortex array as a whole gets released from the pinning centers and starts moving. The onset of this collective transport requires a completely new type of understanding, sometimes termed "nonequilibrium critical phenomena."

We employed the recently developed mapping between boson world-lines and the flux motion problem to use QMC simulations to analyze the localization of both a single and interacting flux line in the presence of both point and columnar disorder. Measurements of the transverse flux line wandering as a function of disorder for the case of a single flux line via boson world line simulations allow us to determine the possible existence of a critical ratio of the columnar to point disorder strength to localize the bosons. Turning on the interaction between bosons, we can study the boundaries between the various phases.

The other technique, suited primarily to study the transport in these materials, is the Molecular Dynamics (MD) simulation. It follows the motion of vortices in real time, as opposed to the QMC technique, which works in imaginary time; and nontrivial continuation techniques are needed to find the real-time behavior. The MD approach provides direct access to the details of the processes, such as the distribution of velocities and locations of the vortices. The data suggest that long power-law tails are showing up in these distribution functions, which will necessitate unusual care in keeping track of the so-called "rare events" in the vortex flow. While there were previous attempts to capture the dynamics of vortices, every evidence suggests that MD is the most effective tool to capture the transport properties.

Importance to LANL's Science and Technology Base and National R&D Needs

This work will have an important impact both on basic and applied research: (i) The interplay of disorder and interactions in quantum systems represents deep general questions in theoretical physics with applications to mobility problems, the onset of superfluidity, disordered superconductors, and quantum phase transitions. (ii) The specific problem of flux line motion has crucial applications to the development of superconducting materials with high critical currents. (iii) Software and computational algorithms developed for this particular class of problems will be portable to a range of applications in other fields that use closely analogous QMC and MD techniques, in particular developing software for the efficient submission, monitoring, and analysis of runs.

Scientific Approach and Accomplishments

Large-scale simulations of interacting quantum systems address deep scientific questions at the forefront of superconductivity, magnetism, and the metal-insulator transition that are of importance to modern materials science. The numerical techniques involved are also particularly appropriate for collaborative efforts between the University of California (UC) and Los Alamos National Laboratory (LANL) since, at this technical level, there are many significant advanced scientific computing challenges in which both groups have considerable interest and expertise. As specific goals in High Performance Computing, we investigated

- the restructuring of codes to accommodate parallelism of the evolution of independent system configurations;
- the introduction of parallel control, I/O, and random number generation mechanisms;
- the implementation of parallelized code on a small-scale parallel machine (32-processor Intel Gamma);
- the prediction of performance scalability (linearity of anticipated speedups) to large machines based on 32-processor experience;
- the confirmation of portability to other platforms by testing on a cluster of single-processor workstations;
- the addressing of obstacles to attainment of scalable parallel performance;
- the evaluation of the performance of the parallel QMC and MD codes on a set of different test problems which represent different lattice connectivities, particle densities, and interaction types.

We performed simulations for disordered boson systems and for the related problem of vortices with correlated disorder. Our results for boson systems are summarized in publications [1,2,3], and for the vortex systems in publications [4,5,6]. M. Vekic, supported by this project, also worked on related problems in disordered quantum spin systems and quantum magnetism, publications [7,8,9].

In paper [1], we reported Monte Carlo studies of the critical behaviour of superfluid ^{4}He in aerogel. Modeling aerogel as an incipient percolating cluster and weakening the bonds at the fractal sites, we measured a superfluid density exponent which is roughly consistent with the experimental results. In paper [2] we discussed the issue of the coexistence of superfluidity and charge ordering in interacting boson systems. Paper [3] describes a renormalization group study of the question of whether there is a direct superfluid to Mott insulator transition in the disordered Boson-Hubbard Hamiltonian.

Paper [4] addresses the localization of flux lines caused by splayed columnar pins. We combined a sine-Gordon type renormalization group study with MD simulations to determine T_c from I-V characteristics. The full phase diagram was constructed as a function of the disorder strength, temperature, the interaction strength between vortices, and the magnetic field. In paper [5] we studied numerically the motion of vortices in dirty type II superconductors. In two dimensions at strong driving currents, vortices form highly correlated "static channels" with quasi long range translational order in the transverse direction but only short range longitudinal order. We clearly established the existence of a finite transverse critical current. Paper [6] developed a theory for the quantum gauge glass, a model closely related to XY magnets and bosons in random media. For properly chosen distributions of the site disorder we find two distinct Weak and Strong Glass regions, dominated by long range and local fluctuations, respectively. Strikingly, at the Strong Glass transition the nonlinear susceptibility does not diverge.

Publications [7,8] studied the issue of transitions in which disorder destroys states with long-range antiferromagnetic order. The two-dimensional spin-1/2 quantum Heisenberg antiferromagnetic with random bonds was simulated using Quantum Monte Carlo. Singlet formation on the strong bonds drove the formation of a spin liquid state. Publication [9] described a similar phenomenon in an itinerant model, the Anderson lattice Hamiltonian, as the hybridization between local orbitals and the conduction band increased.

Publications

1. Moon, K., and Girvin, S., "Critical Behaviour of Superfluid ^{4}He in Aerogel," Phys. Rev. Lett. **75**, 1328 (1995).
2. Scalettar, R. T., Batrouni, G. G., Kampf, A. P., and Zimanyi, G. T., "Simultaneous Diagonal and Off-Diagonal Long Range Order in the Boson-Hubbard Model," Phys. Rev. B **51**, 8467 (1995).
3. Pazmandi, R. T., Zimanyi, G. T., and Scalettar, R. T., "Simultaneous Diagonal and Off-Diagonal Long Range Order in the Boson-Hubbard Model," submitted to Phys. Rev. B.
4. Devereaux, T. P., Scalettar, R. T., Zimanyi, G. T., Moon, K., and Loh, E., "Phase Diagram for Splay Glass Superconductivity," Phys. Rev. Lett. **75**, 4768 (1995).
5. Moon, K., Scalettar, R. T., and Zimanyi, G. T., "Dynamical Phases of Driven Vortex Systems," Phys. Rev. Lett. **77**, 2778 (1996).
6. Pazmandi, F., Zimanyi, G. T., and Scalettar, G. T., "Dynamical Phases of Driven Vortex Systems," submitted to Europhys. Lett.
7. Sandvik, A., and Vekic, M., "Disorder Induced Phase Transition in a Two-Dimensional Random Quantum Antiferromagnet," Phys. Rev. Lett. **74**, 1226 (1995).
8. Sandvik, A. W., and Vekic, M., "Quantum Phase Transitions in 2D Antiferromagnets," J. of Low Temp. Phys. **99**, 367 (1995).
9. Vekic, M., Cannon, J. W., Scalapino, D. J., Scalettar, R. T., and Sugar, R. L., "Competition Between Antiferromagnetic Order and Spin Liquid Behavior in the Two-Dimensional Periodic Anderson Model at Half-Filling," Phys. Rev. Lett. **74**, 2367 (1995).