Statistical Mechanics Lectures

Telluride School on Theoretical Chemistry 2013

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My statistical mechanics lectures will present a selection of modern perspectives on the emergent structure and dynamics of complex systems comprising many, many atoms and molecules. As an organizing context I will focus on classical physics of the liquid state, a subject that has inspired mathematical and computational developments which now find myriad applications in chemistry, biology, materials science, and beyond.

The first lecture will review foundational material, establishing a contemporary view on the basics of statistical mechanics as well as a common language and notation for the remaining discussions. It will draw from Chapters 1-4 of David Chandler's Introduction to Modern Statistical Mechanics, adding some rudimentary concepts from the theory of large deviations. It will conclude with an analysis of classical harmonic oscillators and the general structure of linear response they reveal.

The second and third lectures will explore collective fluctuations in liquids that exhibit linear response to a surprising degree -- in effect, the normal modes of the liquid state. These include microscopic density fluctuations as well as polarization fluctuations conventionally described in the context of dielectric continuum theory. Time permitting, I will describe similar approaches to analyzing shape fluctuations of interfaces and membranes, as well as the elastic response of long chain molecules.

The fourth lecture will concern phase transitions, with an emphasis on phenomenology, tools of mean field theory, and the Landau-Ginzburg approach to constructing appropriate continuum descriptions.

The fifth lecture will explore the time dependence of equilibrium fluctuations and their connection with nonequilibrium response. We will consider both the regime of linear response and perspectives on far-from-equilibrium behavior inspired by modern fluctuation theorems.

The final lecture will discuss techniques of computer simulation. I will sketch the operating rules of molecular dynamics as well as Monte Carlo simulations, focusing on their physical underpinnings and the responsible use of advanced sampling methods.