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FOURTH UNIVERSITY OF CALIFORNIA CONFERENCE ON STATISTICAL MECHANICS

March 26-28, 1990

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REPORT

As was agreed with the funding agencies beforehand, no formal proceedings of this conference were produced. Included in this Report are the following items:

1) List of members of Organizing Committee.
2) List of invited speakers.
3) List of registered participants.
4) Conference schedule.
5) Schedule of poster sessions.
6) Abstracts of posters presented.

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Organizing Committee
UCSM90

Prof. K. Dawson, Department of Chemistry, UC Berkeley

Prof. C. Garrod, Department of Physics, UC Davis

Prof. R. Wallis, Department of Physics, UC Irvine

Prof. J. Rudnick, Department of Physics, UCLA

Prof. F. Cummings, Department of Physics, UC Riverside

Prof. K. Lindenberg, Department of Chemistry, UC San Diego

Prof. J. Cardy, Department of Physics, UC Santa Barbara

Prof. M. Nauenberg, Department of Physics, UC Santa Cruz

Prof. D. Campbell, Center for Nonlinear Science, Los Alamos National Laboratory

Prof. B. Alder, Lawrence Livermore National Laboratory,

By per call

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Shlesinger. Office of Naval Research/
code 1112.
VHG 11/02/90

Invited Speakers
UCSM90

Prof. J. Chayes, Department of Physics, UCLA
Prof. T. Spencer, Institute for Advanced Studies, Princeton
Prof. M. Aizenman, Courant Institute of Mathematics, New York University
Prof. D. Cannell, Department of Physics, UC Santa Barbara
Prof. J. Deutsch. Department of Physics, UC Santa Cruz
Prof. W. Gelbart, Department of Chemistry, UCLA
Prof. D. Hone, Physics Department. UC Santa Barbara
Prof. J. Wheeler, Department of Chemistry, UC San Diego
Prof. S. Chakravarty, Department of Physics, UCLA
Prof. D. Haldane, Department of Physics, UC San Diego
Prof. A. P. Young, Department of Physics, UC Santa Cruz
Prof. R. Bruinsma, Department of Physics, UCLA
Prof. C. Knobler, Department of Chemistry, UCLA
Prof. M. Gharib, AMES, UC San Diego
Prof. J. Langer, Institute for Theoretical Physics UC Santa Barbara
Prof. H. Levine, Department of Physics, UC San Diego
Prof. D. Chandler, Dept. of Chemistry, UC Berkeley
Prof. J. Simon, Department of Chemistry, UC San Diego
Prof. K. Wilson, Department of Chemistry, UC San Diego
Prof. G. Shaw, Department of Physics, UC Irvine

Participants
UCSM90

Ken Babcock, Physics Department, UC Santa Barbara

Joel Bader, Department of Chemistry, UC Berkeley

Carey Bagdassarian, Department of Chemistry, UCLA

Angelo Barbieri, Department of Physics, UC Santa Cruz

Robert Barnett, Department of Chemistry, UC Berkeley

Arezki Beldjenna, Department of Physics, UCLA

Arjun Berera, Department of Physics, UC Berkeley

Guillermo Castilla, Department of Physics, UCLA

Ariel Chialvo, Department of Chemical Engineering, Princeton

Pedro Colmenares, Institute of Theoretical Dynamics UC Davis

Dr. L. Rene Corrales, Department of Chemistry, University of Texas, Austin

Dr. M. E. Costas-Basin, Department of Chemistry & Biochemistry, UCLA

Mark Cowan, Physics Department, UCLA

Roger Drake, Physics Department, UC Santa Barbara

Keivan Esfarjani, Physics Department, University of Delaware

Sakkar Eva, Physics Department, UCLA

Fabio Ferri, Physics Department, UC Santa Barbara

Michael Flatté, Physics Department, UC Santa Barbara

José A. Fornés, Department of Physiology & Biophysics, California College of Medicine, UC Irvine

Dr. Barry Frank, Physics Department, Concordia University, Montreal

Barbara Friskin, Physics Department, UC Santa Barbara

Alejandro Garcia, Physics Department, San Jose State

Jaime Garcia, Department of Chemistry, UCLA

Claude Garrod, Department of Physics, UC Davis

Prof. John Gehlen, Department of Chemistry, UC Berkeley

Martin Gelfand, Physics Department, UCLA

Michael Geller, Physics Department, UC Santa Barbara

Brad Gertner, Department of Chemistry UC La Jolla

Leonardo Golubović Physics Department, UC

Kenneth Hui, Department of Chemistry, UC Berkeley

Byungnam Kahng, Department of Chemistry, UC Berkeley

Upali Karunasiri, Department of Physics, UCLA

Peter Kopietz, Department of Physics, UCLA
Flora Koukiou, Dept of Physics, Harvard
Xiaodan Leng, Department of Physics, UC Irvine
Shoudan Liang, Department of Physics, University of Illinois, Urbana
Thomas Madden, Department of Physics, UC Santa Cruz
Domingos H. Marchetti, Department of Mathematics, Rutgers
Hernan Martinez, Department of Physics, UC San Diego
John McGrann, Department of Physics, UC Irvine
David Mitchell, Joseph Henry Laboratory, Department of Physics, Princeton
Jacob Morris, Department of Physics, UCLA
Rajamani S Narayanan, Department of Physics, UC Davis
Eric Nylund, Department of Chemistry, UC San Diego
Peter D. Olmsted, Department of Physics, University of Illinois, Looomis Lab, Urbana
Raj Pathria, Department of Physics, University of Waterloo, Ontario
Enrique Peacock-Lopez, Department of Chemistry, Williams College
Zhang Qing, Department of Chemistry, UC Berkeley
Wouter-Jan Rappel, INLS UC San Diego
Bill Reynolds, INLS, UC San Diego
Prof. Juan Carlos Reina, Department of Physics, Texas A & M University
Joseph Rudnick, Department of Physics, UCLA
George Ruppeiner, Division of Natural Sciences New College, Sarasota
Jonathan Selinger, Department of Physics, UCLA
Robin Selinger, Department of Chemistry, UCLA
Wen-Shyan Sheu, Department of Chemistry, UC San Diego
Kurt Shuler, Department of Chemistry, UC San Diego
Dr. E. Siegel, SPD, San Francisco
Duane Siemens, Physics Department, UC Davis
Ralph A. Smith, Physics Department, U C San Diego
Erik Sorensenm, Physics Department, UC Santa Cruz
Keith Stine, Department of Chemistry, UC
Li-piin Sung, Department of Physics, UC Santa Barbara
Shubha Tewari, Physics Department, UCLA
Craig A. Tracy, Department of Mathematics, UC Davis
Yuhai Tu, Department of Physics, UC San Diego
Ramin Vakilian, Institute of Theoretical Dynamics, UC Davis
Christian van den Broeck, Department of Chemistry, UC San Diego

