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During the grant period we have carried out research on the properties of equilibrium and nonequilibrium plasmas. A large part of our work was focused on the basic problem of ionization by time periodic fields. An understanding of this process is improtant for the development and optimal utilization of plasmas in various areas relevant to AFOSR.

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FINAL PROGRESS REPORT

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BASIC STUDIES IN PLASMA PHYSICS

February 1, 1998—January 31, 2001

by

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SUMMARY

During the grant period we have carried out research on the properties of equilibrium and nonequilibrium plasmas. A large part of our work was focused on the basic problem of ionization by time periodic fields. An understanding of this process is important for the development and optimal utilization of plasmas in various areas relevant to AFOSR.

We also continued our general program of applying the methods of statistical mechanics to phenomena which take place when neutral and ionized atoms and electrons interact strongly with external fields and with each other. These show intrinsic nonlinear cooperative behavior and our work utilized a variety of techniques: rigorous mathematical analysis, simplifying approximations and computer simulations.

We present below brief summaries of some papers published recently or submitted for publication. A list of publications follows these summaries.

1) Ionization of a Model Atom by Perturbations of the Potential

We study the time evolution of the wave function of a particle bound by an attractive δ-function potential when it is subjected to time dependent forcing. The simplicity of this model permits certain nonperturbative calculations to be carried out analytically both in one and three dimensions. Thus we prove that this system will be fully ionized by a time periodic variation of the attractive potential of arbitrary strength r and frequency ω. Starting with the system in the bound state, the survival probability is for small r given by $e^{-\Gamma t}$ for times of order $\Gamma^{-1} \sim r^{-2n}$, where n is the minimum number of "photons" required for ionization (with large modifications at resonances). For late times the decay is like t^{-3} with the power law modulated by oscillations. As r increases the time over which there is exponential decay becomes shorter and the power law behavior starts earlier. While our rigorous results are for a simplified model comparison with analytical works and with experiments indicate that many features are general.

2) Charge Fluctuations in the Two-Dimensional One-Component Plasma

We study, via computer simulations, the fluctuations in the net electric charge, in a two dimensional one component plasma (OCP) with uniform background charge density $-e\rho$, in a region Λ inside a much larger overall neutral system. Setting $e = 1$ this is the same as the fluctuations in N_Λ, the number of mobile particles of charge e. As expected the distribution of N_Λ has, for large Λ, a Gaussian form with a variance which grows only as $\hat{\kappa}|\partial\Lambda|$, where $|\partial\Lambda|$ is the length of the perimeter of Λ. The properties of this system depend only on the coupling parameter Γ. Our simulations show that when the coupling parameter Γ increases, $\hat{\kappa}(\Gamma)$ decreases to an asymptotic value $\hat{\kappa}(\infty) \sim \hat{\kappa}(2)/2$ which is equal (or very close) to that obtained for the corresponding variance of particles on a rigid triangular lattice. Thus, for large Γ, the characteristic length $\xi_L = 2\hat{\kappa}/\rho$ associated with charge fluctuations behaves very differently from that of the Debye length, $\xi_D \sim 1/\sqrt{\Gamma}$, which it approaches as $\Gamma \to 0$. The pair correlation function of the OCP is also studied.

3) Binary Fluids with Long Range Segregating Interaction I: Derivation of Kinetic and Hydrodynamic Equation

We study the evolution of a two component fluid consisting of particles which interact via strong short range (hard core) and weak long range pair potentials. At low temperatures the equilibrium state of the system is one in which there are two coexisting phases. Under suitable choices of space-time scalings and system parameters we obtain a teract via strong short range (hard core) and weak long range pair potentials. At low temperatures the equilibrium state of the system is one in which there are two coexisting phases. Under suitable choices of space-time scalings and system parameters we obtain a mesoscopic kinetic Vlasov-Boltzmann equation for the one particle position and velocity distribution functions, appropriate for a description of the phase segregation kinetics in this system. Further scalings then yield Vlasov-Euler and incompressible Vlasov-Navier-Stokes equations. We also obtain, via the usual truncation of the Chapman-Enskog expansion, compressible Vlasov-Navier-Stokes equations.

