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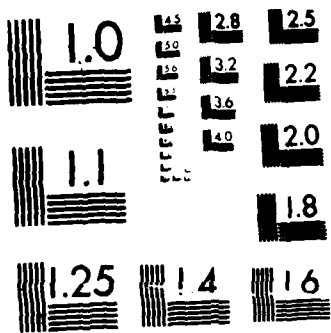
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Progress was made on the statistical mechanics of the Zakharov model which describes the interaction of an electromagnetic wave with a plasma. The model leads to a nonlinear set of partial differential equations which resemble in some ways equations arising in nonlinear field theories which have been studied by statistical mechanical methods. Some very exact results for this model have been obtained in 1-D and computer simulations are being carried out on it. A new program has been launched involving both theoretical analysis and computer simulations on interacting quantum systems. Keywords:

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FINAL SCIENTIFIC REPORT

AFOSR GRANT 82-0016C **AFOSR·TR· 87 - 0 5 1 3**

TITLE: STATISTICAL MECHANICS OF COLLECTIVE PHENOMENA IN PLASMAS

NOVEMBER 1, 1983 – OCTOBER 31, 1986

by

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INTRODUCTION

Our work during this period continued to have as its main objective the study of the thermodynamics and structure of plasmas; equilibrium and time dependent. We used both rigorous analysis and approximation schemes.

In addition we started a new program involving both theoretical analyses and computer simulations on interacting quantum systems. Our first publication in this field will appear in the Rapid Communication section of Physical Review in February 1987. We have also made progress on the statistical mechanics of the Zakharov model which describes the interaction of an electromagnetic wave with a plasma. The model leads to a nonlinear set of partial differential equations which resemble in some ways equations arising in nonlinear field theories which have been studied by statistical mechanical methods. We have obtained some very exact results for this model in one dimension and are now carrying out some computer simulations on it.

The general nature of the dynamics describe a quantum system in interaction with a heat reservoir is also being investigated in some simple model system. We are currently writing up a report on this work.

1. Correlation Functions for Nematic Liquid Crystals

   (Joel L. Lebowitz and John W. Perram)

   We show that the correlation functions of a system of hard ellipsoids whose axes are constrained to be parallel are simply related to the corresponding functions of a hard sphere fluid with the same packing fraction. The existence of simple, accurate approximations for the latter system make the oriented ellipsoid fluid a suitable "reference system" for the nematically ordered phase of liquid crystals [1-3] and other orientationally ordered molecular fluids such as polar fluids in an external field. The properties of such fluids, with a given angular distribution $f(\underset{\sim}{\omega})$, may then be obtained via "standard" perturbation theory. Methods for obtaining $f(\underset{\sim}{\omega})$ near the perfectly ordered state are discussed.

   (Jour. Molec. Phys., 50, 6, 1207, 1983)

2. One-Dimensional Models of Anisotropic Fluids

   (Joel L. Lebowitz and Jerome K. Percus)

   Equilibrium properties of fluids of approximately spherical molecules can be adequately described over a wide range of temperatures and densities by the classical statistical mechanics of point particles interacting via spherical pair potentials. The situation is less satisfactory for highly nonspherical molecular fluids. It is the aim of this paper to seek some such comparison test by considering a situation in which the fluid is confined to a very narrow channel.

3. Sphericalization of Nonspherical Interactions

    (Joel L. Lebowitz and Jerome K. Percus)

    A density and temperature-independent spherically symmetric reference potential is constructed for an interacting classical fluid of nonspherical molecules. It annuls the first order correction to the free energy and, in special cases, the second as well. The potential is a limiting form of that used successfully for N_2 by Shaw et al., and reproduces numerically the Y_4 approximation of Barboy and Gelbart for homonuclear dumbell molecules.

    (J. Chem. Phys., 79(1), 1983)

4. Equivalent Potentials for Equations of State for Fluids of Nonspherical Molecules

    (G. O. Williams, J. L. Lebowitz and J. K. Percus)

    We analyze the extent to which the equation of state and other thermodynamic properties of systems of hard nonspherical molecules can be obtained from a density independent hard sphere reference system. We conclude that the median and Barker-Henderson prescriptions effectively reproduce all data now available. We discuss the motivation for these two formulations in detail.

