SWEDISH—UKRAINIAN SEMINAR
in THEORETICAL PHYSICS

April 2, 2024

Program*

10.00–10.05 – Opening

10.05–10.45 – **Anders Irbäck** (Computational Biology and Biological Physics, Lund University, Sweden) **"Folding and design of lattice proteins using quantum annealing"**

10.45–11.25 – **Taras Patsahan** (Institute of Condensed Matter Physics, NAS of Ukraine, Lviv, Ukraine) **"Soft-core colloidal particles with competing interactions near confining surfaces: computer simulations and field theory approach"**

11.25–11.40 – Coffee break

11.40–12.20 – **Ralf Eichhorn** (AlbaNova University Center Nordita, Sweden) **"How thermodynamics becomes stochastic — a short exploration of recent advances in statistical physics"**

12.20–13.00 – **Elmar Petrov** (Bogolyubov Institute For Theoretical Physics, NAS of Ukraine, Kyiv, Ukraine) **"Barrier and superexchange models for the analysis of tunneling current through a molecular wire"**

***EE Time, CE Time is one hour earlier**

Folding and design of lattice proteins using quantum annealing

Anders Irbäck

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Quantum annealing is a promising approach for obtaining good approximate solutions to difficult optimization problems. Protein folding and design represent such problems. For testing new methods for these tasks, the minimal lattice-based hydrophobic/polar (HP) model is well suited, as it is challenging despite its simplicity. In this talk, I first describe a scalable mapping of the lattice protein folding problem onto a suitable binary spin representation for quantum annealing. I then present results obtained with this mapping on a D-Wave Advantage system. Using the hybrid quantum-classical solver offered by D-Wave, it was possible to fold and design HP proteins with up to 64 amino acids, with 100% success rate. When relying only on the quantum processing unit (QPU), the results were less impressive. The longest HP protein successfully folded with this approach had 14 amino acids. To shed light on the pure QPU results, we investigated the effects of control errors caused by an imperfect implementation of the intended Hamiltonian on the QPU, by numerically analyzing the Schrödinger equation. We found that the simulated success rates in the presence of control noise semi-quantitatively reproduce the modest pure QPU results for larger chains.

Soft-core colloidal particles with competing interactions near confining surfaces: computer simulations and field theory approach

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Models of colloids with competing interactions, which are characterized by short-range attraction and long-range repulsion (the so-called SALR pair potential) [1], have been the focus of extensive research due to their ability to describe spontaneous emergence in a homogeneous fluid of mesostructured phases of different morphologies [2]. A popular SALR model is that of a two-Yukawa hard sphere fluid. Such a potential provides a reasonable description of dispersions of charged colloidal particles in the presence of a depletant, and it is possible to tune its interaction parameters by varying physical conditions [3]. In contrast, in this work we propose to study colloids interacting with a three-Yukawa potential (3Y model) of the SALR form. Such a model with a soft core takes into account the possibility of partial overlap between two particles. Examples of respective systems include, but are not limited to, protein molecules, soft colloids, polymer grafted nanoparticles, star and branched polymers, microgels. A soft-core potential also has the advantage of making it possible to perform analytical calculations.

We report a study of the 3Y SALR model for soft-core colloids in the bulk and near a confining flat surface using both simulation and theoretical approaches. Using computer simulations, we have examined the system under consideration in a wide range of density and temperature values. We show that at low temperatures various well-known mesostructures, such as lamellar and gyroidal phases, hexagonally packed cylindrical phases, cubically ordered and disordered clusters are formed. In the case of the system near confining surfaces or between two walls, the self-assembly effects become more pronounced and may be observed at temperatures that are noticeably higher than in the bulk.

To describe structural properties of a 3Y SALR colloids at high temperatures, a classical field theory [4-6] is employed. Explicit analytical expressions for the pair correlation function and the density profile are derived. These expressions contain only parameters of the pair potential and the thermodynamic state, thus providing a link between microscopic parameters of the system and respective measurable quantities. Thermodynamic conditions for the applicability of the theoretical approximations employed are discussed. The results found are tested against computer simulations data.

References

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[3] J.-M. Bomont, J.-L. Bretonnet, D. Costa, J.-P. Hansen, J. Chem. Phys., 137 (2021) 011101.
[4] I. Kravtsiv, T. Patsahan, M. Holovko and D. Di Caprio. J. Chem. Phys., 142 (2015) 194708.
[5] D. di Caprio, I. Kravtsiv, T. Patsahan, M. Holovko, Mol. Phys., 114 (2016) 2500.
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How thermodynamics becomes stochastic — a short exploration of recent advances in statistical physics

Ralf Eichhorn

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Stochastic thermodynamics is a newly established discipline in statistical physics. It explores fundamental aspects of non-equilibrium processes by applying and extending concepts from equilibrium thermodynamics to the non-equilibrium realm, typically on the level of single particle trajectories. This approach provides an adequate framework for investigating the behaviour of ``small systems'' on mesoscopic scales for which thermal fluctuations may have a significant or even dominant effect on the overall system properties. We consider such small systems consisting of so-called Brownian particles (like colloids in suspension or biological macromolecules in a living cell). After introducing the standard model for Brownian motion, we briefly describe the ideas and concepts leading to a (trajectory-wise) thermodynamic characterization of Brownian motion, and finally elaborate on central results from stochastic thermodynamics. As a refinement of the second law of thermodynamics, the most famous amongst these results are probably the fluctuation theorems.

BARRIER AND SUPEREXCHANGE MODELS FOR THE ANALYSIS OF TUNNELING CURRENT THROUGH A MOLECULAR WIRE

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Abstract

A modified model of superexchange electron transfer is discussed, which can be used to elucidate the mechanism of formation of a non-resonant tunneling current through a molecular wire embedded between metal electrodes. It is shown how tunneling electron transfer can be controlled by shifting the energy levels of the terminal units of the molecular chain in relation to the position of the delocalized orbitals of the chain and the Fermi levels of the metal electrodes. Using the example of a molecular wire containing a bridged alkane chain, it is shown that the model leads to current-voltage characteristics that are in good agreement with the experimental results on the attenuation of the tunneling current in the chain depending on its length. In addition, conditions have been found under which the modified superexchange model leads to results following from the Simmons model of tunneling through a rectangular barrier or the McConnell model of deep superexchange tunneling.