MONTE CARLO FREE ENERGY ESTIMATES USING NON-BOLTZMANN SAMPLING: APPLICATION TO THE SUB-CRITICAL LENNARD-JONES FLUID

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Received 22 July 1974

The paper reports a Monte Carlo technique for estimation of the free energies of fluids by sampling on distributions designed for this purpose, rather than on the usual Boltzmann distribution. As an illustration of its use, the free energy of a Lennard-Jones fluid in the liquid-vapour coexistence region has been estimated by relating it to that of the inverse-twelve (soft sphere) fluid, which itself shows no condensation.