

Samuela Pasquali's Research Activity

Scientific Interests

My research activity has developed in the field of statistical physics applied to biological systems, in particular on theoretical approach to polymer folding and solvent representation. My interests have focused on various aspects of the folding problem, bringing me to work on protein folding, RNA folding, on statistical mechanical aspects of folding of confined homopolymers, and, more recently, on the role played by the solvent on the folding process.

One of the areas I have been particularly interested in is the topological aspect of the possible folds and on how topology influences the folding ability of the molecule. I developed a perturbative approach for systematically organizing long-range interactions along the chain. Understanding the hierarchy of long-range interactions is key to the understanding of the fold and the folding process of the molecule. Interestingly the first order of this perturbation generates the topologies of simple RNAs, i.e. RNAs without pseudoknots. This work was developed in the context of homopolymers both in order to understand what are the general features of such perturbative approach and because it is more accessible mathematically, but a similar investigation for heteropolymers is what will start bridging pure statistical mechanics and real biological molecules, since now sequence would also be taken into account.

I have also been involved in studies more specifically directed to either proteins or RNA. In the field of proteins I have worked with lattice models addressing the question of folding and misfolding, a very up to date problem given the variety of diseases that crucially depend on the misfolding of a single protein, like Alzheimer and mad cow disease. Regarding RNA, my focus has been on the relation between sequence and structure of ribozymes. For most RNAs, tertiary structure is just a spatial organization of secondary structure, and there is experimental evidence that secondary structure formation and tertiary structure formation are separate transitions. This allows us to center our attention on RNA secondary structures where the concept of topology of the molecule is well defined.

At the moment my work is focused on fluctuation-induced interactions (dispersion forces), with a particular interest in systems where a high dielectric contrast is present. In collaboration with the "*Max Planck Institute for complex systems*" in Dresden and with the "*École Normale Supérieure*" in Lyon, I have been developing both theoretical and numerical methods to study these interactions at finite temperature, using the tools of statistical mechanics.

Current activities

As main project of my Postdoc at the "*Laboratoire de physico-chimie théorique*" of the "*École Supérieure de Physique et de Chimie Industrielles de la Ville de Paris (ES-*

PCI”, under the supervision of Anthony C. Maggs (directeur de recherche CNRS), I work at the development of efficient calculations of long range dipolar forces and of electrostatic forces in biological systems.

For highly polarizable materials, like water, static Van der Waals forces, or thermal Casimir forces, become significant and can play an important role in biological processes such as folding and membranes interaction. Starting from a purely classical partition function, expressed in terms of the displacement field D , we analyze the interactions between finite macroscopic objects of arbitrary shape due to their different dielectric properties. Using a path integral quantization, this approach is then extended to quantum interactions as well, both in the non-retarded (near-field) and in the retarded regimes. We have developed an on-lattice theory and two separate numerical methods based on it. These methods are both efficient and generalizable to systems which are well beyond those which can be studied with the standard methods commonly used in the context of the Casimir effect.

We have recently started a collaboration with the group of “*Microfluidics, MEMS and Nanostructures*” at ESPCI to apply our numerical methods to the study of the interactions of oil droplets in microchanells.

In collaboration with professor J.K. Percus at New York University, I continue working on the subject of confined homopolymer. We have developed a variational formulation that allows us to consider to more realistic systems. Using a saddle point approximation and a variational principle, we can find mean field density profiles for the equilibrium configuration taken by the polymer as a function of confinement and long-range interactions.

Motivated by the current interest on random RNA, in collaboration with F. Krzakala at ESPCI, I study the ability of secondary structures to distinguish between “natural” RNAs and random RNAs. Using the concept of graph topology, we have developed an algorithm combining secondary structure folding and graph analysis to gather a better understanding on the specificity of naturally selected RNA.