4) **Scaling Dynamics of a Massive Piston in a Gas**

We study the dynamical system consisting of N non-interacting point particles of mass m, in a cubical domain Ω_L of sides L, separated into two regions by an idealized movable wall: a massive particle (piston), of cross-sectional area L^2 and mass $M_L \sim L^2$. The piston is constrained to move along the x-axis and undergoes elastic collisions with the gas particles. We find that, under suitable initial conditions, there is, in the limit $L \to \infty$, a scaling regime with time and space scaled by L, in which the motion of the piston and the one particle distribution of the gas satisfy autonomous coupled equations.

5) **Large Deviations for Quantum Systems**

We consider a general d-dimensional quantum system of particles in a very large container. We prove that, under suitable conditions, the fluctuations in the density of particles in a subdomain Λ of the container are described by a large deviation function related to the pressure of the system. That is, untypical densities occur with an exponentially small probability in the volume of Λ, with the coefficient in the exponent given by the appropriate thermodynamic potential. Furthermore, small fluctuations satisfy the central limit theorem.

6) Properties of Stationary Nonequilibrium States in the Thermostatted Periodic Lorentz Gas I: The One Particle System

We study numerically and analytically the properties of the stationary state of a particle moving under the influence of an electric field **E** in a two dimensional periodic Lorentz gas with the energy kept constant by a Gaussian thermostat. Numerically the current appears to be a continuous function of **E** whose derivative varies very irregularly, possibly in a discontinuous manner. We argue for the non differentiability of the current as a function of **E** utilizing a symbolic description of the dynamics based on the discontinuities of the collision map. The decay of correlations and the behavior of the diffusion constant are also investigated.

7) Dynamics of Mesoscopic Precipitate Lattices in Phase Separating-Alloys under External Load

We investigate, via three-dimensional atomistic computer simulations, phase separation in an alloy under external load. A regular two-dimensional array of cylindrical precipitates, forming a mesoscopic precipitate lattice, evolves in the case of applied tensile stress by the movement of mesoscopic lattice defects. A striking similarity to ordinary crystals is found in the movement of "meso-dislocations", but new mechanisms are also observed. Point defects such as "meso-vacancies" or "meso-interstitials" are created or annihilated locally by merging and splitting of precipitates. When the system is subjected to compressive stress, we observe stacking faults in the mesoscopic one-dimensional array of plate-like precipitates.

8) Fourier's Law

We present a selective overview of the current state of our knowledge (more precisely of our ignorance) regarding the derivation of Fourier's Law, $\mathbf{J}(\mathbf{r}) = -\kappa\nabla T(\mathbf{r})$; $\mathbf{J}$ the heat flux, T the temperature and κ, the heat conductivity. This law is empirically well tested for both fluids and crystals when the temperature varies slowly on the microscopic scale with κ an intrinsic property of a macroscopic system i.e. one which depends only on the system's equilibrium parameters, such as the local temperature and density. There is indeed an expression, Kubo's formula, for κ involving integrals over equilibrium time correlations, derivable in principle from a knowledge of the Hamiltonian of the system, which is believed to be exact. There is however at present no rigorous mathematical derivation of Fourier's law and ipso facto of Kubo's formula for any Hamiltonian or indeed for any model with a deterministic microscopic evolution. The situation is better for stochastic models.

9) Macroscopic Evolution of Particle Systems with Short and Long Range Interactions

We consider a lattice gas with general short range interactions and a Kac potential $J_\gamma(r)$ of range γ^{-1}, $\gamma > 0$, evolving via particles hopping to nearest neighbor empty sites with rates which satisfy detailed balance with respect to the equilibrium measure. Scaling space like γ^{-1} and time like γ^{-2}, we prove that in the limit $\gamma \to 0$ the macroscopic density profile $\rho(r,t)$ satisfies the equation

$$\frac{\partial}{\partial t}\rho(r,t) = \nabla \cdot \left[\sigma_s(\rho)\nabla\frac{\delta\mathcal{F}(\rho)}{\delta\rho(r)}\right]. \qquad (*)$$

Here $\sigma_s(\rho)$ is the mobility of the reference system, the one with $J \equiv 0$, and $\mathcal{F}(\rho) =$