Zhen-Gang Wang, Department of Chemistry, UC San Diego
Matthias Wollensak, Department of Physics, UCLA
David Tai-Wei Wu, Department of Chemistry, UC Berkeley
Ten-Ming Wu, Department of Physics, UC San Diego
Yumin Yang, INLS, UC San Diego
Dr. Zhenyu Zhang, Department of Chemistry, UC Santa Barbara

FOURTH UNIVERSITY OF CALIFORNIA CONFERENCE ON STATISTICAL MECHANICS

SCHEDULE

All talks will be held in Broida Hall 1610. The poster sessions will be in the Engineering II Conference Room.

MONDAY, MARCH 26

8:30–9:00	Registration

Morning Session: *Quantum Spins*

9:00–9:45	A. P. Young (UCSC) *Simulations of Quantum Antiferromagnets*
9:45–10:30	D. Haldane (UCSD) *One-dimensional Quantum Spin Chains*
10:30–11:00	Break - Refreshments served
11:00–11:45	S. Chakravarty (UCLA) *Nonlinear σ-models for quantum spins*
11:45–1:30	**Poster Session I**, Engineering II Conference Room. **Boxed lunch will be served to all** *registered* **participants.**

Afternoon Session: *Molecularly Complex Systems*

1.30–2:15	J. Deutsch (UCSC) *The Physics of Electrophoresis*
2:15–3:00	D. Hone (UCSB) *Conjugated Polymers in Solution: Conduction and Contortion*
3:00–3:45	W. Gelbart (UCLA) *Effects of Flow on Micellar Self-Assembly*
3:45–4:15	Break - Refreshments served
4:15–5:00	J. Wheeler (UCSD) *Phase Transitions and Critical Phenomena in Molecularly Complex Liquids*
5:00–5:45	D. Cannell (UCSB) *Tricritical Phenomena in Water-Alcohol-Oil Mixtures* (with R. Drake)

TUESDAY, MARCH 27

Morning Session: *Rigorous Results*

9:00–9:45	T. Spencer (Institute for Advanced Studies) *Localization and Dynamical Systems*
9:45–10:30	J. Chayes (UCLA) *The Wulff Construction and Two-Dimensional Percolation*
10:30–11:00	Break - Refreshments served
11:00–11:45	M. Aizenman (NYU) *Equilibrium Effects of Static Disorder*
11:45–1:30	**Poster Session II**, Engineering II Conference Room. **Boxed lunch will be served to all** *registered* **participants.**

OVER

Afternoon Session: *Pattern Formation*

1:30–2:15	H. Levine (UCSD) *Pattern Selection in Chemically Reactive Systems*
2:15–3:00	M. Gharib (UCSD) *Pattern Formation in Laminar and Turbulent Flows*
3:00–3:45	C. Knobler (UCLA) *Phase Transitions and Pattern Formation in Langmuir Monola*
3:45–4:15	Break - Refreshments served
4:15–5:00	R. Bruinsma (UCLA) *Thin-Film Growth and the Shadow Model*
5:00–5:45	J. Langer (UCSB) *A Mechanical Model of an Earthquake Fault* (with J. Carlson)

Evening

6:00–8:00	**Reception at the Faculty Club.**

WEDNESDAY MARCH 28

Morning Session: *Dynamical Processes in Fluids*

9.00–9:45	K. Wilson (UCSD) *Fluctuations and Chemical Reaction Dynamics*
9:45–10:30	D. Chandler (UCB) *The Sign Problem and Barrier Crossing in a Quantum Fluid (Water?)*
10:30–11:00	Break - Refreshments served
11:00–11:45	J. Simon (UCSD) *Solvent Dynamics and Electron Transfer Reactions*

Final Session

11:45–12:30	G. Shaw (UCI) *Models of Higher Brain Function*
12:30	**Conference ends.**

FOURTH UNIVERSITY OF CALIFORNIA
CONFERENCE ON STATISTICAL MECHANICS

POSTER SESSIONS

Engineering II Conference Room

Poster Session I, Monday March 26, 11:45–1:30

Babcock K* & Westervelt R M, *Avalanche Dynamics and Self-Organization in a Magnetic Froth*

Bader J, *Nuclear Tunneling in Electron Transfer*

Beldjenna A*, Rudnick J & Gaspari G, *The Shapes of Random Walks with Fixed End-to-End Distance*

Chialvo* A A & Debenedetti P G, *Determination of Excess Properties and Infinite Dilution Quantities from Computer Simulation via Single Charging-Integral Approach*

Costas M E*, Varea C & Robledo, *Mean Field Properties of Fluids, Nematic Liquids and Microemulsions*

Fornés J* & Procopio J, *Local Transient Fluctuational Density as Producing Ionic Flow Through Cell Membranes*

Frisken B J*, Ferri F* & Cannell D, *Binary Mixtures in Silica Gels*

Garcia A* & Penland C, *Fluctuating Hydrodynamics and the Principal Oscillation Pattern Analysis*

Garcia J M* & Greer S, *Equilibrium Polymerization at a Phase Transition*

Gelfand M, *Series Investigations of Frustrated Square-Lattice Antiferromagnets*

Golubovic L* & Bruinsma R, *Surface Diffusion and Fluctations of Growing Interfaces*

