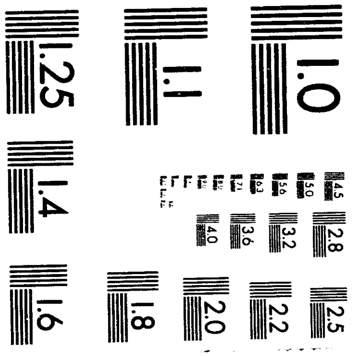
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1 of 1

Progress Report for 030191–090193

Grant No. DE–FG03–85ER45197

1. **Project Title**: Numerical Simulation of Quantum Many-Body Systems

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2. **Principal Project Personnel**

D.J. Scalapino and R.L. Sugar are the Principal Investigators in this project. J.R. Schrieffer was a P.I. until 1/1/92, when he left UCSB to become a University Professor in the University of Florida system. Scalapino and Sugar have focused on the development and implementation of numerical techniques, such as quantum Monte Carlo, to study the physical properties of interacting many-body systems.

3. **Additional Project Personnel**

W.D. Toussaint, Professor of Physics at the University of Arizona, spends one summer month at UCSB working with us on the development of algorithms and measurement techniques. Toussaint is one of the leading experts in the simulation of quantum field theories.

Postdoctoral physicists who have worked with our group include:

	Ph.D. Degree	Present Position
S. White	Cornell	Asst. Prof., U.C. Irvine
R. Fye	U.C. San Diego	Sandia
A. Moreo	Univ. Nac. de Cuyo, Argentina	Asst. Prof., Florida State

These postdoctoral workers carried out large-scale simulations on various models of strongly interacting electron systems and worked closely with the graduate students.

This project has benefitted from an IBM grant which provided Postdoctoral Fellowship support. Du Pont, Xerox, and UCSB have also contributed to visitor and computational support.

Since the inception of this project, we have supported five UCSB graduate students who have received Ph.D. degrees for their work on numerical simulation of many-body systems.

	Thesis Title	Present Position
E. Loh	Monte Carlo Simulation of the 2D Spin 1/2 XY Model	Thinking Machines
W. Gill	Ferromagnetism in a Degenerate Hubbard Model	Prof., National University, Korea
R. Scalettar	A New Algorithm for the Numerical Simulations of Fermions	Assoc. Prof., U.C. Davis
M. Jarrell	Impurity Enhancement of Superconductivity	Asst. Prof., U. Cincinnati
N. Bulut	Magnetic Fluctuations in Layered Cuprates	Res. Asst. Prof., Univ. of Illinois
R. Noack	Competition between Superconductivity and CDW Order in the 2D Holstein Model	Postdoc, U.C. Irvine

At present, Sean Quinlan, a UCSB graduate student, is working on a layered electron gas model of the cuprate oxide superconductors for his thesis. In addition, during the past year, Anders Sandvik, a Fulbright scholar, worked on simulation techniques for Hubbard systems with random impurities. During the present grant N. Bulut worked as a postdoctoral fellow for one year. He is now a research assistant professor at the University of Illinois.

4. **Project Review**

Understanding the physical properties of strongly interacting many-electron systems remains one of the central goals of condensed matter physics. In this project, we have developed and implemented numerical techniques, such as quantum Monte Carlo simulations [12,22,23],* to study basic models of interacting electrons: the one-band Hubbard model for positive [15,24] and negative U [8,14], the three-band CuO_2 Hubbard model [1,2], the Holstein electron-phonon model [6], the periodic Anderson model, and the Kondo lattice [4,9]. Such models exhibit a rich variety of physical properties. For example, the half-filled Holstein model undergoes a Peierls-charge-density wave transition. While away from half-filling there is competition between superconductivity and the Peierls-charge-density wave phase. The ground state of the half-filled 2D Hubbard model has long-range antiferromagnetic order. Away from half-filling, it has been found to have an attractive interaction in the singlet $d_{x^2-y^2}$ pairing channel [21,26,28,29], and it provides a model for the high-temperature cuprate superconductors. Similarly, it is believed that the periodic Anderson model and the Kondo lattice model provide a framework for understanding the heavy fermion materials which can exhibit antiferromagnetic and superconducting phases.

Because of the strong coupling and the interplay between the different correlations, it is possible to tip these delicately balanced systems in favor of a given correlated state by the approximations one makes. Thus it is important to develop systematic, controlled calculations for these models. Numerical calculations provide an important approach for

* Bracketed numbers refer to references listed in 5. Publications.

determining the properties of such models. In the following section we will review our work on these problems.