$\int[f_s(\rho(r)) - \frac{1}{2}\rho(r)\int J(r-r')\rho(r')\mathrm{d}r\mathrm{d}r']$, where $f_s(\rho)$ is the (strictly convex) free energy density of the reference system. This result holds also if $\mathcal{F}$ achieves its minimum on non constant density profiles and this includes the cases in which *phase segregation* occurs. Using the same techniques we also derive hydrodynamic equations for the densities of a two component A-B mixture with long range repulsive interactions between A and B particles. The equations for the densities ρ_A and ρ_B are of the form (*). They describe, at low temperatures, the demixing transition in which segregation takes place via vacancies, i.e. jumps to empty sites. In the limit of *very few* vacancies the problem becomes similar to phase segregation in a continuum system in the so called *incompressible limit.*

10) Microscopic Computer Simulations of Directional Coarsening in Face-centered Cubic Alloys

We carried out Monte Carlo simulations of phase separation in a three-dimensional binary alloy with misfitting phases subjected to uniaxial stress. A lattice of cylindrical or plate-like precipitates is formed at the mesoscale, as observed in real alloys. The rate of precipitate growth is much slower than the conventional $R(t) \sim t^{\frac{1}{3}}$ behavior in systems with no elastic misfit. Once a well-defined precipitate microstructure is formed, the reversal of external applied load has only a small effect.

11) Bounded Fluctuations and Translation Symmetry Breaking I

We present general results for one-dimensional systems of point charges (signed point measures) on the line with a translation invariant distribution μ for which the variance of the total charge in an interval is uniformly bounded (instead of increasing with the interval length). When the charges are restricted to multiples of a common unit, and their average charge density does not vanish, then the boundedness of the variance implies translation-symmetry breaking — in the sense that there exists a function of the charge configuration that is nontrivially periodic under translations — and hence that μ is not "mixing." Analogous results are formulated also for one dimensional lattice systems under some constraints on the values of the charges at the lattice sites and their averages. The general results apply to one-dimensional Coulomb systems, and to certain spin chains, putting on common grounds different instances of symmetry breaking encountered there.

12) Bounded Fluctuations and Translation Symmetry Breaking II

The variance of the particle number (equivalently the total charge) in a domain of length $\mathcal{L}$ of a one-component plasma (OCP) on a cylinder of circumference W at the reciprocal temperature $\beta = 2$, is shown to remain bounded as $\mathcal{L} \to \infty$. This exactly solvable system with average density ρ has a density profile which is periodic with period $(\rho W)^{-1}$ along the axis of the infinitely long cylinder. This illustrates the connection between bounded variance and periodicity in (quasi) one-dimensional systems. When $W \to \infty$ the system approaches the two-dimensional OCP and the variance in a domain Λ grows like its perimeter $|\partial\Lambda|$İn this limit, the system is translation invariant with rapid decay of correlations.

13) Surface-Directed Spinodal Decomposition in Binary Fluid Mixtures

We consider the phase separation of binary fluids in contact with a surface which is preferentially wetted by one of the components of the mixture. We review the results available for this problem and present new numerical results obtained using a novel simulation technique for the 3-dimensional problem.

14) **Spatial Structure in Low Dimensions for Diffusion Limited Two-Particle Reactions**

Consider the system of particles on $\mathbb{Z}^d$ where particles are of two types, A and B, and execute simple random walks in continuous time. Particles do not interact with their own type, but when a type A particle meets a type B particle, both disappear. Initially, particles are assumed to be distributed according to homogeneous Poisson random fields, with equal intensities for the two types. This system serves as a model for the chemical reaction $A + B \to inert$. In our earlier work the densities of the two types of particles were shown to decay asymptotically like $1/t^{d/4}$ for $d < 4$ and $1/t$ for $d \geq 4$, as $t \to \infty$. This change in behavior from low to high dimensions corresponds to a change in spatial structure. In $d < 4$, particle types segregate, with only one type present locally. After suitable rescaling, the process converges to a limit, with density given by a Gaussian process. In $d > 4$, both particle types are, at large times, present locally in concentrations not depending on the type, location or realization. In $d = 4$, both particle types are present locally, but with varying concentrations. Here, we analyze this behavior in $d < 4$; the behavior for $d \geq 4$ will be handled in a future work.