    (J. Chem. Phys. 81(4), 1984)

5. Thermodynamics of Homonuclear Diatomic Fluids from the Angular Median Potential

    (David MacGowan, Eduardo M. Waisman, Joel L. Lebowitz and Jerome K. Percus)

    The use of the angular median potential as a temperature-independent spherical reference system for approximating molecular fluids is tested for its predictions of thermodynamics. Calculations have been carried out for a wide range of homonuclear diatomics with continuous atom-atom potentials believed to be representative of the full range of simulation data available for such systems. The results for the pressure are surprisingly good both in the detonation regime and around the triple point. In the latter case, however, the internal energies for highly elongated molecules with attractive potential wells are considerably too positive. Comparison with other perturbation theories indicates that the median reference system gives better pressures but poorer energies than RAM, and that in many cases, especially for purely repulsive potentials, it gives results of comparable accuracy to those obtained with nonspherical reference systems.

    (J. Chem. Phys. 80(6), 1984)

6.   The Two-Dimensional One-Component Plasma in an Inhomogeneous
     Background: Exact Results

     (A. Alastuey and J. L. Lebowitz)

         We study the general inhomogeneous two-dimensional jellium

where the background density varies in one space direction only.   At

 = 2, explicit functional representations of the one- and two-body

densities of the particles are derived in terms of the electrostatic

potential created by the background.   The present model can be used

for describing a large variety of charged interfaces.

(J. Physique 45, 1859, December 1984)

7.   Low-Frequency Electric Microfield Distributions in Plasmas

     (Carlos A. Iglesias, Hugh E. DeWitt, Joel L. Lebowitz,
      David MacGowan and William B. Hubbard)

         We evaluate the low-frequency component electric micro-

field distribution at a charged point, i.e., the field distribu-

tion due to ions, possibly of different species, which interact

through an electron-screened potential.   The method employed

is an adaptation of the adjustable-parameter exponential (APEX)

approximation previously developed for the high-frequency

component and involves a noninteracting-quasiparticle representa-

tion of the electron-screened ions designed to yield the correct

second moment of the microfield distribution.   The APEX results

are compared to Monte Carlo simulations, and we find good agree-

ment.

(Phys. Rev. A, 31, 3, March 1985)

8. **Long-Wavelength Oscillations in an Inhomogeneous One-Component Plasma**

   (Joel L. Lebowitz and Ph. A. Martin)

The perfect screening of charge fluctuations in an equilibrium plasma is extended to the time-displaced structure function of a general inhomogeneous one-component plasma. We find that the long-wavelength modes oscillate undamped with a single frequency $\bar{\omega}, \bar{\omega}^2$ being an angular average of squares of plasma frequencies $\omega_p^2 = 4\pi e^2 p/m$ in uniform systems with density p. Our results are derived rigorously from the Bogoliubov-Born-Green-Kirkwood-Yvon hierarchy under some reasonable assumptions on the spatial decay of correlations and contain as special cases previously obtained results of this kind.

(Phys. Rev. Letts., <u>54</u>, 14, 8 April 1985)

9. **The Ideally Polarizable Interface: Integral Equations**

   (M. L. Rosinberg, L. Blum and J. L. Lebowitz)

The integral equations used in the microscopic theory of the electric double layer were extended to the case of an impermeable interfacr separating two conducting media (ionic solutions or plasma). This system is a model for an ideally polarizable interface. Exact relations are given for the contact values of the one particle density function, and also for the pair correlation functions. We solve numerically the Poisson-Boltzmann (PB), the hypernetted chain (HNC), and mean spherical (MSA) approximations, and compare the results to the exact solution of the one component plasma in two dimensions.

(J. Chem. Phys. <u>83(2)</u>, 15 July 1985)

10. Time-Dependent Correlations in an Inhomogeneous One-Component Plasma

(B. Jancovici, J. L. Lebowitz and Ph. A. Martin)

Sum rules describing perfect screening at equilibrium in a classical plasma were extended to the time displaced structure function of an inhomogeneous one-component plasma. We found that there are long-wavelength modes which oscillate undamped with a single frequency $\bar{\omega}\,\bar{\omega}^{-2}$ being an angular average of the squared plasma frequency at infinity. Our results were derived heuristically, allowing also for quantum effects, from linear response theory, and rigorously from the classical BBGKY hierarchy under some reasonable assumptions on the spatial decay of correlations. Special cases were investigated, in particular plasmas bounded by walls of varied shapes.

The sum rules express the macroscopic property of screening which is possessed by Coulomb fluids. They can be derived by using linear response theory and assuming that an external charge introduced in the fluid induces a polarization charge which cancels the external one. More rigorous derivations using the BGY hierarchy can be given under suitable clustering assumptions.