Kahng B* & Dawson K A, *Roughening Transition of the Isotropic Frustrated Ising Model*

Koukiou F, *Random Interactions and Phase Transitions*

Leng X* & Shaw G L, *Music Composition and Models of the Cortex Using Physical System Analogies*

Liang S, *Monte Carlo Simulations of the Correlation Functions for Heisenberg Spin Chains* at $T = 0$

* indicates person presenting poster

over

Poster Session II, Tuesday March 27, 11:45–1:30

Deutsch J M & Madden T L*, *The Diffusion Coefficient of a Reptating Polymer*

Marchetti D *Rigorous Proof of Power-Law Behavior in Kosterlitz-Thouless Phase*

McGrann J*, Shaw G L, Silverman D J & Pearson J C, *Phase Transitions in the Trion Model of Cortical Organization*

Peacock-Lopez E* & Swartz M, *Two-dimensional Reactive Systems: Rapid Bimolecular Processes on Spherical Surfaces*

Quing Zhang* & Silbey R J, *Symmetry Breaking in a Simple Electron-Phonon Model with Electron Correlations*

Selinger J V* & Bruinsma R J, *Hexagonal and Disordered Phases of Semiflexible Chains*

Selinger R L B, *To be announced*

Sheu W-S*, Lindenberg K & Kopelman R, *Scaling Properties of Diffusion Limited Reaction*

Siemens D, *Thermodynamic Equations of State for the Kinetic and Potential Energies of a System of Charged Particles*

Smith R, *Phase Transition Behavior in a Negative Temperature Guiding Center Plasma or Vortex Gas*

Stephenson J, *Asymptotic Formulae for Cycles in the Logistic Map*

Sung L* & Cannell D, *Universality in Solutions of Linear Polymers*

Tewari S* & Chakravarty S, *Crossover from Heisenberg to Ising Critical Behavior in* K_2NiF_4

van den Broeck C, *To be announced*

Wang Z G, *Curvature Elasticity of Diblock Polymer Monolayers and Bilayers*

Hui K, Wu D* & Chandler D, *Renormalized Step Length of Polymers with Self-Interactions*

Wu T-M*, Brown D & Lindenberg K, *An Exactly Solvable Model of Dissipative Quantum Tunneling*

Levine H & Yang Y*, *A Rising Bubble in a Tube*

Abstract for Poster
for the 4th Annual University of California
Conference on Statistical Mechanics
26-28 March 1990

Avalanche Dynamics and Self-Organization in a Magnetic Froth

K.L. BABCOCK* and R.M. WESTERVELT, *Harvard University.*

Uniaxial magnetic garnet films support an experimentally accessible system of two-dimensional domain patterns that evolve in response to external magnetic fields. This poster will describe observations of the coarsening of disordered cellular domain patterns in an increasing bias field.[1] The patterns coarsen via the shrinking and elimination of cells with fewer than six sides, a process topologically similar to that observed in soap froths and the annealing of polycrystalline materials. Novel to the domain patterns are structures containing trapped magnetic bubbles which act as stable five-fold vertices. These "bubble traps" resist elimination, and so provide a barrier to the coarsening that allows the patterns to settle into stationary, metastable states. Bias increments destabilize these states, leading to avalanche-like reorganizations in which cells are destroyed by a domino effect. The avalanche dynamics are self-organizing: for significant ranges of bias field and cell density, the stationary patterns are barely stable with respect to small bias increments. The avalanche sizes and lifetimes span more than two decades and have distributions that are best described as power laws over a limited range. These features suggest that this is an experimental manifestation of self-organized criticality.[2] The self-organizing dynamics also lead to scaling in the structure of the patterns: the fraction of cells that are bubble traps remains nearly constant over a two-decade drop in cell density.[3]

* Currently at the University of California at Santa Barbara, Dept. of Physics.

[1] K.L. Babcock and R.M. Westervelt, Phys. Rev. A **40**, 2022 (1989).

[2] P. Bak, C. Tang, and K. Wiesenfeld, Phys. Rev. Lett. **59**, 381 (1987).

[3] K.L. Babcock and R.M. Westervelt, Phys. Rev. A **41**, Feb. 15 (1990).

THE SHAPES OF RANDOM WALKS WITH FIXED END-TO-END DISTANCE

Arezki Beldjenna and Joseph Rudnick

Department of Physics
University of California at Los Angeles
Los Angeles, CA 90024

and

George Gaspari

Department of Physics
University of California at Santa Cruz
Santa Cruz, CA 95064

ABSTRACT

Anisotropies of random walks embedded in d spatial dimensions and with fixed end-to-end distance are discussed. As a representation of polymers, these walks correspond to long chain molecules whose heads and tails are fixed in space. An exact analytical expression for the asphericity, valid in an arbitrary spatial dimensionality, is presented. We also present expressions for the average principal radii of gyration to first order in $1/d$. The results reveal two regimes that depend on the fixed length. They recover the results for both unrestricted open and closed random walks.

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Determination of Excess Properties and Infinite Dilution Quantities fron Computer Simulation via Single Charging-Integral Approach

by

Ariel A. Chialvo and Pablo G. Debenedetti
Department of Chemical Engineering
Princeton University
Princeton, NJ 08544-5263

Rigorous statistical mechanical expressions are derived to evaluate activity coefficients, partial molar volumes and partial molar enthalpies at infinite dilution via NPT molecular-based computer simulation. These equations are based on the recently proposed single charging-integral method for the determination of excess properties in multicomponent model systems [1].

The distinguishing feature of the new method, in contrast to conventional ones, is that there is no need for simulations at infinite dilution or for unreliable extrapolation in order to obtain infinite dilution quantities.

Since the single charging-integral method is based on the coupling parameter concept, the approach avoids all of the problems commonly associated with particle insertion methods.

