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POWRE: Driven Nonequilibrium Systems with Quenched Disorder: A Renormalization-Group Study

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Principal Investigator: McKay, Susan R. **Award ID:** 9720482

Organization: University of Maine

POWRE: Driven Nonequilibrium Systems with Quenched Disorder: A Renormalization-Group Study

Project Participants

Senior Personnel

Name: McKay, Susan
Worked for more than 160 Hours: Yes
Contribution to Project:
Susan R. McKay has directed the research on this project, including supervising the three graduate students and one undergraduate working on the research. Her involvement has been ongoing throughout the 18-month period of the grant and the one-year extension of time. She has received 2 months summer salary support through this grant (7/98 and 6/99). Scientifically, she has contributed by providing both the general direction and many specific ideas for the project, teaching the students related concepts in statistical mechanics, working with them to interpret results, developing methods, assisting with programming, assisting students in preparing presentations, and drafting publications with students related to this work.

Post-doc

Graduate Student

Name: Georgiev, Ivan
Worked for more than 160 Hours: Yes
Contribution to Project:
Ivan is a Ph.D. candidate in the Department of Physics and Astronomy and has worked on the project as part of his Ph.D. thesis research under the direction of Professor Susan McKay. His contributions have been in the development of position-space renormalization-group approaches for nonequilibrium systems. He has applied this type of approach to an exactly solvable one-dimensional system and, because the results were very encouraging, is pursuing a two-dimensional method that is similar. He is also exploring the treatment of noise within this renormalization-group framework. He has done simulations of the model for comparison with renormalization-group results and he has continued our investigation of the effects of noise by simulations, which was begun by undergraduate Ben Dwyer. Ivan did not receive salary/stipend support from the grant, but he benefitted from the computer upgrades provided by the grant. He is currently supported by a University Graduate Research Assistantship (a maximum of one award provided each year to each department through a competition). During the course of the project he has also been supported by departmental scholarships and a teaching assistantship.
Ivan has completed all of his required courses and Ph.D. qualifying exams; his expected graduation date is May, 2002.

Name: Javeri, Vrishali
Worked for more than 160 Hours: Yes
Contribution to Project:
Vrishali is a Ph.D. candidate in the Department of Physics and Astronomy and has worked on this project as part of her dissertation research under the direction of Professor Susan McKay. She was supported by the project during the summer of 1998 and the 1998-9 academic year. She is currently supported by a teaching assistantship and she has also received departmental scholarship support while working on this project. She has worked to optimize the spatial and temporal rescaling transformations proposed for the three-state model in two dimensions. Vrishali has completed all of her required courses and Ph.D. qualifying exams; her expected graduation date is May, 2002.

Name: Seshaaiyar, Geetha
Worked for more than 160 Hours: Yes
Contribution to Project:
Geetha was a Ph.D. candidate in the Department of Physics and Astronomy doing her dissertation research under the direction of Professor Susan McKay. She did the initial simulations of the three-state model with interactions and began testing methods for accomplishing the spatial

and temporal rescaling for a renormalization-group approach to this model. Geetha left graduate school at the University of Maine in 1999 and took a position as a computer programmer in Michigan, close to where her husband was a student in medical school. She tried to continue research on the project in absentia, but was unable to make progress working in that mode.

Undergraduate Student

Name: Dwyer, Benjamin
Worked for more than 160 Hours: Yes
Contribution to Project:
Benjamin Dwyer was hired as a summer research intern to work on the project during the summer of 1998. He chose to continue this research for his senior project during 1998-1999. He was supported by this grant during July and August of 1998. Ben wrote programs to simulate the behavior of the three-state model in the presence of Gaussian noise in the electric field. He determined the effects of quenched randomness and slowly varying randomness in the electric field on the phase diagrams of the system. He presented this work at the APS Centennial Meeting (March, 1999) and he was selected to represent the Department of Physics and Astronomy at the University of Maine's Undegraduate Research Conference (May, 1999). (Each department holds a competition and the winner gives a talk as part of a college-wide conference held on campus.) His travel to the March Meeting was supported in part by an APS Travel Grant to Undergraduates.

Organizational Partners

Other Collaborators or Contacts

No formal collaborators. Professors Beate Schmittmann and Royce Zia from Virginia Tech have served as very helpful informal contacts at several points during the project.

Activities and Findings

Project Activities and Findings:
The objectives of this project are to investigate general questions related to the phase diagrams and criticality of driven nonequilibrium systems, explore the effects of quenched randomness on these phase diagrams, and develop dynamic renormalization-group methods which can be applied to these systems. The major activities that we have done to move toward accomplishing these objectives are listed below. In parentheses after each activity are the initials of students primarily involved in that portion of the research. The findings section includes more detailed descriptions of the models studied.
1. Simulations of a driven three-state model with repulsive bilinear interactions (GS).
2. Introduction of a renormalization-group approach that rescales a 3x9 block of the three-state model without interactions to a 1x3 block to probe steady-state behavior with two rescaled parameters, the electric field strength and the comparative particle-particle/particle hole exchange rate parameter, gamma (GS).
3. Increase in the parameter space by taking a matrix approach to mapping particular 1x3 blocks in the original length scale to 1x3 blocks in the rescaled system (GS, VPJ).
4. Modification of this approach to better retain correlations perpendicular to the electric field and thus attempt to match the field dependence of the phase diagram better (VPJ).
5. Exploration of alternate spatial rescaling strategies to determine which works best compared to phase diagrams obtained from simulation; this investigation is still in progress (VPJ).
6. Simulations of the driven three-state model with Gaussian random noise in the electric field (BND, GS); we are still running some simulations on large lattices to explore finite size effects (ITG).
7. Simulations of the two-dimensional driven two-state model with particles permitted to enter and exit at the boundaries (ITG).
8. Development of a renormalization-group solution for this model in one dimension for comparison with exact solution (ITG).
9. Investigation of this model with quenched randomness in one and two dimensions; this work is still in progress (ITG).
10. Exploration of approaches related to the solution in item (7) for higher dimensional systems (ITG).

Presentations related to this research:

'The Effects of Repulsive Nearest Neighbor Interactions on the Phase Diagram of the Blume-Emery-Griffiths Model with Biased Diffusion' by Geetha Seshaaiyar and Susan R. McKay; presented by SRM at the 20th IUPAP International Conference on Statistical Physics; Paris, France (July, 1998).
'The Impact of a Quenched Random Driving Field on the Three-State Lattice Gas' by Benjamin N. Dwyer, Geetha Seshaaiyar, and Susan R. McKay; presented by BND at the Centennial Meeting of the American Physical Society; Atlanta, GA (March, 1999).
[Bull. Am. Phys. Soc. 44 713 (1999)]
'The Effects of Quenched Randomness on Phase Transitions in the Driven Diffusive Three-State Lattice Gas' by Benjamin N. Dwyer and Susan R. McKay; presented by SRM at the 19th Annual International Conference on Chaos and Nonlinear Dynamics, Santa Fe NM (January, 2000).
In addition, the three graduate students involved all gave presentations at the University of Maine Graduate Research Exposition (1999, 2000 or both).
Benjamin Dwyer was selected to present his research related to this project at the University's College of Liberal Arts Undergraduate Research Conference (May, 1999).

