Workshop of Mathematical Analysis, Modeling, and Computations on Liquid Crystals and Related Topics

August 8--9, 2015
Beijing Normal University, Beijing

*Sponsor*
- Beijing Normal University
- Peking University
- The Joint Math Institute of NYU/Shanghai

*Organizers*
- Fanghua Lin : Courant Institute of Mathematical Sciences, New York University/New York University, Shanghai
- Pingwen Zhang : Peking University
- Chun Liu : Penn State University
- Changyou Wang : Purdue University
- Hui Zhang : Beijing Normal University
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<td>Onsager principle as a tool of approximation</td>
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<td>Masao Doi; Peter Palffy-Muhoray</td>
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<td>‘Hard’ density functional theory for nematic liquid crystals</td>
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<td>New results from a different perspective on the Poisson-Boltzmann equation</td>
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<td>Fanghua Lin</td>
<td>Recent developments in analysis of complex fluids</td>
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<td>Pingwen Zhang</td>
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<td>Wormlike-chain model and theory of liquid-crystal polymers</td>
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<td>Jeff Z. Y. Chen</td>
<td>Zhong-can Ou-yang</td>
<td>Overview of the study of complex shapes of fluid membranes, the Helfrich variation model and new applications</td>
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Onsager Principle as a Tool of Approximation

Masao Doi

Center of Soft Matter Physics and its Applications, Beihang University, Beijing, China

In the celebrated paper on the reciprocal relation for the kinetic coefficients in irreversible processes, Onsager extended Rayleigh's principle of the least energy dissipation to general irreversible processes. The principle has been shown to be useful in deriving basic equations which describe non-linear and non-equilibrium phenomena in soft matter[1,2,3]. Here I want to show that the principle is useful in getting an approximation solution. Examples are selected from the problems of diffusion[4], gel dynamics[4], droplet motion on substrates[5] and meniscus rise between flexible walls.

REFERENCES
5. Xiamnin Xu, Yana Di and Masao Doi, in preparation.
‘Hard’ density functional theory for nematic liquid crystals

Peter Palffy-Muhoray

Liquid Crystal Institute, Kent State University

Xiaoyu Zheng.
Dept. of Mathematical Sciences, Kent State University

Interparticle interactions in condensed matter can be regarded to consist of long range attractive forces originating in London dispersion, and short range repulsive forces originating in Pauli exclusion. Although particles with short range interactions are usually modelled as impenetrable rigid solid bodies, density functional theories typically allow configurations with arbitrarily high particle densities. In our ‘hard’ density functional formalism, to be presented here, the free energy expression contains a logarithm whose argument vanishes for certain configurations; arbitrarily high densities and certain configurations are therefore strictly disallowed. We present the model, discuss the implications of the ‘hard’ aspect, and provide results from numerical calculations. Discontinuities of the derivatives of the orientational distribution function resulting from the hardness is of particular interest.
New results from a different perspective on the Poisson-Boltzmann equation

Maijia Liao¹, Li Wan¹, Shixin Xu², Chun Liu³, and Ping Sheng¹

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³Department of Mathematics, Pennsylvania State University, University Park, Pennsylvania 16802, USA

Electrokinetics is a phenomenon that results from charge separation at the fluid-solid interface, e.g., the silica-water interface. An electrical double layer is formed as the consequence of the charge separation. The mathematical treatment of the electrical double layer is traditionally handled by the Poisson-Boltzmann (PB) equation, with a zeta potential boundary condition set at the fluid-solid interface. Such a treatment effectively cut the electrical double layer into two parts: the Debye layer and the surface charge, with the Debye layer treated by the PB equation, and the surface charge layer serving as a passive neutralizing element. Such a treatment can give rise to problems when the fluid channel width is less than two Debye lengths. Also, it is common knowledge that the zeta potential can be affected by the salt concentration and acidity of the fluid, a fact which cannot be accurately accounted for by the traditional PB equation framework.

We propose a new perspective on the PB equation that is based on treating the electrical double layer as a synergistic whole. Our computational domain is overall electrically neutral, which contrasts with computational domain of the traditional PB equation, which is charged. A charge-conserving PB equation is derived from the Poisson-Nernst-Planck (PNP) equations. To achieve charge separation we introduce a surface potential trap that is charge neutral, with a height that is designed to capture the energy involved in the electrical charge separation process. A complete formulation of the problem involves the additional definition of a surface dissociation charge density and a global chemical potential derived from the condition of global charge neutrality.

