Tobias Kuna (Reading)

Density expansion of the truncated and the direct correlation function

Abstract
Particle systems interacting via translation invariant pair potentials are among the most intractable point processes if one is outside the high temperature low activity regime (HTLAR). In particular, the liquid regime is of paramount interest in chemistry and engineering, but the available theory is phenomenological. Chemists and physicists have derived a rather satisfactory description for the thermodynamics of simple liquids which works far outside the HTLAR exploiting correlation functions and postulation relations between them based on formal expansion in the density. However, it is also acknowledged that *"the manipulations involved in obtaining these infinite sums ... have been carried out in a purely formal way and we have not examined the important but difficult questions of convergence and the legitimacy of the rearrangement of terms"* even in HTLAR. Mathematically the difficulty is to find for a sum e^{n^2} terms (each of them an n-dimensional integral) a bound of order $e^{n \ln(n)}$. The required cancelations are based on combinatorial identities for families of graphs and have to hold exactly to make this estimation possible. This is joint work with Dimitrios Tsagkarogiannis.