A. The Hubbard Model

Monte Carlo calculations of the particle-particle and particle-hole irreducible vertices were carried out. Combining these results with the Monte Carlo single-particle Green's function, we determined the eigenvalues and eigenfunctions of the particle-particle and particle-hole Bethe-Salpeter equations [21] for an 8×8 Hubbard lattice with $U/t = 4$ and 8. At half-filling the dominant eigenvalue occurs in the particle-hole channel with center of mass momentum $Q = (\pi, \pi)$ and corresponds to the formation of antiferromagnetic spin correlations. In the singlet particle-particle channel at a filling $\langle n \rangle = 0.87$, the leading even-frequency instability occurred in the $d_{x^2-y^2}$ channel.

A comparison [26,28,29] of the momentum transfer and frequency dependence of the irreducible particle-particle vertex Γ for $U = 4t$, and a filling $\langle n \rangle = 0.87$ showed that Γ could be approximated by a single spin-fluctuation exchange form

$$\Gamma(q, \omega_m) = U + \tfrac{3}{2} g^2 U^2 \chi(q, \omega_m)$$

with χ the Monte Carlo determined spin susceptibility and g a renormalization factor of order 0.8. This result provides support for theories in which the pairing interation in the doped Hubbard model is viewed as arising from the exchange of single nearly antiferromagnetic spin fluctuations. Conserving approximations built around this picture of the effective interaction lead to $d_{x^2-y^2}$ pairing at temperatures $T \simeq 0.02\,t$, where t is the one-electron hopping. While our Monte Carlo calculations are unable to run at these low temperatures, we can run at temperatures at which the antiferromagnetic correlations are established and the basic structure of the pairing interaction is developed. Our numerical results imply that if the doped Hubbard model goes superconducting it will have a $d_{x^2-y^2}$ gap.

At present we are completing work on the single-particle spectral weight $A(p, \omega)$ and the density of states $N(\omega)$ for $U = 4t$ and $8t$ on an 8×8 lattice. Here Monte Carlo data for $G(p, \omega_n)$ is analytically continued using a maximum entropy algorithm. We have also carried out Lanczos calculations [15] of the single-particle density of states $N(\omega)$ and the conductivity $\sigma(\omega)$ for 4×4 Hubbard clusters. While the conductivity and the resulting Drude weight appear similar to the experimental observations on the cuprates (in particular the Drude weight grows as x rather than $1 - x$), the density of states differs from photoemission data. We believe that this difference is associated with Madalung energy shifts and surface effects. However, it remains to be understood and may suggest that some essential features are missing from the Hubbard model.

We also carried out studies of 1D Hubbard rings [7] for both $U > 0$ and $U < 0$ as well as studies of the 2D negative-U Hubbard model [8,14].

B. The 3-Band Hubbard Model for CuO_2

We carried out simulations of the three-band Hubbard model of a CuO_2 sheet [1,2]. In this work we found that when the on-site Cu Coulomb interaction U exceeded the splitting Δ of the O and Cu site energies, the system exhibited a charge-transfer gap at a filling of one hole per CuO_2 unit. At this filling the antiferromagnetic correlations were dominant. As holes were added and the sheet was doped, the antiferromagnetic correlations decreased, and we found evidence for an attractive pairing interaction in both the $d_{x^2-y^2}$ and extended s channels. However, we found no evidence indicating the growth of long-range pair-field correlations at the temperatures which could be reached. We also examined the effect of a near-neighbor Cu-O Coulomb interaction V. We found that for $V < t_{\text{Cu-O}}$, there was no evidence that V induced a charge-fluctuation-mediated pairing interaction. The "fermion sign" problem prevented us from exploring larger V (*i.e.*, $V > t_{\text{Cu-O}}$). We are presently carrying out new calculations for this model in which we will study the effective particle-particle interaction. We plan to examine the $d_{x^2-y^2}$ pairing strength and its dependence on doping and the relative occupation of the Cu and O sites.

C. Other Work

We have studied the 1D Kondo lattice at half-filling and analyzed the competition between RKKY antiferromagnetic ordering and Kondo singlet formation. We find evidence for a gap and short-range spin correlations [4]. We have also studied the 1D periodic Anderson model and developed a perturbation theory which we have compared with Monte Carlo results [5]. Additionally, work was carried out on the effect of impurities on the properties of the one-dimensional Hubbard model [27].

We have completed work on an electron-phonon model, the 2D Holstein model [6]. Here we showed how the pairing correlations at first increased as the band filling approached half-filling and then suddenly decreased very near half-filling as the charge-density-wave (CDW) Peierls correlations became dominant. We found at half-filling that there was a finite temperature phase transition to a CDW-Peierls phase. We believe that this provides a description of strong-coupling superconductors which can undergo lattice distortions if pushed too far towards strong coupling.

