Joint CQSE and CASTS Seminar

Weekly Seminar
Mar. 31, 2017 (Friday)

TIME Mar. 31, 2017, 14:30 ~ 15:30
TITLE Two-dimensional melting: New algorithms, new insights
SPEAKER Prof. Werner Krauth
Statistical Physics Laboratory, Department of Physics, Ecole normale supérieure, Paris, France
PLACE Rm716, CCMS & New Physics Building, NTU

Abstract

The hard-disk model has exerted outstanding influence on computational physics and statistical mechanics. Decades ago, hard disks were the first system to be studied by Markov-chain Monte Carlo methods (1) and by molecular dynamics (2). It was in hard disks, through numerical simulations, that a two-dimensional melting transition was first seen to occur (3) even though such systems cannot develop long-range crystalline order. This provided the starting point for the Kosterlitz-Thouless theory (4). Analysis of the system was made difficult by the absence of adequate simulation methods. In recent years, we developed the powerful event-chain algorithm (5) which allowed us to prove (6) that hard disks melt with a first-order transition from the liquid to the hexatic and a continuous transition from the hexatic to the solid. We thus confirm the existence of a hexatic phase yet show that the classic KTHNY theory does not apply. Subsequent work for soft-sphere potentials yields a generic theory of two-dimensional melting (7).

The event-chain algorithm is a first example of a class of "Beyond-Metropolis" (8) methods that violate detailed balance, yet satisfy global balance (the Markov chains are irreversible). Equilibrium is reached as a steady state with non-vanishing probability flows. The widely used filter. The system energy is not computed, providing a fresh perspective for long-range interactions (9). Moves are infinitesimal and persistent, implementing the lifting concept (10). The resulting general class of fast algorithms overcomes the Markov-chain Monte Carlo algorithm's limitations of the detailed-balance condition and goes beyond hybrid Monte Carlo.

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