We show that such a reformulation of the problem can yield quantitative, yet simple, accounts of experimentally observed phenomena such as the repulsive force between two approaching charged surfaces, the isoelectronic point, and the appearance of the Donnan potential in nanochannels.

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Octupolar Order Tensors

Epifanio G. Virga

Department of Mathematics, University of Pavia, Pavia, Italy

Unconventional liquid crystals, such as tetrahedratic nematics, require a more refined mathematical description of the molecular orientational order established in their condensed phases than can be possibly afforded by the classical quadrupolar tensor of the second moments of the probability density function. The first refinement that comes to mind appeals to the distribution of the probability third moments, which is described by a symmetric, completely traceless third-rank tensor. This lecture will describe the general representation of such tensors, in both two an three space dimensions, building upon an appropriate notion of generalized eigenvalues and eigenvectors.

Planar discontinuities for liquid crystals

John Ball

University of Oxford

The talk will discuss various situations in which it may be reasonable to allow the director to jump across surfaces, together with related issues concerning the description of defects and choice of function spaces in models of liquid crystals. This is joint work with Stephen Bedford.
Recent developments in analysis of complex fluids

Fanghua Lin

Courant Institute of Mathematical Sciences, New York University/
New York University, Shanghai

Some recent analytic results concerning complex fluid flows would be discussed in this talk. I shall be concentrated on the classical Oldroyd B-model of the incompressible viscoelastic fluids. The mathematical studies of this model are closely related to that for liquid crystals, incompressible magneto-hydrodynamic equations.... Even in the case of two dimensions, the basic mathematical problems are challenging, despite well-known theory that had been developed long ago for the classical incompressible fluid flows described by the Navier-Stokes equations, and that they have been open since the time these equations were posed. Here I shall discuss some of my recent joint works with Xianpeng Hu regarding local and global well posedness questions in 2D case. I shall also take this opportunity to discuss a few other results in both 2D and 3D cases.

Wormlike-chain model and theory of liquid-crystal polymers

Jeff Z. Y. Chen

Department of Physics and Astronomy
University of Waterloo
Waterloo, Ontario, Canada N2L3G1

In this talk, we review the progress in understanding directionally and spatially coupled structures of liquid-crystal polymers, on the basis of the self-consistent field theory of wormlike chains. A comparison between this formalism and other theoretical tools is made. Nematic defect structures predicted from the theory is discussed, along with open questions that need to be further addressed.
Overview of the study of complex shapes of fluid membranes, the 
Helfrich variation model and new applications

Zhong-can Ou-Yang

Institute of Theoretical Physics, Chinese Academy of Sciences, Beijing 100190, 
China

Shape problems stemmed from real bio- and abiotic materials in nature initial many nice theories in sciences. The observation of law of constant angle of crystal planes by N. Stensen (1669) leads to G. Wulff (1901) construction for convex crystal shape. The beautiful shapes of soap films observed by J. Plateau (1803) emerges a “golden age” in the study of minimal surface. The investigation on the rise of a liquid in a capillary tube generates T. Young (1805) and P.S. Laplace (1806) theory on a surface of constant mean curvature which predicts liquid bubble to be sphere only (Alexandrov (1950’s)). However, a long-standing problem in physiology, why the red blood cells (RBCs) in human bodies are always in a rotationally symmetric and biconcave shape, has puzzled peoples for more than 100 years. It is finally solved by W. Helfrich (1973) who recognized membrane being a liquid crystal (LC) film and derived from curvature elastic theory of LC a free energy of fluid membranes (FM). The variation with the energy leads a generalized Young-Laplac shape equation (Ou-Yang and Helfrich, 1987). J.C.C. Nitsche (1993) regarded Helfrich FM theory as the renewal of the Poisson’s elastic shell theory in his encyclopedic book on minimal surface. In this talk some progress of our study following Helfrich variation model for 25 years are reported. We found that the Helfrich FM theory predicts not only the exact solution for RCB shape but also a special kind of torus vesicle which have soon afterwards confirmed by experimental observations. Especially, the Helfrich variation model was successfully extended to investigate the complex structures in other soft matters such as the formation of focal conic domains in smectic LC, helical carbon nanotubes, the tube to sphere transition in peptide nanostructures, and Icosahedral self-assemblies in virus capsids.
The Interface and Defects of Liquid Crystals

Pingwen Zhang

School of Mathematical Sciences
Peking University
Beijing, 100871

The interface and defects in liquid crystals are of great practical importance and theoretical interest. The spectral methods can be used to capture the global pattern and local profile of defects. We try to establish the connections between microscopic and macroscopic theories of liquid crystals including the interface and defects.