D. Algorithms

One of our long term objectives under this grant has been to develop algorithms and calculational techniques for the study of strongly correlated electron systems. During the past three years we have developed techniques for determining within our numerical simulations whether a system is insulating, metallic or superconducting; for distinguishing between Fermi and non-Fermi liquids; for calculating effective particle-particle and particle-hole interactions; and for extracting real time information from numerical calculations of imaginary time correlations functions.

The most challenging algorithmic problem which we presently face is the "fermion sign problem." In order to perform a numerical simulation involving fermions it is necessary to first integrate or trace out the fermion degrees of freedom. This can be done if the Hamiltonian is quadratic in the fermion degrees of freedom or can be made so through the introduction of auxiliary bosonic or spin degrees of freedom through a Hubbard–Stratonovich transformation. One is then left with an integral (sum) over the Hubbard–Stratonovich or dynamical bosonic (spin) degrees of freedom. The integrand (summand) is proportional to a product of the fermion determinants for the spin up and spin down electrons. In some models a discrete symmetry forces the product of the fermion determinants and therefore the measure of the bosonic integrals (spin sums) to be positive definite. Examples include the single-band Hubbard model with a repulsive Coulomb interaction at half-filling; the single-band Hubbard model with an attractive interaction, and electron-phonon models in which the spin-up and spin-down electrons have identical couplings to the phonon field, with arbitary filling. For these models simulations can be carried out in a straight forward manner using importance sampling techniques. However, when no such symmetry exists, the product of the fermion determinants is in general not positive definite. This is the case for the single–band Hubbard model with a repulsive interaction away from half-filling, and for a number of other models of interest. It is still possible to carry out numerical simulations for such models by taking the sampling probability to be proportional to the magnitude of the fermion determinants and including the sign in the measurements. Unfortunately, the expectation value of the sign decreases exponentially with the inverse temperature, $\beta = 1/T$, so simulations of such models are restricted to relatively high temperatures. One is simply overwhelmed by statistical fluctuations at low temperatures. During the past three years we have tried a number of new approaches to the sign problem including alternative Hubbard–Stratonovich transformations, partial resummation techniques, and improved methods for extracting signals from noisy estimators. We have not yet obtained an affective algorithm for studying systems afflicted with the sign problem at low temperatures. Obtaining such an algorithm will be one of the focuses of our future work.

5. Publications

The following publications have resulted from DOE grant DE–FG03–85ER45197.

1. Antiferromagnetic, Charge-Transfer, and Pairing Correlations in the 3-Band Hubbard Model, R.T. Scalettar, D.J. Scalapino, R.L. Sugar, and S.R. White, *Phys. Rev. B* **44**, 770 (1991).
2. Quantum Monte Carlo Simulations of a CuO_2 Model, R.T. Scalettar, D.J. Scalapino, R.L. Sugar, and S.R. White, *Internat. J. Supercomp. Appl.* **5**, 36–45 (1991).
3. Results from Numerical Simulations of the 2D Hubbard Model, D.J. Scalapino, in *High Temperature Superconductivity proceedings*, K.S. Bedell, D. Coffey, D.E. Meltzer, D. Pines, and J.R. Schrieffer, eds. (Addison Wesley, 1990), 314–372.
4. One-Dimensional Symmetric Kondo Lattice: A Quantum Monte Carlo Study, R.M. Fye and D.J. Scalapino, *Phys. Rev. Lett.* **65**, 3177–3180 (1990).
5. Perturbation Theory of the Electronic Properties in Strongly Correlated Solids, M.M. Steiner, R.C. Albers, D.J. Scalapino, and L.J. Sham, *Phys. Rev. B* **43**, 1637–1650 (1991).
6. Charge-Density-Wave and Pairing Susceptibilities in a Two-Dimensional Electron-Phonon Model, R.M. Noack, D.J. Scalapino, and R.T. Scalettar, *Phys. Rev. Lett.* **66**, 778-781 (1991).
7. Drude Weight, Optical Conductivity, and Flux Properties of One-Dimensional Hubbard Rings, R.M. Fye, M.J. Martins, D.J. Scalapino, J. Wagner, and W. Hanke, *Phys. Rev. B* **44**, 6909–6915 (1991).
8. Two-Dimensional Negative-U Hubbard Model, A. Moreo and D.J. Scalapino, *Phys. Rev. Lett.* **66**, 946–948 (1991).
9. Quantum Monte Carlo Study of the One-Dimensional Symmetric Kondo Lattice, R.M. Fye and D.J. Scalapino, *Phys. Rev. B* **44**, 7486–7498 (1991).
10. Understanding High T_c, J.R. Schrieffer, *Int. J. Mod. Phys. B* **4**, 1611–1628 (1990); also in *Frontiers in Physics, Hight Technology and Mathematics*, H.A. Cerdeira and S.O. Lundquist, eds. (World Scientific, 1990), 288.
11. Approaches to Understanding High Temperature Superconductivity, J.R. Schrieffer, *Int. J. Mod. Phys. B* **5**, 1487–1494 (1991); also in *Proc. TCSUH Workshop - Physics and Mathematics of Anyons* (World Scientific, 1991), 3–10.
12. The Hubbard Model and All That, R.L. Sugar, *Nucl. Phys. B (Proc. Suppl.)* **17**, 39 (1990).
13. Binding of Holes in the Hubbard Model, E. Dagotto, A. Moreo, R.L. Sugar, and D. Toussaint, *Phys. Rev. B* **41**, 811 (1990).
14. Quasi-Particle Gap in a Two-Dimensional Kosterlitz-Thouless Superconductor, A. Moreo, D.J. Scalapino, and S.R. White, *Phys. Rev. B* **45**, 7544–7546 (1992).
15. Numerical Simulations of the Two-Dimensional Hubbard Model: Dynamic Properties, D.J. Scalapino, *Physica C* **185–189**, 104–113 (1991).
16. Superfluid Density and the Drude Weight of the Hubbard Model, D.J. Scalapino, S.R. White, and S.C. Zhang, *Phys. Rev. Lett.* **68**, 2830–2833 (1992).
17. A Generalization of Handscomb's Quantum Monte Carlo Scheme—Application to the 1D Hubbard model, A.W. Sandvik, *J. Phys. A: Math. Gen.* **25**, 3667 (1992).

