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FINAL TECHNICAL REPORT

Summary of Research

Our aim has been that of understanding from first principles the behavior of two-phase interfaces in the absence of gravitational constraints. This is fundamental to our ability to deal with the fluid structures that abound in the real biological, chemical, and physical world.

Since the state of thermal equilibrium is basic to all effective descriptions of the dynamical processes involved, its study heavily colored our initial investigations, culminating with the publication (1) of a detailed analysis of the mean-field hydrodynamic limit of matter, a low resolution caricature of such systems. This was accompanied by more refined treatments (2) in which the inherent interfacial thermal fluctuations that are crucial e.g. to the timing of coalescence processes, were included. The full set of considerations was subsumed under the aegis of the heavily studied density functional theory, but in a framework, that of expanded density functionals (3), in which one is able to focus at will on microscopic, mesoscopic, or macroscopic elements of the structure.

A substantial effort was mounted to determine how familiar hydrodynamic concepts have to be modified and interpreted to make them appropriate to the multi-level structure alluded to above. This was primarily in the context of the microscopic symmetric pressure tensor, which was, for the first time (4), expressed in the invaluable density functional format, and the used (5) to follow the predictions of popular microscopic models of the energetics of interfacial systems. In the course of these investigations, the previous murky relation between pressure tensor and thermodynamics was completely clarified (6).

The process of extending thermodynamic information to intrfacial dynamics was initiated along two paths. One (7) was from the viewpoint of an inertialess lattice gas, resulting in the surprising conclusion that at this level, all transport is governed by precisely the thermodynamic free energy, albeit with a non-trivial effective particle mobility. The other aimed at understanding the fashion in which slow macroscopic motions, accounted for by a time-varying microscopic energy, generate effective hydrodynamic parameters. By examining a solvable model system, it was found (8) that all current procedures for doing so are deficient, and suitable alleviation suggested.

The major effect of this project was to set the stage for the analysis of the substantial dynamical regimes in which extensive equilibrium information provides the dominant background. This produces a smooth junction to the models of Araki and Munakata, Giacomin and Lebowitz, and Oxtoby. It is also crucial to our understanding of the complex interfacial equilibrium configurations required for intermediate stages of two-phase separation, for which the "phase-field" techniques we have been developing are uniquely effective. And it puts us within striking range of the physical experiments that can provide incisive tests of the theoretical framework.

(1) Non-uniform van der Waals Theory, J Stat Phys 78, 1337 (1995)
(with M Kiesling)
(2) The Structure of Density Functionals, J Phys Cond Matt 6, A125 (1994)

Classical Liquid-gas Interface in Thermal Equilibrium, J Stat Phys 78, 1165 (1995)
(3) Density Functional Theory in the Classical Domain, Chap 5 in "Modern Density Functional Theory", ed J Seminaria, Elsevier (1996)
(4) The Stress Tensor for Non-local Field Equations, J Math Phys 37, 1259 (1996)
(5) Stress Tensor of Liquid-vapor States of Inhomogeneous Fluids, Phys Rev E53, 5130 (1996) (with V Romero-Rochin)
(6) Generalized Compresibility Equation, Phys Rev e 48, 1819 (1993) (with LA Pozhar and KE Gubbins)
Local Thermodynamics of Inhomogeneous Fluids at Equilibrium, Phys Rev E51, 261 (1995) (with LA Pozhar and KE Gubbins)
(7) Phase Separation with Conserved Order Parameter, submitted (G Giacomin and JL Lebowitz)
(8) Adiabatic Properties of Distributions, Phys Rev E53, 80 (1996) (with LJ Samaj)