Project Training and Development: (See PDF version submitted by PI at the end of the report)
Simulations of the driven three-state model with repulsive bilinear interactions - In this study, which was begun prior to receiving this funding and continued with support from this grant, we have investigated the effects of interactions on the phase diagrams of the driven three-state model introduced by Korniss, Schmittmann and Zia [J. Stat. Phys. 86, 721 (1997)]. We focused on this model as a prototype of an interacting driven nonequilibrium system and the simulations were done both to explore directly the effects of interactions and for comparison with future renormalization-group results for the same system. In the absence of interactions, this system exhibits a low-current phase with separate stripes of +1, -1, and empty sites perpendicular to the electric field direction. The repulsive bilinear interactions compete directly with this ordering, and we were interested in finding out how they would affect ordering in the system. The simulations show that, instead of reducing the ordered region of the phase diagram, they enhanced order at lower densities and additional striped phases occur, including stripes of checkerboard ordering (alternating +1 and -1, analogous to an antiferromagnetic phase). The competition between the segregating effects of the field and the mixing effects of the interactions led to reentrant phase diagrams as a function of electric field strength. The basic topology of the phase diagrams reported for non-interacting systems remained in the presence of the interactions, with a tricritical phase diagram at low gamma (when particle-particle exchange is relatively improbable) and all second order transitions at high gamma. Our preliminary results from these simulations were published in Phase Transformations and Systems Driven Far From Equilibrium, edited by E. Ma, P. Bellon, M. Atzmon, and R. Trivedi (Materials Research Society, Pittsburgh, PA, 1998), and the more detailed simulations done as part of this project supported these results.

Development of renormalization-group methods for driven nonequilibrium systems - We have tackled this problem using two different approaches. The first identifies dynamical parameters which can be rescaled in order to preserve a physical quantity over the changes in length scale. This approach we have tested most fully on the one-dimensional driven asymmetric chain. In the two-state version of this model, each site is either empty or occupied. If an empty site is to the right of an occupied site, the particle moves to the empty site with probability p. If the right-most site is occupied, the particle exits the chain with probability beta; if the left-most site is empty, a particle enters the chain with probability alpha. We chose this model to use for developing our methods since it can be solved exactly [Derrida and Evans in Nonequilibrium Statistical Mechanics in One Dimension ed. V. Privman, Cambridge University Press, 1997; Schutz and Domany, J. Stat. Phys 72, 277 (1993)] and possesses a non-trivial phase diagram including a multicritical point, and first and second order phase boundaries. Our renormalization-group treatment hinges upon knowledge of the current and general form of the solution in each region of the phase diagram. Mean-field theory yields the exact form of the current in this model; in cases for which an exact solution is not available, mean-field or an alternate approximate approach could be used to suggest a general form for the current. The parameters alpha and beta can be expressed in terms of one-site and two-site probability distributions. Similarly their rescaled values can be expressed in terms of these probability distributions for the spatially renormalized system. For the results included here, a length rescaling factor of three and majority rule are used to implement the transformation. The one-site and two-site probability distributions in the coarse-grained chain can be expressed in terms of three-site and six-site probability distribution functions of the original chain.

The first figure in the attached PDF file shows the known phase diagram for this system. The regions labeled AI and AII are low density and differ only in the way that the density profile approaches the boundary. Similarly, BI and BII are high density; and C indicates a high current phase. The boundary separating the A and B phases coincides with a jump in density of the system, analogous to a first order transition in an equilibrium system. The density and current are both smoothly varying across the boundaries bordering phase C. Figure 2 illustrates the trajectories resulting from our renormalization-group treatment. The method locates the multicritical point at (0.5,0.5) in exact agreement with the known solution, and the exact phase boundaries are also obtained. All of the low current regions flow to a single attractor at (0.0,0.0) and the high current phase C has its own attractor. The critical exponent nu, determined by analyzing flows in the region of the multicritical point (0.5,0.5), from our method is 2.71, compared with 2.00 from the exact solution. Figure 3 illustrates the vicinity of the multicritical point, which is unstable in all directions. Nu was calculated from the ratios of the separation of successive points in the vicinity of the multicritical point. This ratio, r, as a function of iteration, is shown in Figure 4. The lower value is characteristic of the attractor located at (2.93,2.93). We expect this attractor to move toward infinity as the length rescaling factor is increased from three. More information about this work is included in a preprint in preparation for submission to Physical Review Letters within the next month.

Our second approach, which we are applying to the two-dimensional driven three-state model, consists of mapping small units on one length scale onto corresponding units on a coarse grained system. In practice, we construct a set of larger blocks using smaller units (so far, we have used primarily triplets of sites). The dynamical rules of the system are imposed until the distribution of larger blocks reaches a steady state. Then these blocks are coarse grained, using majority rule with center site as a tie breaker in the triplet case, and a mapping is generated numerically between the evolution of triplets on the two length scales. This method involves a larger flow space (27x27 parameters for the triplet case, although many are linked by symmetries), but shows promise as being generally applicable to a variety of systems. Although the method captures a phase transition as a function of density for the three-state system, we are still working on the best way to handle the spatial rescaling and dynamics to yield the appropriate behavior as a function of field. A difficulty which we did not anticipate in doing this type of transformation for a nonequilibrium system is that the smaller blocks often do not behave in ways connected to the larger system. For example, simulations on very small lattices or on rectangular lattices of certain aspect ratios do not show the striped low current phase characteristic of larger systems for the driven three-state model.

Effects of noise on nonequilibrium phase transitions - We have begun this investigation by adding Gaussian random noise in the electric field to the driven three-state model without interactions. Figure 5 indicates a typical phase diagram for the case of quenched noise. In this case, the standard deviation in the distribution of E was 25% of its average value. This phase diagram is quantitatively indistinguishable from the no-noise case. The open circles indicate the width of the hysteresis region obtained along the first order portion of the boundary. The filled circles are points at which a second order transition occurs.

Schmittmann and Zia suggested that, for a system with regular current flow and periodic boundary conditions, particles may see the same noise over and over again and slowly varying noise might be more appropriate in a simulation to approximate the effects of noise on a larger system. To investigate this idea, we repeated the simulations with changes in the noise after every 6250 Monte Carlo steps and after every 12,500 Monte Carlo steps. Figure 6 shows that the second order phase transition is relatively insensitive to these changes in the features of the noise. Along the first order phase boundary, though, as the noise is varied more rapidly, the hysteresis loop shifts to higher mass density, as shown in Figure 7. As the noise is increased, eventually the ordered phase is destroyed. This annihilation of order occurs much earlier when gamma, which controls the rate of particle-particle exchange, is high. Figure 8 and Figure 9 both show results for substantial noise, sigma=100%. Although the transition features are still observable in the low gamma case (Figure 8), they are no longer evident when gamma is increased to 0.4 (Figure 9).