In the present work, we derive a dynamical and quantum-mechanical generalization of sum rules, for inhomogeneous one-component plasmas (OCP). The restriction to OCP's (i.e. to systems of identical particles of charge e and mass m in a fixed background of opposite charge) has to be made because we

use a unique property of these systems: the long-wavelength plasma oscillations are not damped. From a microscopic point of view, this is related to the validity of a dipole sum rule. We can however deal with a large class of inhomogeneous OCP's: we allow the background density $\rho_b(q)$, a function of the position q, to have a value at infinity which may depend upon the direction Ω in which q recedes to infinity. More precisely, $\lim_{r\to\infty} \rho_b(r,\Omega) = \rho_\infty(\Omega)$ exists (for almost every Ω), with $q = (r,\Omega)$, $r = |q|$, $\Omega =$ angles of q. This allows in particular for OCP plasmas bounded by walls of varied shapes.

Defining the usual dynamical structure factor $S(q_1, t | q)$ as the correlation function between the charge density at time t and point q_1 and the charge density at time 0 and point q, we find the proper dynamical and quantum-mechanical generalization which

reduces to the classical limit, and to the quantum-mechanical static limit; the $\overline{\omega}^2$ appearing in these equations is an angular average of the plasma frequency (squared) $\omega_p^2(\Omega)$ at infinity.

Note that a system of real atoms and molecules in which the nuclei are treated as <u>fixed</u> is included in our scheme – provided that they are confined to a bounded region of space. This region is then imagined surrounded by a more smeared out background $\rho_b(r,\Omega)$ which has the limit $\rho_\infty(\Omega)$ as $r \to \infty$.

11. A Solvable Model for Localized Adsorption in a Coulomb System

(M. L. Rosinberg, J. L. Lebowitz and L. Blum)

A model for an interface with localized adsorption is
presented, in which the surface has a distribution of sticky
adhesive sites in contact with a Coulomb fluid. Contrary to the
current literature on the electrical double layer the surface
charge is in dynamic equilibrium with the bulk fluid. The sum-
rules obeyed by the one-and two-body correlation functions are
investigated. Explicit results are obtained for a solvable model,
the two dimensional one-component plasma at reduced temperature 2.
The effect of the granularity of the adsorbed charge on the ad-
sorption isotherm is discussed.

When a solid material such as an electrode plate or a colloid
particle is in contact with an electrolyte solution or a plasma, it
can acquire an electrical charge by specific adsorption of ions.
This adsorbed surface charge modifies the distribution of the ions

and the molecules in the vicinity of the surface and induces a sur-
face potential. In the case of chemisorbed systems (or strong
physisorption) the adsorbed ions are localized on adsorption sites
with a distribution which reflects in some way the structure of the
adsorbent, as for instance a periodic lattice. It is not an easy
task to include this surface charge which is in dynamic equilibrium
with the electrolyte in a statistical mechanical treatment of the
interface. For this reason, in almost all works devoted to the
study of Coulomb systems near a wall, the surface charge is a pre-
scribed "external" charge, uniformly distributed on the wall.
In particular, the adsorbed charges cannot "react" to the bulk
system.

In our work we found an exact solution to a two dimensional model of the true adsorption problem. The Coulomb fluid is the classical one-component plasma (OCP) at the special temperature T for which the coupling constant $\Gamma = \beta e^2 = 2$, $\beta = (K_B T)^{-1}$, and the specific (short range) adsorption potential is the sticky potential of Baxter.

The one component plasma is the simplest model of a Coulomb fluid and recently various physically interesting inhomogeneous situations have been worked out exactly in two dimensions for $\Gamma = 2$. They are restricted, however, to the case where the background density or the external potential varies only in one direction.

We shall consider here the following three situations : i) a semi-infinite plasma in the vicinity of an impenetrable wall (i.e., a line) with continuous adsorption ; ii) an infinite plasma in the vicinity of discrete adsorption sites regularly spaced on a line ; iii) a semi-infinite plasma in the vicinity of an impenetrable wall with discrete adsorption.

While i) is a simple extension of the results obtained in (3,4,5), ii) and iii) are real two dimensional problems and the structure of the fluid (for instance, the one- and two-body distribution functions) will vary both in the directions perpendicular and parallel to the line of sites.