18. Insulator, Metal, or Superconductor: The Criteria, D.J. Scalapino, S.R. White, and S. Zhang, *Phys. Rev. B* **47**, 7995–8007 (1993).
19. Effects of Weak Random Disorder in the 1D Hubbard Model, A.W. Sandvik and D.J. Scalapino, *Phys. Rev. B* **47**, 10090–10098 (1993).
20. Correlation Functions in Periodic Chains, A.W. Sandvik and D.J. Scalapino, *Phys. Rev. B* **47**, 12333–12336 (1993).
21. Bethe-Salpeter Eigenvalues and Amplitudes for the Half-Filled Two-Dimensional Hubbard Model, N. Bulut, D.J. Scalapino, and S.R. White, *Phys. Rev. B* **47**, 14599 (1993).

The following papers, prepared under this grant, are currently in press:

22. Does The Hubbard Model Have the Right Stuff?, D.J. Scalapino, to appear in *Proc. Int. School of Physics "Enrico Fermi,"* Varenna, 1992.
23. Quantum Monte Carlo and the Hubbard Model, D.J. Scalapino, to appear in proceedings of Summer School on Modern Perspectives in Many-Body Physics, Canberra, January 1993 (World Scientific Pub. Co.)
24. Quantum Monte Carlo Study of Spin Correlations in the One-Dimensional Hubbard Model, A.W. Sandvik, D.J. Scalapino, and C. Singh, preprint UCSBTH–93–05, to appear in *Phys. Rev. B*.
25. $d_{x^2-y^2}$ Pairing in the Cuprates?, D.J. Scalapino, to appear in the Proceedings of the Conference on Spectroscopies in Novel Superconductors, *J. Phys. Chem. Solids*.
26. The Effective Electron-Electron Interaction in the 2D Hubbard Model, N. Bulut and D.J. Scalapino, to appear in the Proceedings of the Conference on Spectroscopies in Novel Superconductors, *J. Phys. Chem. Solids*.

The following papers, prepared under this grant, have been submitted for publication:

27. Quantum Monte Carlo Study of the One-Dimensional Hubbard Model with Random Hopping, A.W. Sandvik, D.J. Scalapino, and P. Henelius, submitted to *Phys. Rev. B*.
28. The Effective Electron-Electron Interaction in the Two-Dimensional Hubbard Model, N. Bulut, D.J. Scalapino, and S.R. White, preprint UCSBTH–93–25, submitted to *Phys. Rev. Lett.*
29. Physical Pictures of the Pairing Interaction in the Hubbard Model, N. Bulut, D.J. Scalapino, and S.R. White, submitted to Proceedings of Physics and Chemistry of Molecular and Oxide Superconductors, *J. Supercond.*

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