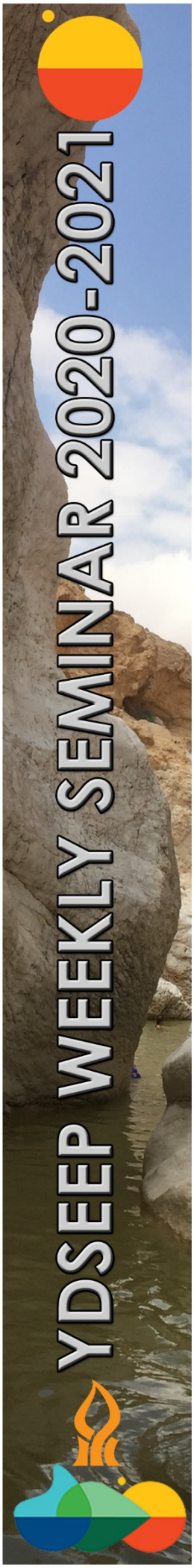

Ben-Gurion University of the Negev
Blaustein Institutes for Desert Research
The Swiss Institute for Dryland Environmental and Energy Research
Alexandre Yersin Department of Solar Energy and Environmental Physics

Title:

Inferring entropy from the structure of particulate systems

Haim Diamant

Chemistry Department, Tel Aviv University

Abstract:

The thermodynamic definition of entropy can be extended to nonequilibrium systems based on its relation to information. To apply this definition in practice requires access to the physical system's microstates, which may be prohibitively inefficient to sample or difficult to obtain experimentally.

It is beneficial, therefore, to relate the entropy to other integrated properties which are accessible out of equilibrium. One of the motivations is to identify subtle structural transitions through their entropy change. We focus on the structure factor, which describes the spatial correlations of density fluctuations and can be directly measured by scattering. The information gained by a given structure factor regarding an otherwise unknown system of particles provides an upper bound for the system's entropy. We find that the maximum-entropy model corresponds to an equilibrium system with an effective pair interaction. Approximate closed-form relations for the effective pair potential and the resulting entropy in terms of the structure factor are obtained.

We demonstrate the applicability of these relations in several examples. The entropy inferred from the structure factor is found to be consistent with other methods, superior for larger system sizes, and accurate in identifying global transitions. We discuss extensions to more complex particulate systems.

Date & Location:
Tuesday, November 30, 2021, at 11:00
Lecture Room – Physics building (entrance floor)