Simulation results for infinite dilution activity coefficients, Henry constants and pure component fugacities of a binary Lennard-Jones mixture are presented and compared with theoretical results from two perturbation schemes [2,3]

[1] Chialvo, A.A., **J. Chem. Phys.**, In press (1990)

[2] Shukla, K.P., **Molec. Phys.**, 62, 1143 (1987)

[3] Fischer, J. and S. Lago, **Chem. Phys.**, 78, 5750 (1983)

Shear Viscosity Calculation via Equilibrium Molecular Dynamics: Einstenian vs. Green-Kubo Formalism

by

Ariel A. Chialvo and Pablo G. Debenedetti
Department of Chemical Engineering
Princeton University
Princeton, NJ 08544-5263

Twenty years after the first report on shear viscosity calculation via Molecular Dynamics [1], there is still controversy over the proper evaluation of this property [2]. An intriguing fact is that despite the numerical advantages of the Einstenian-like (i.e., squared displacement) formalism, most (if not all) work has been done through the application of the Green-Kubo approach. Although the theoretical equivalence between both formalisms was demonstrated by Helfand [3], their relative numerical and computational merits are quite different. Furthemore, the mean squared displacement expression can be written in two theoretically equivalent but numerically very different forms: one given by Helfand [3], and a much less frequently used form given by McQuarrie [4].

In this work, we compare the numerical and computational implications (accuracy, memory requirement, sample size and cutoff-dependence) of the two Einstenian-like equations and of different expressions based on the Green-Kubo formalism. In contrast to Hoheisel and Vogelsang's conclusions [2], we find that the Einstenian formalism gives excellent results and is less computationally demanding than its Green-Kubo counterpart. In addition, we find that the expression given by McQuarrie [4] is numerically more convenient than Helfand's expression [3], since it requires a smaller number of "experiments" (uncorrelated time origins). All of our conclusions are validated by extensive comparisons with literature values for shear viscosity of Lennard-Jones systems.

[1] Alder, B.J. D.M. Gass, and T.E. Wainwright, **J. Chem. Phys.**, 53, 3813 (1970)

[2] Hoheisel, C. , and R. Vogelsand, **Comp. Phys. Rep.**, 8, 1 (1988)

[3] Helfand, E., **Phys. Rev.**, 119, 1 (1960)

[4] McQuarrie, D. , "Statistical Mechanics", Harper&Row, New York (1976)

Abstract for UC Stat. Mech. 1990 conference

Molecular Bonding and Packing of Sulfur

L. René Corrales and Peter J. Rossky

A novel format for modeling the formation of bonds and packing arrangements in covalently bonded materials is introduced and applied to sulfur. The method takes into consideration the implicit contributions from chemical bonding and conventional packing interactions using ideas borrowed from both semi-empirical quantum chemistry and molecular mechanics. This method has the computational advantage of being efficient, inexpensive and broadly applicable. Results for sulfur are presented and contrasted with experimental data and other theoretical methods.

[illegible]

[illegible] compressibility minimum, the specific heat [illegible] minimum, and the correct changes [illegible] temperature and pressure. The qualitative [illegible] agreement [illegible] experimental results shows that the anomalous properties of liquid water are determined, within this model, by the excluded volume and the interaction parameters.

We used the same model to find the nematic-isotropic [illegible] transition: the nematic liquid is considered as a binary mixture in which each component represents a specific molecular orientation. We found that the first order transition can be recovered through a tricritical or a critical end point by applying an external field to the nematic phase.

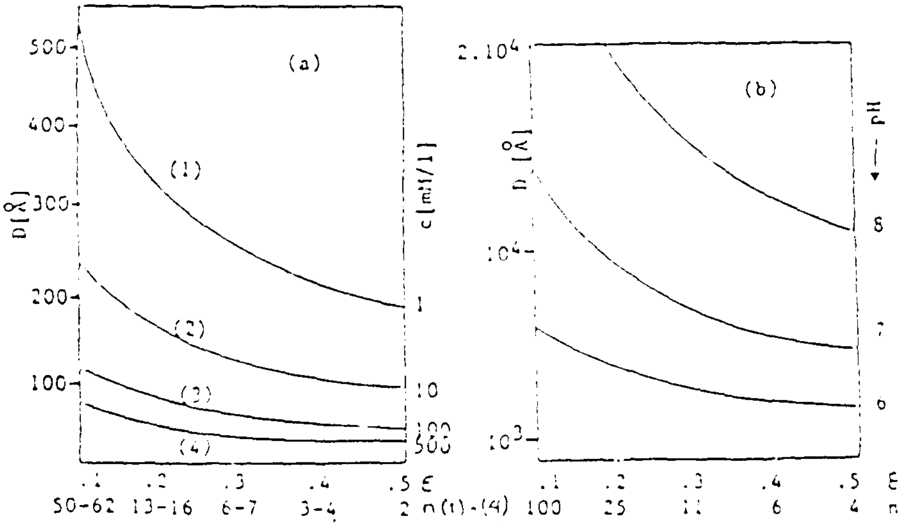
A mean field lattice model is used to predict the phase diagrams of a system that forms microemulsions in different physical situations. The calculated phase progressions and the interfacial properties agree qualitatively with experimental results. We conclude that the ultra-low interfacial tensions we get are due to the presence of a tricritical point near the three phase line. We also discuss the phase diagrams for systems that show ordered phases.

LOCAL TRANSIENT FLUCTUATIONAL DENSITY AS PRODUCING IONIC FLOW THROUGH CELL MEMBRANES.

J.Procopio and J.A.Fornés.
(1) Departamento de Fisiologia e Farmacologia USP-Brazil.(2)Department of Physiology and Biophysics, University of California,Irvine.

We analize some hypothetical conditions in which random fluctuations of ion concentration in restricted regions might lead to transient ion flow through a cell or mitochondrial membrane, and to eventually produce ion concentrations gradients across these structures. We observe from figures that the larger the required relative fluctuation ε , the smaller is the corresponding volume enclosing it. However, there is a broad range of concentrations for which significant fluctuations of c take place in enclosing volumes having diameters comparable to the membrane thickness. In these cases, the dissipation of a fluctuation close to the membrane could result in a transient net flow of the corresponding ion through the channel. In the case of protons the fluctuation in concentration should have considerable significance, due to the very low basal H+ concentration. For example, in a volume of one cubic micrometer there are about 60 free protons at pH 7 and this number should fluctuate between 52 and 68, what should produce significant changes in the local pH.

