CRETE CENTER FOR
QUANTUM COMPLEXITY
AND NANOTECHNOLOGY

ΣΕΜΙΝΑΡΙΟ ΚΕΝΤΡΟΥ ΚΒΑΝΤΙΚΗΣ ΠΟΛΥΠΛΟΚΟΤΗΤΑΣ & ΝΑΝΟΤΕΧΝΟΛΟΓΙΑΣ/
CCQCN SEMINAR

Tuesday, 12 November 2013

11:00-12:00

1st Floor Seminar Room

Counting entropy in molecular systems

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Abstract

In this work, we will present a statistical mechanical formulation that enables the evaluation of the free energy in molecular systems, in a "single" step, by "deleting" all the molecules in the system. The approach can be understood as the statistical mechanics analogue of evaluation of the potential energy in classical mechanics by accounting for the necessary work to transfer all particles one by one to infinite distance. As a result, the free energy of an atomistic system can now be expressed as an ensemble average over a sample of configurations that have been created via an impotence sampling algorithm (e.g. Molecular Dynamics or Monte Carlo). Moreover, the proposed method is capable of evaluating the free energy as a function of the density, from the simulated density down to zero. The relation of the proposed method to the Rosenbluth sampling will be discussed and we will provide the analogy to classical statistical mechanics theorems like the Bennett's and Crooks' theorems (Bennett, C. H. J. Comput. Phys. 1976, 22, 245; Crooks, G. E. Phys. Rev. E 1999, 60, 2721). When the proposed process is envisioned as the transformation of an interacting to a noninteracting system, the proposed scheme reduces to the Jarzynski identity linking the free energy of the system to the "chemical work" related to this transformation.

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