In summary, when quenched randomness is added to the electric field, the zero-noise phase diagram is robust and remains even quantitatively unchanged in the presence of substantial noise. However, slowly varying noise is more destructive to the ordering in the system, particularly when gamma is large enough to make particle-particle exchange occur frequently. The effects of slowly varying noise are evident on the first order boundaries, which are shifted toward higher density as the noise is varied more rapidly. As expected, the interfaces between neighboring stripes become rougher in the presence of noise, and more defects occur within the striped regions.

Research Training:

For Susan McKay, this grant has provided the support to begin an important new research direction. Working on this project has enabled her to learn about related work on nonequilibrium systems and to begin to contribute in this area. This project has suggested important questions that should be explored in more depth, and has also indicated promising directions for the development of improved dynamical renormalization-group approaches. The funding from this grant enabled her to attract additional well-qualified graduate students to her group and hire an undergraduate summer intern. It also enabled her to upgrade the computers that she and her students use for research. This grant and the research that it supported contributed to her promotion from associate to full professor in 1998.

This project provided Benjamin Dwyer with his first exposure to research and gave him extensive experience in computer programming and related skills. He also learned basic ideas of statistical mechanics and simulation methods and how they can be applied to study new types of model systems. In preparing talks and giving them at the APS Centennial Meeting and the University of Maine's Undergraduate Research Conference, Ben learned how to organize a presentation and explain his work to both experts and non-scientists. With both audiences, he fielded questions and showed that he understood his project well. Ben graduated from the University of Maine with a B.S. in Engineering Physics in 1999. He is planning to go to graduate school after working for a few years in his current job, a structural engineering position at a small construction firm in southern Maine.

All three of the Ph.D. students substantially improved their abilities as researchers during their involvement in this project. They have also acquired better computer skills and more familiarity with statistical mechanics and the analytical and numerical methods used to study systems with many degrees of freedom. In addition to their research activities, these three students have also taught introductory physics (and astronomy in the case of Ivan Georgiev) classes and laboratories at times during the project. Both Vrishali and Geetha were selected as trainers for new teaching assistants due to their excellent teaching skills. These students have also learned how to work as a group and help each other during their involvement with the project. They have benefitted from having students working on related aspects of the project with whom to share ideas.

Outreach Activities:

For Susan McKay:

Member of the (University of Maine's) Presidential task force on K-12 Education, working with secondary teachers and principals and other

task force members to improve science and math education in the State.
Director of the University's College of Liberal Arts and Sciences' efforts to obtain funding for Center for Excellence in Math and Science Education Research, a Center that would involve teachers in curriculum design for new teachers, research, and continuing education activities. Leader in the development of a planned MST degree (Master's in Science Teaching) at the University of Maine.
As chair of the Department of Physics and Astronomy, answers or redirects questions from the public related to physics which come into the Department office. (Since the University of Maine offers the only Ph.D. program in physics in the State, people call with questions about physics. Typically several calls per month are received.)
Gives tours and talks with prospective undergraduates about studying physics and the types of careers that physicists have (formally about four times per year; many more informal meetings).
With a Master's student (Nellie Andreeva), developed a set of videos with clips from popular movies and accompanying worksheets illustrating concepts in physics. These are available for high school teachers to borrow and are also used in our introductory courses.
Is working with departmental staff to develop a weather web site that will provide up-to-the-minute weather data from instruments located on the departmental building roof.
Departmental representative for the New England Board of Higher Education's Minority Doctoral Scholars Program; recruited one student through this program.
Obtained internal financial support and worked with departmental faculty to host an Annual Maine High School Physics Teachers Meeting each spring.
Served as a science fair judge for the University's Upward Bound Math/Science Summer Program.

For Vrishali Javeri:
Served on the (University) President's Council on Women; provided advice on improving the campus climate for women students.
Served as a presenter in the Expanding Your Horizons Program, which introduces middle school girls to scientific research and career opportunities.
Served as a physics liason for the Summer Upward Bound program at the University of Maine.

For Geetha Seshaaiyar:
Served as a presenter in the Expanding Your Horizons Program, which introduces middle school girls to scientific research and career opportunities.

For Ivan Georgiev:
Has taught in the general education astronomy labs and worked with interested non-science majors at the teaching observatory on campus.

Journal Publications

Ivan T. Georgiev and Susan R. McKay, "A Position-Space Renormalization-Group Approach for Driven Diffusive Systems Applied to the One-Dimensional Driven Asymmetric Chain", *Physical Review Letters*, p. , vol. , ().) To be submitted, October 2000

Books or Other One-time Publications

Web/Internet Sites

URL(s):

Description:

Other Specific Products

Contributions

Contributions within Discipline:
The findings from this research have contributed to the understanding of nonequilibrium phase transitions in three important ways. First, this study has probed the effects of interactions on driven diffusive systems. Since interactions of some type are generally present in real systems, the findings from our work that interactions can enhance ordering and create new types of ordered phases are significant. Somewhat surprising

was the increase in the striped phase region when interactions were added that competed with the ordering field. Secondly, we have shown how ideas from equilibrium position-space renormalization group can be applied to determine steady-state behavior, criticality and phase diagrams for driven diffusive systems. The one-dimensional approximate renormalization-group solution that we have developed, based upon a spatial rescaling factor of three and temporal rescaling at each length scale until a steady state occurs, shows excellent agreement with the known solution for the model studied. This approach looks very promising and we are in the process of applying it to the same system with noise and trying to generalize it to two-dimensional systems. Thirdly, our investigations of noise in driven diffusive systems indicate that the ordering previously reported is robust in the presence of quenched randomness in the electric field. Slowly varying noise has some effect on the first order transitions, but did not impact the second order transitions until the amplitude of the noise was large enough to destroy the transition entirely. Thus, this work contributes to knowledge of ordering and criticality in specific nonequilibrium models and introduces a new general approach for studying these systems.

Contributions to Other Disciplines:

The development of new methods to determine the properties of nonequilibrium model systems is important for disciplines other than physics. Nonequilibrium systems are ubiquitous in biology, chemistry, materials science and engineering. Driven diffusive models such as those studied in this project can show dramatic differences in their transport properties in their distinct phases. Materials with such phase diagrams could have important applications, just as the transitions in ferrofluid thin films have been used as magnetic-field-driven switches. Thus, a basic understanding of transitions in these model systems will lead to better models for a variety of systems in other disciplines, such as membrane transport and traffic flow. Findings related to the behavior of these systems when quenched randomness is present are also important for other disciplines. Such research indicates when noise, often resulting from impurities, must be controlled or when it can be used to enhance desirable properties.