(Partially supported by CNPq-Brazil grant 200463/89-6/BF).



FLUCTUATION SIZE (D) VERSUS ITS RELATIVE AMPLITUDE ($\varepsilon = \frac{\delta c}{c}$) AND NUMBER OF THE PARTICLES INVOLVED (n) FOR TYPICAL VALUES OF CONCENTRATIONS (c) AND pH OF BIOLOGICAL SYSTEMS. (a) IONIC FLUCTUATION IN GENERAL (b) PROTONIC FLUCTUATIONS.

BINARY MIXTURES IN SILICA GELS

B.J. Frisken, F. Ferri and D.S. Cannell
Department of Physics, UCSB

We have studied the pretransitional behavior of the binary mixture of lutidine and water in silica gels. The gels used were made by polymerization of TMOS (tetramethylorthosilicate) in water. Static light scattering studies show that these gels are fractal on length scales ranging up to a crossover length which can be varied from 200-4000 Å by gelation conditions. At length scales greater than the crossover length, the gels act as a randomly distributed collection of fractal objects. Samples were prepared so that the lutidine volume fraction in the gels was within 1% of that expected in a sample at bulk critical concentration. The behavior of the mixture in the gel in the one phase region was then studied by static light scattering. It was found that the distribution of the intensity of scattered light with scattering vector **q** resembled the form of that of the bare gel, with an amplitude at **q**=0 which showed power law divergence as the transition temperature of the bulk mixture was approached. Possible explanations for this power law behavior will be discussed.

Fluctuating Hydrodynamics and the Principal Oscillation Pattern analysis

Alejandro Garcia
Dept. Physics, San Jose State Univ., San Jose CA 95192-0106

Cecile Penland
CIRES, Univ. of Colorado, Boulder CO 80309-0216

Principal Oscillation Pattern (POP) analysis was recently introduced in climatology to analyze timeseries $x_i(t)$ produced by systems whose dynamics is described by the stochastic differential equation, $\dot{x}_i = B_{ij} x_j + \xi_i$. The matrix **B** gives the deterministic feedback and ξ is a white noise with covariance $<\xi_i(t)\xi_j(t')> = Q_{ij}\, \delta(t-t')$. The POP method was applied to data from a Direct Simulation Monte Carlo program. The system was a dilute gas with 50,000 particles in a Rayleigh-Bénard configuration. The POP analysis correctly obtained the feedback matrix, **B**, as given by the Navier-Stokes equations and the covariance matrix, **Q**, as given by Landau-Lifshitz fluctuating hydrodynamics. We discuss how the method may be used to empirically compute amplitude equation coefficients from data.

SERIES INVESTIGATIONS OF FRUSTRATED SQUARE-LATTICE ANTIFERROMAGNETS

The zero-temperature properties of the square-lattice, S=1/2 Heisenberg model with antiferromagnetic first and second (diagonal) neighbor interactions have proven to be remarkably elusive. For $J_1 \approx 2J_2$, there are at least three proposals for the nature of the ground state (disordered, helical, spontaneously dimerized), and finite-size studies have yielded conflicting conclusions. We report on series expansions in coupling constants about a variety of trivial (explicitly dimerized) Hamiltonians. The calculations suggest that in the disputed regime, the model is spontaneously dimerized, but only weakly so. Furthermore, there appear to be *several* relatively large correlation lengths.

SURFACE DIFFUSION AND FLUCTUATIONS OF GROWING INTERFACES

Leonardo Golubovic and *Robijn Bruinsma*
Physics Department and Solid State Science Center
University of California,Los Angeles,CA 90024

Abstract

A model is proposed for the growth of realistic interfaces relaxing dominantly by surface diffusion. We show that the thermal noise can produce large scale orientational fluctuations in the active zone of the growth. We relate them to the experimentally observed undersurface networks of voids which we characterize by a structural lengthscale of the order of the orientational persistence length.

Roughening transition of the isotropic frustrated Ising model

B. Kahng and K. A. Dawson

Department of Chemistry, P. O. Box 224, University of California
Berkeley, CA 94720

Abstract

We study the roughening transition behavior with the isotropic competing Ising Hamiltonian [1−2], $\mathcal{H} = -J \sum_{nn} s_i s_j - 2M \sum_{dnn} s_i s_j - M \sum_{nnn} s_i s_j$, where nn, dnn, nnn mean the nearest neighbor, the diagonal neighbor, the linearly next nearest neighbor respectively, and $J > 0$ and $-\infty < M < \infty$. Low temperature expansions are performed in the three dimensional cubic lattice for moments of the interface width and for the interface density. The results are compared to a Sine-Gordon renormalization group calculation of the analogous solid-on-solid model. By comparison with Monte Carlo simulation results [3], it is likely that the roughening transition line in the $(j \equiv J/kT, m \equiv M/kT)$ plane passes through the Lifshitz point, and is very close to part of the phase boundary between paramagnetic and modulated phases. We discuss the implications for the phase-structure and the interfacial profile in the vicinity of the Lifshitz point.

References

1. B. Widom, *J. Chem Phys.* **84**, 6943 (1986).
2. K. A. Dawson, M. D. Lipkin, and B. Widom, *J. Chem Phys.* **88**, 5149 (1988).
3. K. A. Dawson, B. Walker, and A. Berera, *Physica* (in press).

About negative moments of current distribution in random resistor networks

Byungnam Kahng

Department of Chemistry
University of California, Berkeley, CA 94720†
Center for Polymer Studies and Department of Physics
Boston University, Boston MA 02215

*

Abstract

We investigate the size dependent behavior for negative moments of current distribution in random resistor networks. With the extreme value statistics idea, we derive the explicit form of the current distribution in small current regime. The distribution is found to be the Weibull distribution $n(x) \sim \exp(-x^m)$, with $m > 1$ and $x \equiv -\log i/\log L$. L is the system size. Using this distribution function, we show breakdown of multifractal behavior in negative moments regime and non-occurrence of thermodynamic phase transition.