The method that we use for solving this problem involves infinite expansions in terms of the n-body correlation functions of the unperturbed fluid (i.e. without adsorption sites). While this solution is valid for any fluid subject to an external one-body potential of Baxter's type, this is so, however, only in a formal sense since the n-body correlation functions are generally unknown quantities. The two-dimensional OCP at $\Gamma = 2$ is a rare exception : the gaussian structure of the correlation functions (4,11) makes the infinite expansions summable.

12. Monte Carlo Simulation of Hard Spheroids

   (J. W. Perram, M. S. Wertheim, J. L. Lebowitz and G. O. Williams)

   We present Monte Carlo simulations of the equation of state and radial distribution function for a model fluid composed of hard spheroids.

   (Chem. Phys. Letts., 105, 3, 1984)

13. Exact Results for the Two-Dimensional Two-Component Plasma

   (D. Nicolaides)

   The free energy and correlation functions of a two-dimensional two-component plasma are explicitly computed at the special temperature $T_o = e^2/2k_B$.

   (Phys. Letts., 103A, 1, 1984)

14. Exact Results for the Two-Dimensional One-Component Plasma

   (D. Nicolaides)

   We show that the free energy and correlation functions of the 2D OCP at the special temperature $T_o = e^2/2k_B$ can be explicitly computed by solving a free-field Dirac equation.

   (Phys. Letts., 103A, 5, 1984)

15. Fluids with Highly Directional Attractive Forces.   I.
    Statistical Thermodynamics

    (M. S. Wertheim)

A new formulation of statistical thermodynamics is
derived for classical fluids of molecules that tend to
associate into dimers and possibly higher s-mers due to
highly directional attraction. A breakup of the pair
potential into repulsive and highly directionally
attractive parts is introduced into the expansion of
the logarithm of the grand partition function in
fugacity graphs. The bonding by the directional attraction
is used to classify the graphs and to introduce a topo-
logical reduction which results in the replacement of the
fugacity by two variables: singlet density ρ and monomer
density ρ_0. Results for the thermodynamic functions as
functionals of ρ and ρ_0 are given in the form of graph
sums. Pair correlations are analyzed in terms of a new
matrix analog of the direct correlation function. It is
shown that the low density limit is treated exactly,
while major difficulties arise when the Mayer expansion,
which employs only ρ, is used. The intricate resummations
required for the Mayer expansion are illustrated for the
case where dimers are the only association products.
(Jour. Stat. Phys., <u>35</u>, 19, 1984)

16. Fluids with Highly Directional Attractive Forces. II.
Thermodynamic Perturbation Theory and Integral Equations

(M. S. Wertheim)

The formalism of statistical thermodynamics developed
in the preceding paper is used as a basis for deriving
tractable approximations. The system treated is one where
repulsion and highly directional attraction due to a single
molecular site combine to allow the formation of dimers,
but no higher s-mers. We derive thermodynamic perturbation
theory, using the system interacting with only the repulsive
potential as a reference system. Two distinct integral
equations for the pair correlation are derived. The first
one treats both parts of the interaction approximately;
the other one employs the repulsive reference system used
in perturbation theory. We show that each of these integral
equations permits the calculation of an important thermo-
dynamic function directly from the solution at a single
state of density and temperature. In the first case this
applies to a pressure consistent with the compressibility
relation, in the second to the excess Helmholtz free
energy over the reference system.

(Jour. Stat. Phys., 35, 35, 1984)

17. Sum Rules for Inhomogeneous Coulomb Fluids, and Ideal Conductor Boundary Conditions

(B. Jancovici)

The charge correlation function of an inhomogeneous fluid was shown to obey a sum rule involving electrical multipole moments of arbitrary order; this sum rule is a further generalization of the Stillinger-Lovett second-moment condition. An application is given for a fluid bounded by an ideal conductor wall; it is shown how the chemical potentials control both the bulk and surface properties.

(Submitted to J. Phys., France)

18. The Dipole Phase in the Two-Dimensional Hierarchical Coulomb Gas: Analyticity and Correlations Decay

(G. Benfatto, G. Gallavotti and F. Nicolo)

We illustrate the mechanism producing the dipole phase in a two dimensional Coulomb system by a detailed analysis of a hierarchical model. We prove the analyticity of the pressure and of the correlations for $\alpha^2 \equiv \beta e^2 > 8\pi$ (i.e. right above the usually conjectured value for the Kosterlitz-Thouless phase transition). We find also a power law decay for the correlations with exponent $\alpha^2/2\pi$ as the hierarchical distance goes to infinity.

(Commun. Math. Phys. 106, 277, 1986)

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