Contributions to Human Resource Development:

This project has provided opportunities for three Ph.D. students (two women) and one undergraduate to participate in research. The funding for this research (through the POWRE program) helped support the research career of Dr. Susan McKay who, during the course of the award, was promoted from associate to full professor and was selected as department chair. In her position as department chair, she has actively recruited students from underrepresented groups and worked hard to create a departmental climate that will aid retention of women and minorities in the Department's undergraduate and graduate programs. The group of graduate students and Professor McKay have participated in significant outreach activities, listed above, which impact pre-college teachers, young people, and non-science majors.

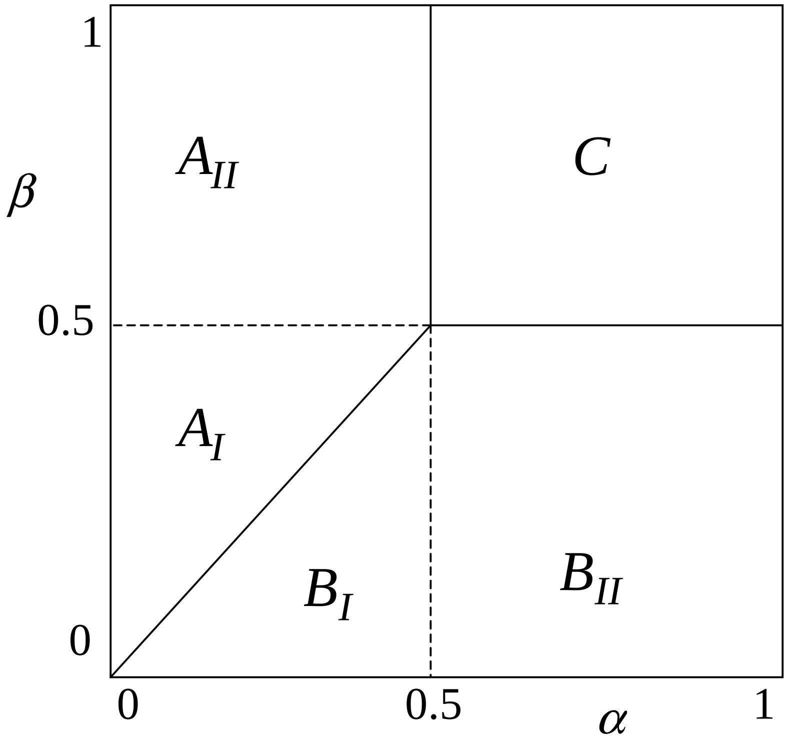
Contributions to Science and Technology Infrastructure:

None not already discussed above.

Beyond Science and Engineering:

Categories for which nothing is reported:

Organizational Partners
Any Book
Any Product
Contributions: Beyond Science or Engineering



1
A_{II}
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β
0.5
A_I
B_I
B_{II}
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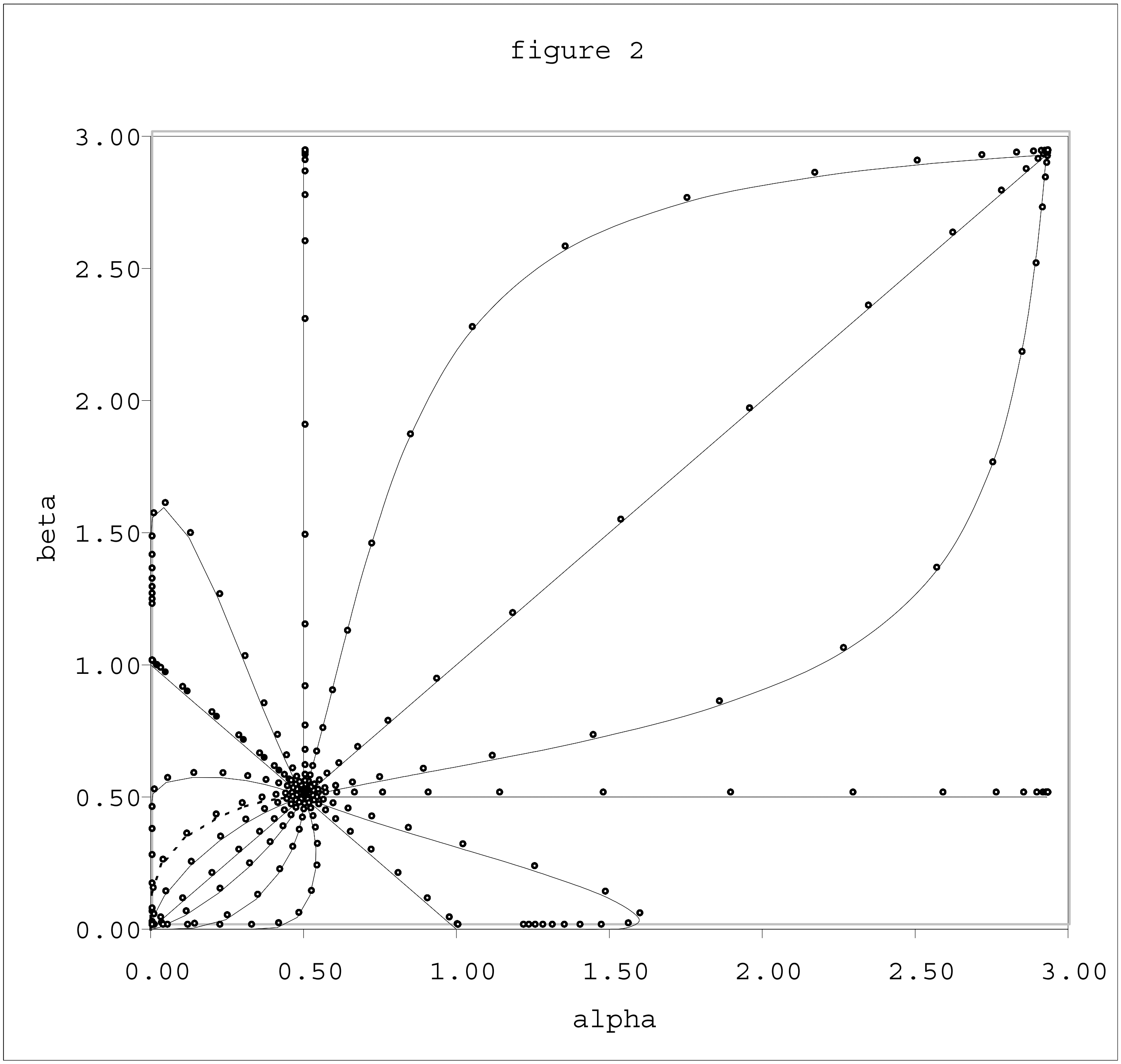
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beta
alpha
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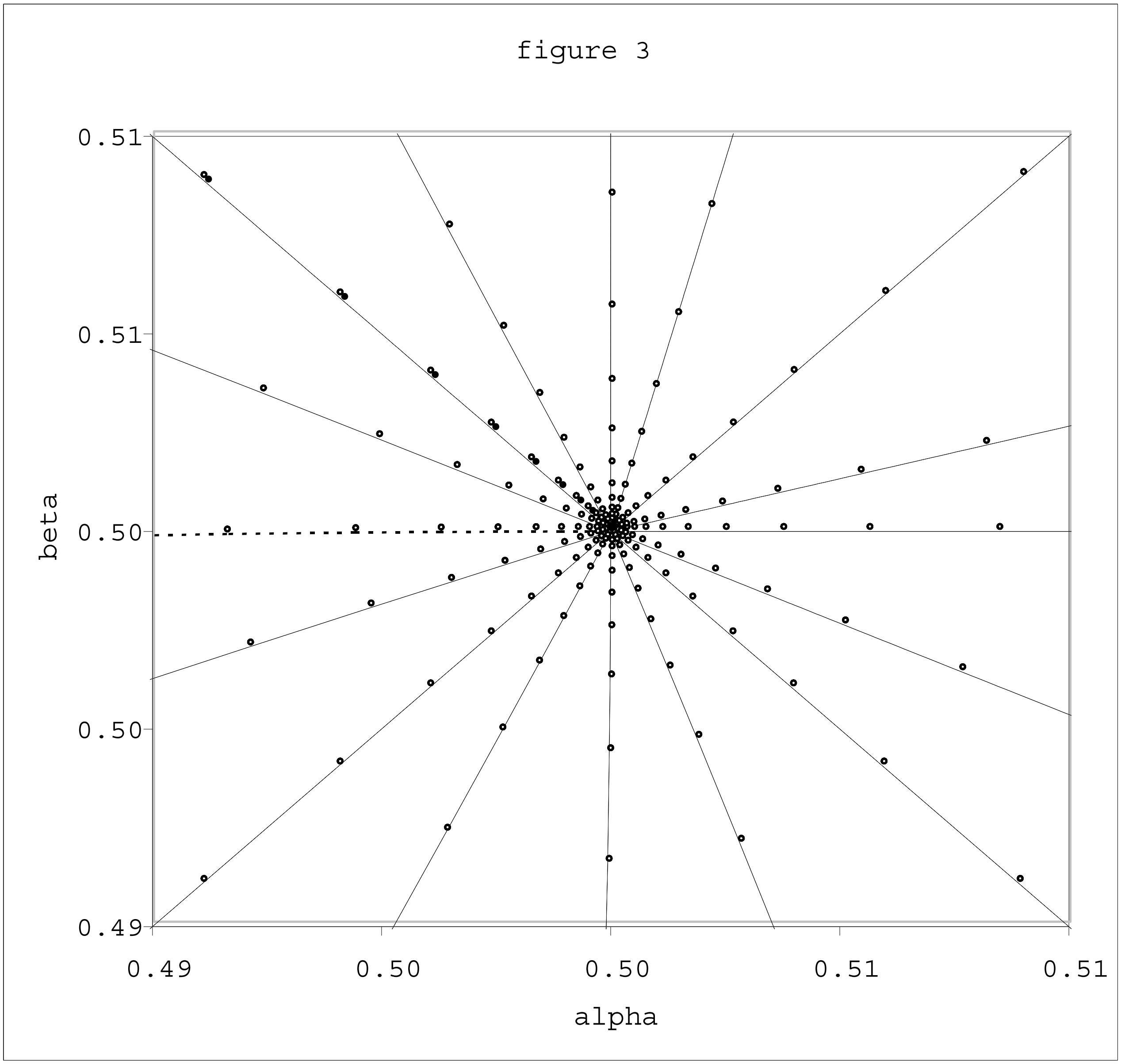
0.50
1.00
1.50
2.00
2.50
3.00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0.49
beta
0.49
0.50
0.50
0.51
0.51
alpha