P.A.C.S. numbers: 64.60.Ak,05.50.+q,05.60.+w

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* † present address

Abstract for the UC Conference on Statistical Mechanics, Santa Babra,1990

MUSIC COMPOSITION AND MODELS OF CORTEX USING PHYSICAL SYSTEM ANALOGIES

Xiaodan Leng and Gordon L. Shaw, Center for the Neurobiology of Learning and Memory and Physics Department University of California, Irvine, Irvine, CA 91717.
Eric Wright Irvine Conservatory of Music, 711 Farad St. Costa Mesa, CA 91627

Based on the Fisher's ANNNI model of physical spin system and guided by the Mountcastle cortical principle of columnar organization we had developed the trion model [G. Shaw, D. Silverman and J. Pearson, PNAS 82,2364 (1985)] for the firing activity of groups of neurons; an essential feature of the trion network is that it is highly structured in time and in spatial connections. The trion model has been shown to be useful for understanding aspects of memory and pattern recognition. To study the properties of interconnected networks of the trion model we incorporated the MILA model [J. Patera, G. Shaw, R. Slansky, and X. Leng, Phys. Rev. A40, 1073 (1989) whose underlying structure is the weight systems of zero-level representations of affine Kac-Moody algebras] to modulate the firing activity of interacting cortical columns. Turning now to higher cognitive processes, we map spatio-temporal firing pattern evolutions of the model onto pitches and instruments to produce music. The preliminary results are striking: 1) The trion music is very pleasant to listen to; 2) One set of connections among the trions produces music sounding like a waltz, another set gives a minuet; 3) Different mappings of

Monte Carlo Calculations of the Correlation Functions for Heisenberg Spin Chains at T=0

Shoudan Liang , Department of Physics and Material Research
Laboratory, University of Illinois at Urbana-Champaign, 1110
West Green Street, Urbana, Illinois 61801.

Abstract: We computed the ground state spin-spin correlation function for the one dimensional antiferromagnetic Heisenberg model of spin 1/2, 1 and 3/2. The spin-1 chain has a disordered ground state with a correlation length of 6.2 lattice spacing whereas the spin-1/2 and the spin-3/2 chains both have $(ln(r))^{\sigma}/r$ decaying correlation functions. The logarithmic corrections are different for the spin-1/2 and the spin-3/2 chains. Finite-size scaling is used to analyze the data for chains of up to 128 spins.

Existence of Néel Order at T=0 in the spin-1/2 antiferromagnetic Heisenberg Model on a Square Lattice

Shoudan Liang . Department of Physics and Material Research Laboratory, University of Illinois at Urbana-Champaign, 1110 West Green Street, Urbana, Illinois 61801.

Abstract: We have computed spin-spin correlation function for the ground state of the spin-1/2 antiferromagnetic Heisenberg model on a 32×32 square lattice using a projection Monte Carlo method. Kennedy, Lieb and Shastry have shown that if the ground state is not Néel ordered, the two point function must satisfy an upper bound. Our correlation function at short distance (less than 4.5) violates this bound which implies that the ground state must have long ranged Néel order. We have also estimated the staggered magnetization to be $m^{+}=0.304\pm0.04$ in the thermodynamic limit.

ABSTRACT FOR SUBMISSION TO UC STATISTICAL MECHANICS CONFERENCE

THE DIFFUSION COEFFICIENT OF A REPTATING POLYMER.

J.M. Deutsch and **T.L. Madden**. University of California at Santa Cruz, Santa Cruz, CA, 95064.

The dynamics of a polymer in a network of entanglements is studied. The viscosity and diffusion coefficient were studied in the repton model for up to 75 links. First we derive the correct procedure for calculating the three dimensional diffusion coefficient in this model. We find that the diffusion coefficient scales as $L^{-2.3\pm0.1}$. This result is in marked contrast to the asymptotic L^{-2} prediction of reptation. We see that the asymptotic behavior of the diffusion coefficient must have corrections of the order of $L^{-1/2}$. This implies that fluctuations in the tube length cannot provide an adequate explanation for the experimental data. The viscosity is found to scale as $L^{3.49\pm0.13}$, in accord with experimental data and other numerical results.

Abstract for the UC Conference on Statistical Mechanics
Santa Barbara, Ca. March 1990

PHASE TRANSITIONS IN THE TRION MODEL OF CORTICAL ORGANIZATION

John McGrann, Gordon L. Shaw, Dennis J. Silverman
Department of Physics, University of California, Irvine
Irvine, Ca. 92717

John C. Pearson
David Sarnoff Research Center, Princeton, NJ 08543

The trion model [Shaw, Silverman, Pearson, PNAS 82,2364,(1985)], based on an analogy with Fisher's ANNNI physical spin system [Fisher,Selke, Phys. Rev. Lett.,44,(1980)], has been motivated by such cortical principles as Mountcastle's columnar organization. The trion represents a localized group of neurons with three levels of firing activity which has spatial-temporal connections that are highly structured. Networks of a small number of trions (with structured interactions and firing dependent on activity at two previous time steps) support a repertoire of hundreds of quasi-stable, periodic firing patterns, MPs (which can be learned). We report striking phenomena with variation in "temperature" T: There exist a series of "phase transitions" at precise values T(n) giving new repertoires of MPs, and the average time for any initial firing configuration to project onto an MP shows a quite sharp change at each T(n). When the connections are made random these phenomena disappear.

Symmetry Breaking in a Simple Electron-Phonon Model with Electron Correlations

Qing Zhang* and Robert J. Silbey
Department of Chemistry
Massachusetts Institute of Technology
Cambridge MA 02139

Abstract

We consider a simple model which contains both electron phonon coupling, electron transfer, and electron correlation, which can be a prototype of a mixed valence system with 3 nearby electronic states. We treated the adiabatic solution, simple corrections to that, and the effect of symmetry breaking terms on the solutions. We find that the adiabatic solutions in the symmetric case can show a (false) symmetry breaking which is removed in the nonadiabatic calculation. These solutions are extremely unstable with respect to the addition of a nonsymmetric term in the Hamiltonian.

