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Fine-Lattice Discretization for Fluid Simulations: Convergence of Critical Parameters. YOUNG C. KIM, MICHAEL E. FISHER, Inst. Phys. Sci. Tech., University of Maryland, MD 20742 — In simulating continuum fluids with long-range interactions, such as plasmas and electrolytes, that undergo phase separation and criticality, it is computationally advantageous to confine the particles to the sites of a lattice of fine spacing, a_0, relative to their size, a.[1,2] But, how does the discretization parameter, $\zeta \equiv a/a_0$ (typically,[1] ≥ 5) affect the values of the critical temperature and density, etc.? A heuristic argument,[2] essentially exact in $d = 1$ and 2 dimensions, shows that for models with hard-core potentials, both $T_c(\zeta)$ and $\rho_c(\zeta)$ converge to their continuum limits as $1/\zeta^{(d+1)/2}$ for $d \leq 3$ when $\zeta \to \infty$. However, the behavior of the error for $d \geq 2$ (related to a classical problem in number theory) is highly erratic. Exact results for $d = 1$ illuminate the issues and reveal that optimal choices for ζ can improve the rate of convergence by factors of $1/\zeta$.[2] For $d \geq 2$, the convergence of the *second virial coefficients* to their continuum values exhibit similar erratic behavior which transfers to T_c and ρ_c. This can be used in to enhance extrapolation to $\zeta \to \infty$. Data for the hard-core or *restricted primitive model* electrolyte have thereby been used to establish that (contrary to recent suggestions) the criticality is of Ising-type — as against classical, XY, etc.

1. Y. C. Kim and M. E. Fisher, Phys. Rev. Lett. **92**, 185703 (2004).
2. S. Moghaddam, Y. C. Kim and M. E. Fisher, J. Phys. Chem. B (2005) [in press].

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