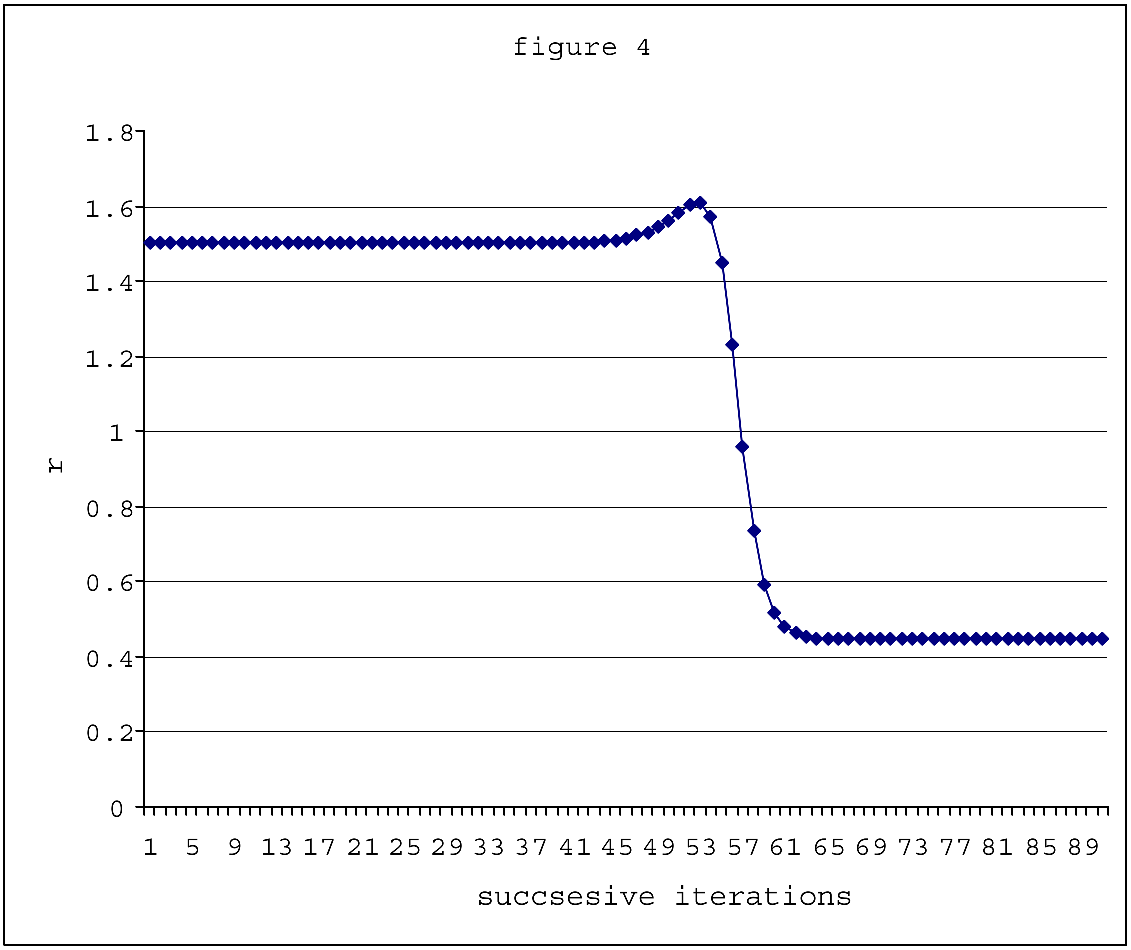
figure 4
1.8
1.6
1.4
1.2
1
0.8
0.6
0.4
0.2
0
r
1 5 9 13 17 21 25 29 33 37 41 45 49 53 57 61 65 69 73 77 81 85 89
succsesive iterations