* Current address: Department of Chemistry, UC Berkeley
Berkeley, CA 94720

ABSTRACT

Title of Poster ~~Dissertation~~: EQUILIBRIUM POLYMERIZATION AS A PHASE TRANSITION

Jaime Ruiz Garcia, Doctor of Philosophy, 1989

Dissertation directed by: Sandra C. Greer
Professor
Department of Chemistry

Recently, Wheeler et al. have proposed a theory to describe equilibrium polymerization reactions. The theory is based on the formal limit n -> 0 of the n-vector model of magnetism. Wheeler et al. have predicted that the equilibrium polymerization reaction can be treated as a phase transition, analogous to the phase transitions observed in magnetic systems.

Several predictions of Wheeler et al. have been experimentally tested in sulfur and sulfur solutions, e. g., the phase diagrams, the divergence of the heat capacity at the polymerization transition, etc.. There are some discrepancies between the theory and the experimental data available in the literature for the sulfur systems.

evidence of the presence of a tricritical point. However, some discrepancies still exist. We have not a good explanation for these differences; thus more work is still needed.

Abstract for Poster at the

University of California Statistical Mechanics Conference

HEXAGONAL AND DISORDERED PHASES OF SEMIFLEXIBLE CHAINS. J. V. Selinger and R. F. Bruinsma, UCLA.*--We consider the statistical mechanics of a system of semiflexible chains, which can represent polymer liquid crystals, long-chain biomolecules, stiff worm-like micelles, or columns of discotic liquid crystals. In the orderered phase, these systems can form a hexagonal lattice; in the disordered phases, they can become nematic or isotropic fluids. We calculate the structure factor and the orientational correlation function in the hexagonal and nematic phases using continuum elastic theory. In the hexagonal phase, the structure factor exhibits Bragg peaks surrounded by diffuse thermal scattering. The diffuse line shape is related to the elastic constants of the lattice. In the nematic phase, the structure factor exhibits a similar line shape as the wavevector $q \to 0$. In general, the elastic constants depend on the type of interaction between the chains. We derive these constants for a pure excluded-volume repulsion. We then use a variational theory to model the first-order transitions among the hexagonal, nematic, and isotropic phases. This theory leads to a phase diagram in terms of pressure (or concentration) and persistence length.

*Supported by the UCLA Solid State Science Center.

SCALING PROPERTIES OF DIFFUSION-LIMITED REACTION

by

Wen-Shyan Sheu [*], Katja Lindenberg [*] and Raoul Kopelman [**]

[*] Department of Chemistry, B-040 and
Institute for Nonlinear Science, R-002
University of California, San Diego
La Jolla, CA 92093

[**] Department of Chemistry,
The University of Michigan,
Ann Arbor, MI 48109

Abstract

A simple novel scaling argument for diffusion-limited reactions for both $A + A \rightarrow 0$ and $A + B \rightarrow 0$ is developed. Asymptotic behaviors of species densities without source input and reaction orders with source input are discussed. It is shown how the structures of spatial distributions of particles affect reaction rates. As a result, the asymptotic behavior of the density for $A + B \rightarrow 0$ without source input is found to depend on the fractal dimension, a dependence that does not seem to have been noted before.

ABSTRACT FOR THE POSTER SESSION

Thermodynamic Equations of State for the Kinetic and Potential Energies of a System of Charged Particles

DUANE P. SIEMENS
Department of Physics
University of California
Davis, CA 95616

ABSTRACT

In this paper we consider a system of N charged particles confined to a volume V. We prove the following relationship between the thermodynamic averages of the kinetic energy, $< \mathcal{T} >$, and potential energy, $< \mathcal{V} >$,

$$2 < \mathcal{T} > + < \mathcal{V} > -3PV = 0,$$

where P is the pressure. Using this relationship we relate the average kinetic and potential energies to measurable thermodynamic quantities. We also derive an analogous realtionship for a given species of particle in a multi-species system. We further consider the effect of a constant external magnetic field.

PHASE TRANSITION BEHAVIOR IN A NEGATIVE TEMPERATURE GUIDING CENTER PLASMA OR VORTEX GAS[1]

Ralph A. Smith

Physics Dep't. B-019. UCSD. La Jolla. CA 92093

The thermal equilibria of a two-dimensional, single-species, guiding-center plasma or gas of parallel line vortices, bounded by a circular equipotential surface, are considered in the microcanonical ensemble. The system is a model for a magnetically confined nonneutral plasma, or an extended vortex column in an ideal fluid. At sufficiently large energies (for specified canonical angular momentum), the statistically predominant configurations are displaced macroscopically from the axis. The transition between symmetric and asymmetric equilibria resembles a second-order phase transition, and occurs at formally negative temperatures. It is related to a bifurcation in the mean-field description. An analysis of fluctuations suggests that the transition is of the Gaussian type, in the limit of large particle number. The theory is compared with microcanonical Monte Carlo simulations.

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[1] Work supported by O.N.R. N00014-82-K-0621 and N.S.F. PHY87-06358; Computations done at the San Diego Supercomputer Center

UNIVERSALITY IN SOLUTIONS OF LINEAR POLYMERS*

Lipiin Sung and David S. Cannell
Department of Physics, University of California, Santa Barbara, CA 93106

The universal properties of linear polymer solutions have been intensively investigated both experimentally and theoretically. For appropriate solutions, it is known that the reduced characteristic length ξ/R_G is a function only of reduced concentration B_2C, where C is the concentration, and B_2 is the second virial coefficient. The reduced characteristic length is the ratio of the characteristic length ξ, determined by the angular dependence of scattered radiation, to the radius of gyration of an isolated coil, R_G. At low concentration $\xi = R_G/\sqrt{3}$. It is also known that the product of the molecular weight, M_W, and osmotic susceptibility $\left(\frac{\partial \Pi}{\partial C}\right)_T$ is also a function only of B_2C for appropriate solutions. The quantity $\left(\frac{\partial \Pi}{\partial C}\right)_T$ can be obtained from the absolute scattered intensity. Universal behavior is observed[1] over a wide concentration range independent of either molecular weight or the solvent quality for polystyrene both in Toluene (good solvent) and in MEK (marginal solvent). Furthermore, real-space renormalization group calculations[2] using no adjustable parameters agree with these findings. The aim of the present work is to extend the study of the universality of linear polymers to polymers in θ solvents by varying the temperature (T) of the polystyrene-cyclohexane system from $T \gg \theta$ to $T = \theta$, at which B_2 vanishes. We are currently investigating the crossover behavior from good solvent to θ solvent as temperature changes, and we hope to quantify the breakdown of universality as T approaches θ.