15) **Precipitate Size Distribution in Alloys with and without Lattice Misfit**

We investigate, via three-dimensional atomistic computer simulations, the influence of a lattice misfit between precipitated and matrix on the precipitate size distribution during phase separation in a binary alloy. The elastic interactions are modeled by springs connecting nearest neighbor atoms. The difference in size between the two species of atoms, specified by the misfit parameter δ, leads to effective long range interactions. Performing simulations with five different values of δ we find a broadening of the scaled precipitate size distribution for $\delta > 0.5\%$ in comparison with the case of no misfit. Additionally, the size of the largest precipitate in the system increases with increasing misfit. We also observe a percolated network-like precipitate structure for a concentration of solute atoms as low as $c_A = 0.2$ at large misfit. We interpret these effects as due to an increased tendency of the precipitates to coalesce, which is caused by their non-spherical shape, their alignment along the $\langle 100 \rangle$-directions and their regular arrangement.

16) **Free Energy Functional for Nonequilibrium Systems : An Exactly Solvable Case**

We consider the steady state of an open system in which there is a flux of matter between two reservoirs at different chemical potentials. For a large system of size N, the probability of any macroscopic density profile $\rho(x)$ is $\exp[-N\mathcal{F}(\{\rho\})]$; $\mathcal{F}$ thus generalizes to nonequilibrium systems the notion of free energy density for equilibrium systems. Our exact expression for $\mathcal{F}$ is a nonlocal functional of ρ, which yields the macroscopically long range correlations in the nonequilibrium steady state previously predicted by fluctuating hydrodynamics and observed experimentally.

17) **Blocking Measures for Asymmetric Exclusion Processes via Coupling**

We give sufficient conditions on the rates of two asymmetric exclusion processes such that the existence of a blocking invariant measure for the first implies the existence of such a measure for the second. The main tool is a coupling between the two processes under which the first dominates the second in an appropriate sense. In an appendix we construct a class of processes for which the existence of a blocking measure can be proven directly;

these are candidates for comparison processes in applications of the main result.

18) **Diffusion Effects on the Breakdown of a Linear Amplifier Model Driven by the Square of a Gaussian Field**

We investigate solutions to the equation $\partial_t \mathcal{E} - \mathcal{D}\Delta\mathcal{E} = \lambda S^2 \mathcal{E}$, where $S(x,t)$ is a Gaussian stochastic field with covariance $C(x-x',t,t')$, and $x \in R^d$. It is shown that the coupling $\lambda_{cN}(t)$ at which the N-th moment $\langle \mathcal{E}^N(x,t)\rangle$ diverges at time t, is always less or equal for $\mathcal{D} > 0$ than for $\mathcal{D} = 0$. Equality holds under some reasonable assumptions on C and, in this case, $\lambda_{cN}(t) = N\lambda_c(t)$ where $\lambda_c(t)$ is the value of λ at which $\langle \exp[\lambda \int_0^t S^2(0,s)ds]\rangle$ diverges. The $\mathcal{D} = 0$ case is solved for a class of S. The dependence of $\lambda_{cN}(t)$ on d is analyzed. Similar behavior is conjectured when diffusion is replaced by diffraction, $\mathcal{D} \to i\mathcal{D}$, the case of interest for backscattering instabilities in laser-plasma interaction.

19) **Thermodynamic Entropy Production Fluctuation in a Two Dimensional Shear Flow Model**

We investigate fluctuations in the momentum flux across a surface perpendicular to the velocity gradient in a stationary shear flow maintained by either thermostated deterministic or by stochastic boundary conditions. In the deterministic system the Gallavotti-Cohen (GC) relation for the probability of large deviations, which holds for the phase space volume contraction giving the Gibbs ensemble entropy production, never seems to hold for the flux which gives the hydrodynamic entropy production. In the stochastic case the GC relation is found to hold for the total flux, as predicted by extensions of the GC theorem but not for the flux across part of the surface. The latter appear to satisfy a modified

GC relation. Similar results are obtained for the heat flux in a steady state produced by stochastic boundaries at different temperatures.

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