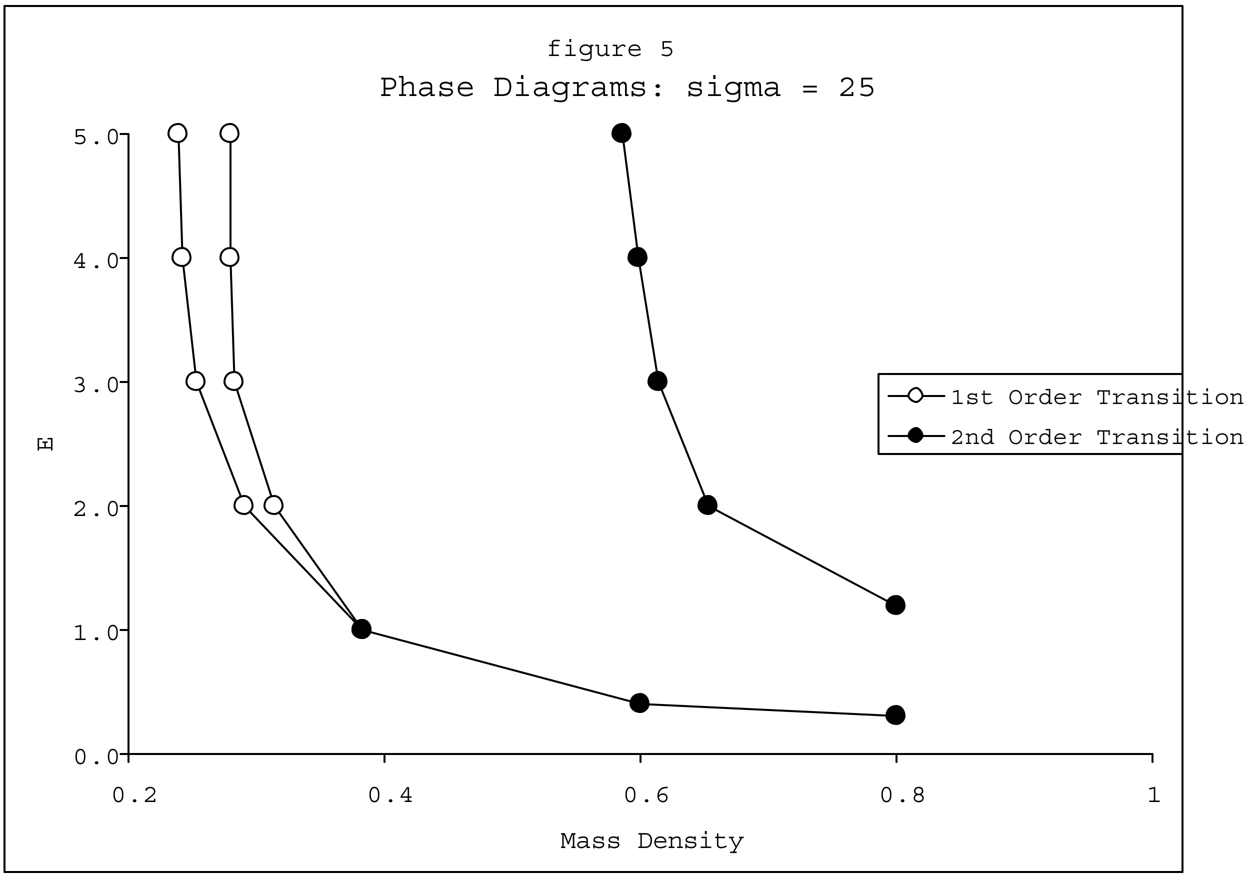
figure 5
Phase Diagrams: sigma = 25
5.0
4.0
3.0
2.0
1.0
0.0
E
0.2
0.4
0.6
0.8
1
Mass Density
1st Order Transition
2nd Order Transition

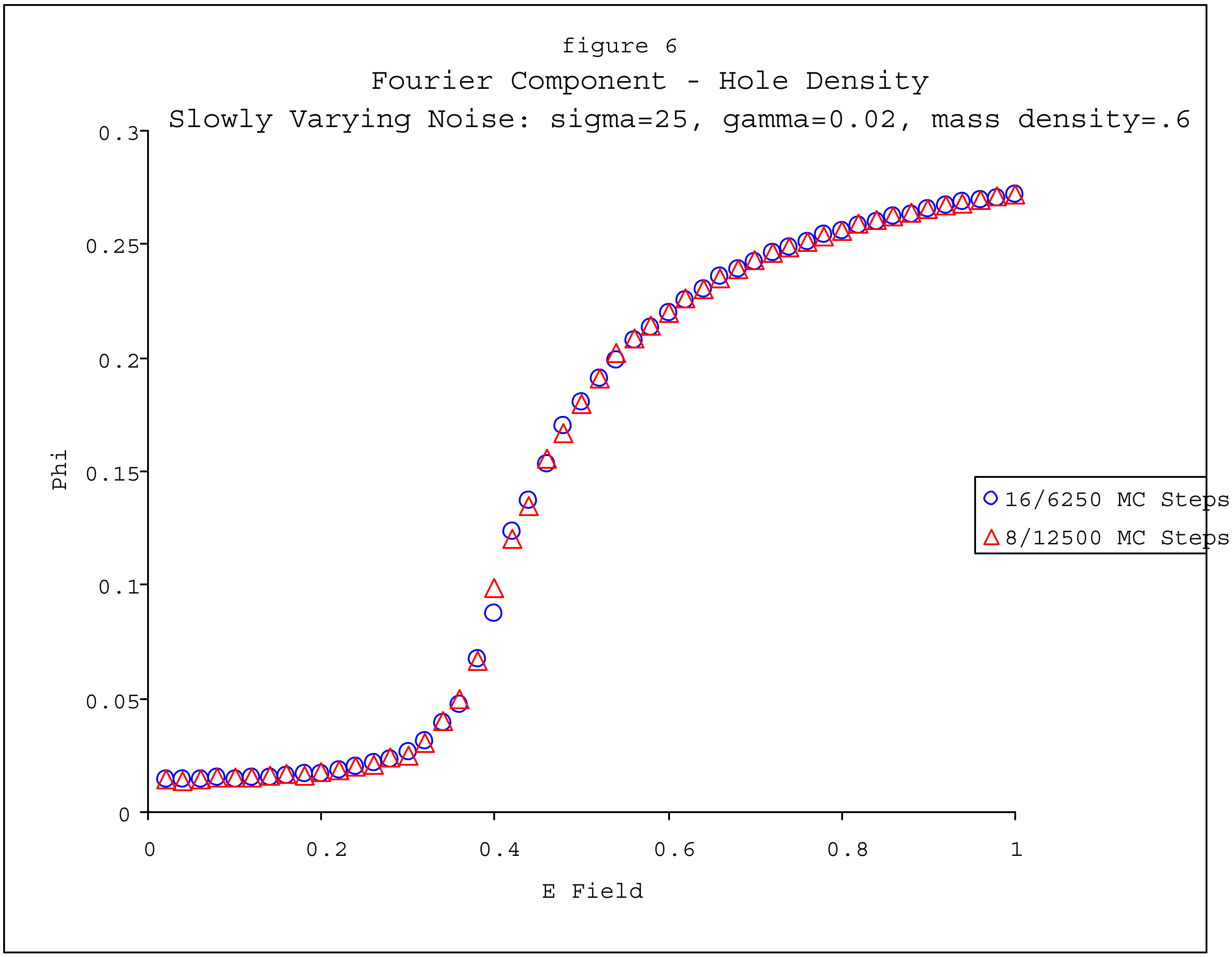
figure 6
Fourier Component - Hole Density
Slowly Varying Noise: sigma=25, gamma=0.02, mass density=.6
Phi
0
0.05
0.1
0.15
0.2
0.25
0.3
0
0.2
0.4
0.6
0.8
1
E Field
16/6250 MC Steps
8/12500 MC Steps