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[1] P. Wiltzius, H.R. Haller, D.S. Cannell and D.W. Schaefer, *Phys. Rev. Lett.* **51**, 1183 (1983).

[2] T. Ohta, A. Nakanishi, *J. Phys. A* **16**, 4155 (1983); L. Schaefer, *Macromolecules* **17**, 1357 (1984); T. Ohta, Y. Oono, *Phys. Lett.* **89A**, 460 (1982).

*This research is supported by National Science Foundation Grant No. DMR-87-14591.

I would like to submit the following two
abstracs for the corresponding poster.

"Two-dimensional reactive systems: Rapid bimolecular processes on spherical surfaces"

by

Enrique Peacock-Lopez and Michael Swartz
Department of Chemistry
Williams College
Williamstown, MA 01267

Abstract

Bimolecular reactions in two dimensions are studied using the fluctuation-dissipation theory. In particular, we calculate the rate constant and the radial distribucion function for a dimerization reaction on a spherical surface of radius R. We analyze the effect of the curvature to reactivity.

Crossover from Heisenberg to Ising critical behaviour in (K_2NiF_4)

Shubha Tewari and Sudip Chakravarty
Department of Physics
University of California at Los Angeles
Los Angeles, CA 90024

Abstract

It is known from experiments done on (K_2NiF_4), a planar antiferromagnet, that there exists a crossover from 2D Heisenberg to 2D Ising critical behaviour above the 3D Neel transition temperature. Using a nearest neighbour Heisenberg model with anisotropy, we do a spin wave calculation and estimate the anisotropy from a comparison with measurements of the spin wave gap. We then map this on to a quantum non-linear σ-model in 2+1 dimensions, which describes the long wavelength, low temperature properties of this system. Integrating out quantum fluctuations we obtain an effective classical model with renormalised parameters. The Heisenberg to Ising crossover temperature is determined. A renormalisation group calculation is done to determine the crossover correlation length.

Abstract Submitted
for the 4th UC Conference
on Statistical Mechanics
26-28 March 1990

Curvature elasticity of diblock copolymer monolayers and bilayers. Zhen-Gang Wang, Department of Chemistry, UCLA --- Curvature expansion of the free energy for diblock copolymers aggregated into monolayers and bilayers, is studied. The theory makes use of the recent results for grafted chains obtained by Milner et al., and allows variation in the area per chain molecule with curvatures. Elastic coefficients such as the bending modulus, the Gaussian bending modulus and the spontaneous curvature, are calculated for a number of situations involving different conditions for the chains (melt or swollen). In the case of bilayers, we show that, if each monolayer has a strong tendency to curve convexly towards the solvent, the flat geometry can become unstable; the curvature free energy rather favors the formation of spherical vesicles over the flat bilayer. Relevence of this study to microemulsion using diblock copolymer as compatilizer, is discussed.

Abstract Submitted
for the 4th UC Conference
on Statistical Mechanics
26-28 March 1990

A statistical mechanical approach to fracture. Robin Blumberg Selinger, Zhen-Gang Wang, William M. Gelbart, Department of Chemistry, UCLA. --- We present a quasi-equilibrium model of fracture of solid materials at finite temperature and under uni-directional tension. Our approach is motivated by the assumption that a solid under stress is metastable thermodynamically. To maintain this metastable state, tension must be applied at a rate fast enough so that thermodynamic phase transitions such as evaporation and melting do not take place, and yet slow enough so that local molecular rearrangement is possible for local ergodicity as required by the statistical thermodynamic approach. The solid is modeled as an elastic bond network and fracture is envisioned as the proliferation and aggregation of broken bonds under tension. We solve a one-dimensional model exactly and carry out Monte Carlo simulations for a two-dimensional network. Characteristic properties such as the stress-strain curve and its dependence on temperature are obtained. We also discuss our results in connection with the Griffith theory for fracture and theory of nucleation.

POSTER ABSTRACT
for UC Conference on Statistical Mechanics

Ken Hui, David Wu and David Chandler
Dept. of Chemistry, UC Berkeley

A procedure for obtaining the renormalized step length, l, (or polymer length L) is developed for polymers with attractive (or repulsive) self-interactions. We apply this method to calculate the interior-point correlation function. Using the isomorphism between a ring polymer and an electron in a fluid, we arrive at an expression for the diffusion constant.

AN EXACTLY SOLVABLE MODEL OF DISSIPATIVE QUANTUM TUNNELING

by

Ten-Ming Wu [*], David W. Brown [**] and Katja Lindenberg [**,+]

[*] Department of Physics, B-019
[**] Institute for Nonlinear Science, R-002 and
[+] Department of Chemistry, B-040
University of California, San Diego
La Jolla, CA 92093

Abstract

We present an exactly solvable model of dissipative quantum tunneling in a two-level system coupled with a phonon bath. The model is motivated by the problem of excimer formation in dimerized molecular crystals such as α-perylene. The spectral function shows the system in the one dimensional case to be of the "ohmic" type. The decay behavior for this dissipative tunneling model may be Gaussian, power-law and/or exponential, depending on the coupling strength and the initial temperature of the lattice.

A Rising Bubble in a Tube

Herbert Levine and Yumin Yang

Department of Physics
and
Institute for Nonlinear Science

University of California, San Diego 92093

November 1, 1989

Abstract

We study the rise of an infinitely long bubble in a vertical cylindrical tube full of inviscid fluid. We demonstrate numerically that the rising velocity of the bubble is determined by the surface tension through a solvability mechanism. Our numerical results are in good agreement with the experimental ones.