Zeitschrift: Helvetica Physica Acta

Band: 62 (1989)

Heft: 6-7

Artikel: Simulation of the liquid-gas transition with finite size analysis

Autor: Rovere, M. / Binder, K. / Heermann, D.W.

DOI: https://doi.org/10.5169/seals-116089

SIMULATION OF THE LIQUID-GAS TRANSITION WITH FINITE SIZE ANALYSIS

M. Rovere, Dip. Fisica Teorica Trieste (Italy)
K. Binder , Institut für Physik Uni. Mainz FRG
D.W. Heermann, Institut für Physik Uni. Wuppertal

Abstract

We extend methods of finite size analysis to the simulation of the liquid-gas transition in a realistic model for a fluid. We show that it is possible to locate the coexistence curve and estimate the critical point.

1- Block analysis

We perform a M.C. simulation of the liquid-vapour transition in a 2D Lennard-Jones fluid. The simulation cell is divided in subsystems (blocks) of different sizes and we compute the density in each block. In this way we can obtain the distribution functions (D.F.) of the density for blocks of different size. Above the critical point the D.F. are gaussians centred at the total fixed density[1]. When we go down with the temperature, the D.F. evolve to a double peak structure (fig 1), which indicates the presence of two coexisting phases as can be seen in fig.2, where a configuration is represented at $T = 0.45$ below T_c.

2- The two phase region

By varying the external density, we move along an isotherm. The two peaks remain centred at the same densities, which correspond to the coexisting low and high density phases (fig. 3). In this way the coexistence curve can be drawn from the D.F. data taken at different temperatures below T_c.

From the D.F. we can evaluate the reduced fourth-order cumulant $U(L, \rho, T)$, which depends on the density ρ, the temperature and the size of the blocks L (fig.4). At the critical point U goes to an universal value, indipendent on the size, and one can estimate the values of the critical parameters[2].

References

[1] M.Rovere,D.W.Heermann and K.Binder *Europhys.Lett.* **6**,585(1988).

[2] M.Rovere,D.W.Heermann and K.Binder ,*in preparation.*

Fig. 1

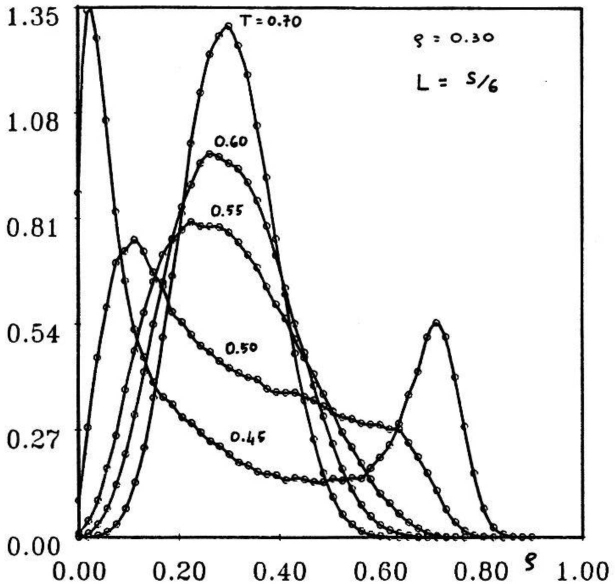

Fig. 2

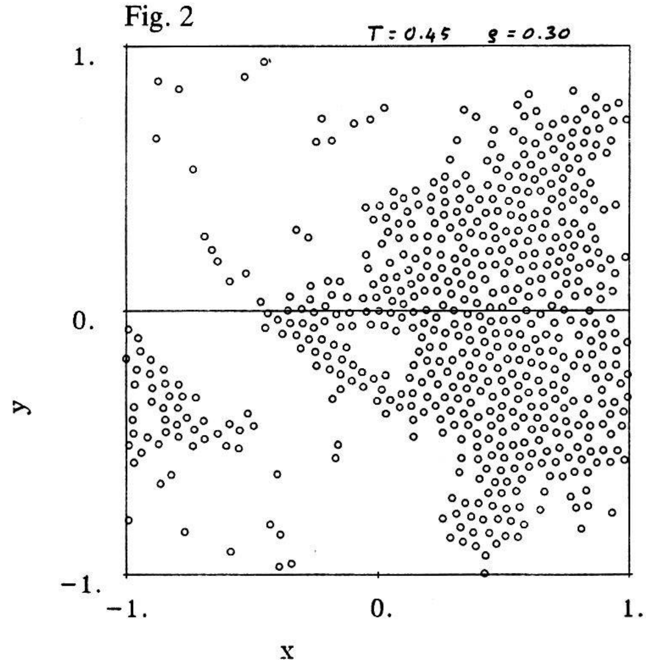

Fig. 3

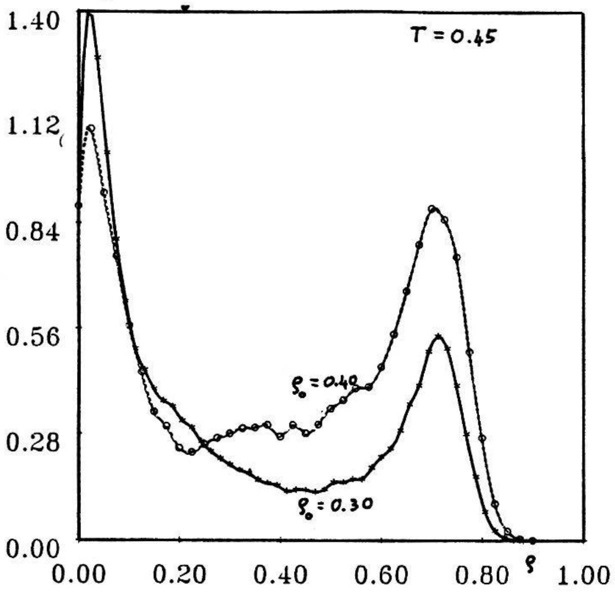

Fig. 4