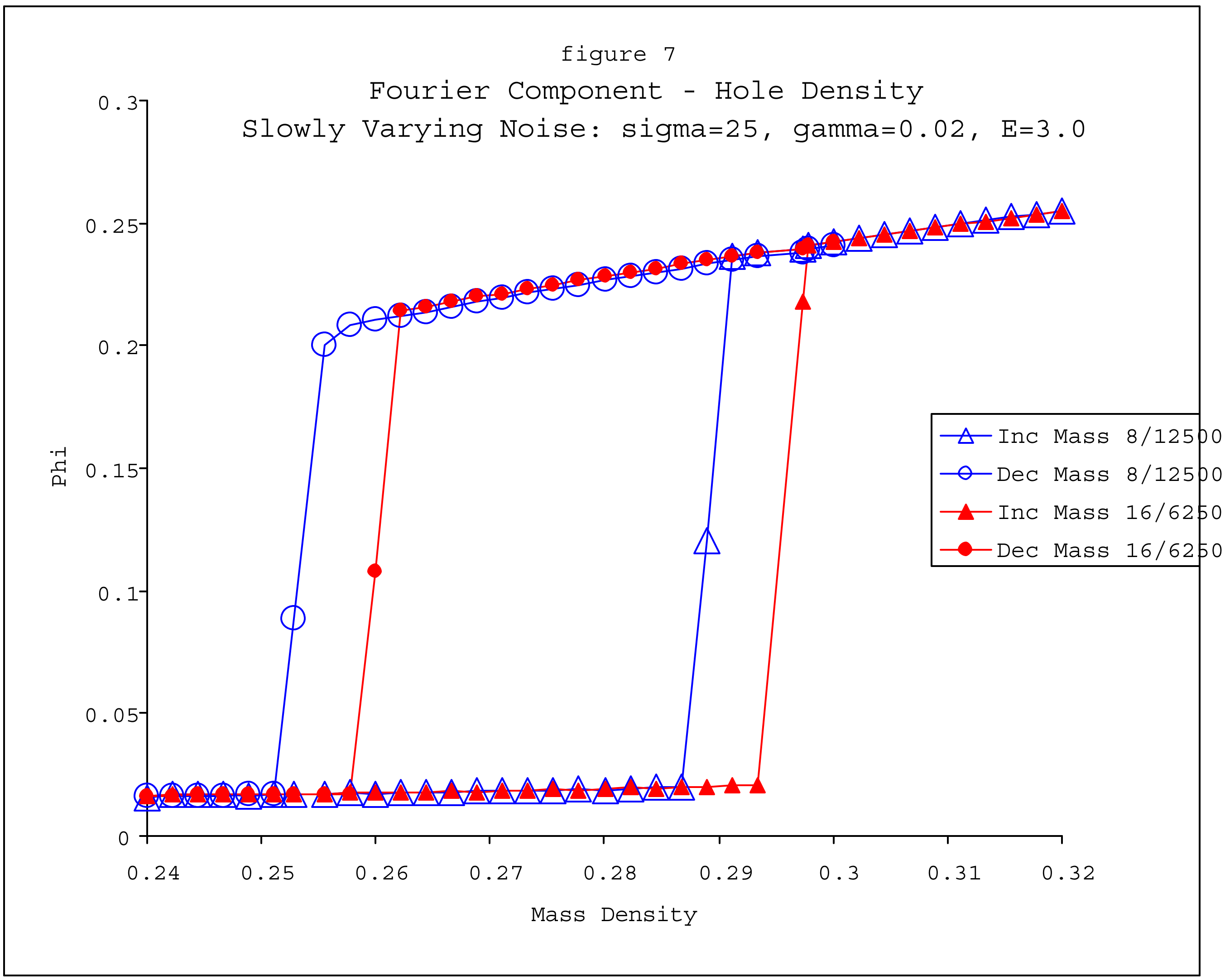
figure 7
Fourier Component - Hole Density
Slowly Varying Noise: sigma=25, gamma=0.02, E=3.0
Phi
Mass Density
0
0.05
0.1
0.15
0.2
0.25
0.3
0.24
0.25
0.26
0.27
0.28
0.29
0.3
0.31
0.32
Inc Mass 8/12500
Dec Mass 8/12500
Inc Mass 16/6250
Dec Mass 16/6250

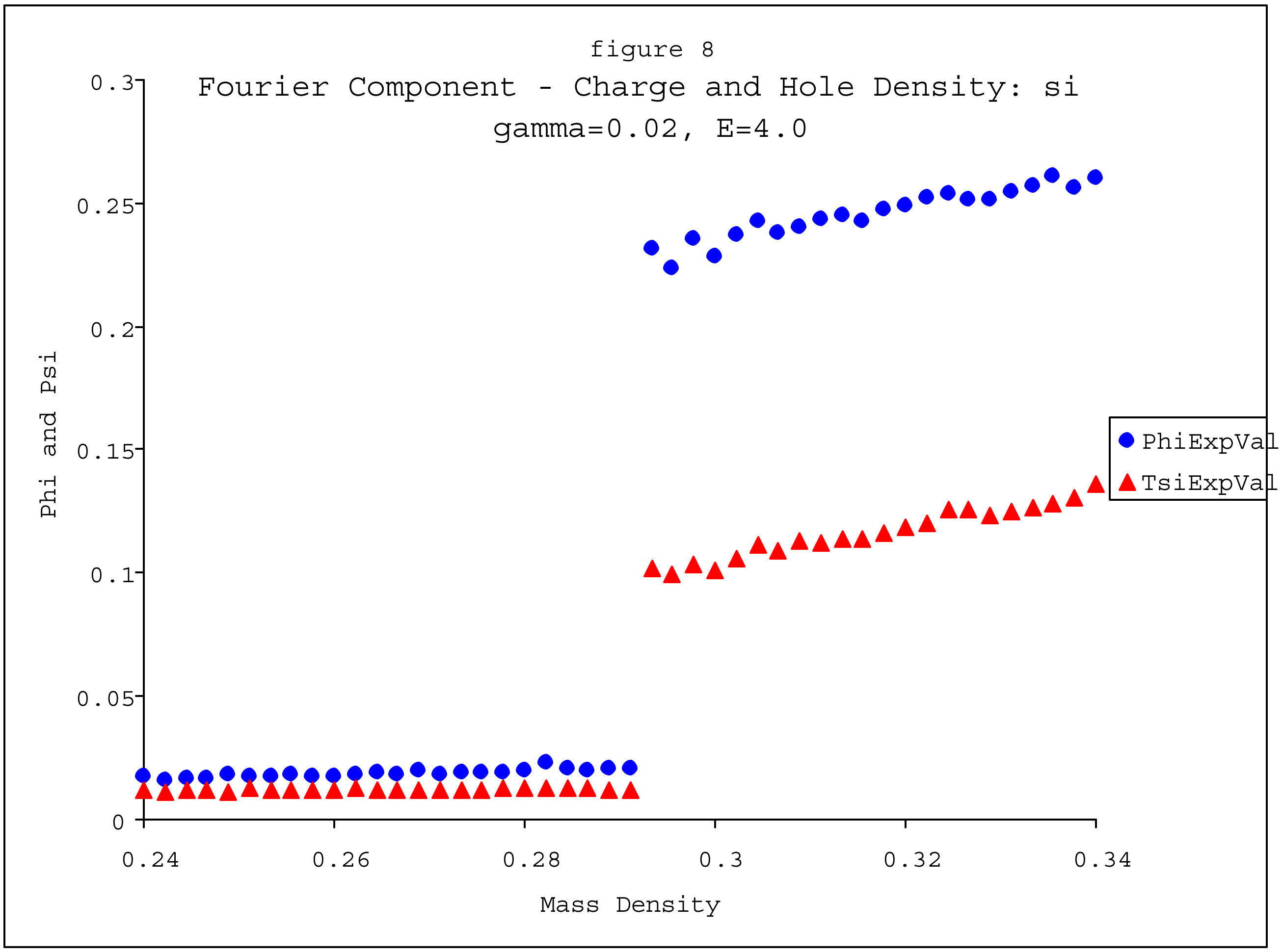
figure 8
Fourier Component - Charge and Hole Density: si
gamma=0.02, E=4.0
0.3
0.25
0.2
0.15
0.1
0.05
0
Phi and Psi
0.24
0.26
0.28
0.3
0.32
0.34
Mass Density
PhiExpVal
TsiExpVal

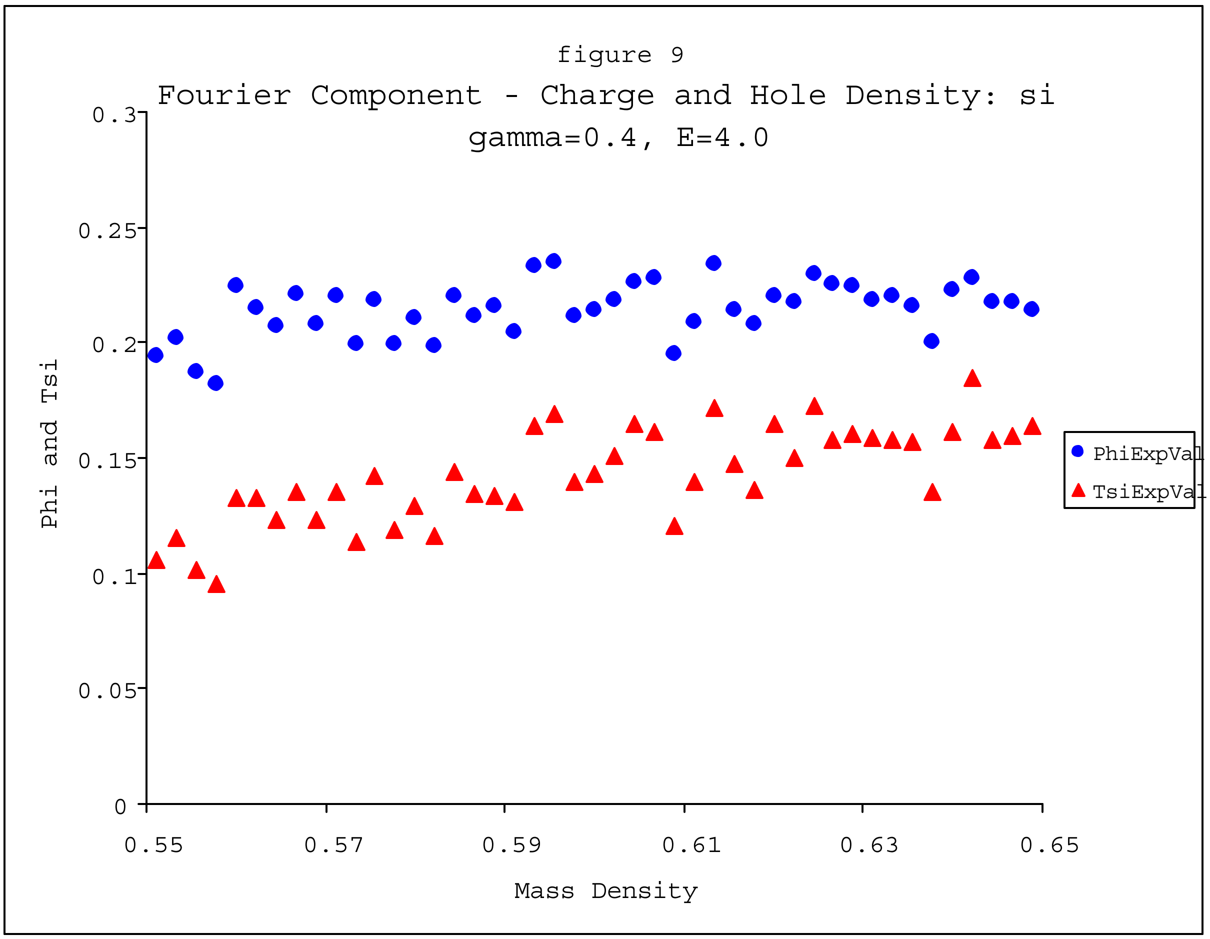
figure 9
Fourier Component - Charge and Hole Density: si
gamma=0.4, E=4.0
Phi and Tsi
Mass Density
0
0.05
0.1
0.15
0.2
0.25
0.3
0.55
0.57
0.59
0.61
0.63
0.65
PhiExpVal
TsiExpVal