455b Finite-Size Scaling Monte Carlo Simulations of Tricritical Behavior

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Knowledge of the coexistence curves of fluid models and the points (ordinary critical or higher-order multi-critical) at which two (or more) distinct phases become identical is a problem of considerable theoretical and practical interest. While implementation of finite-size scaling theories in Monte Carlo simulations has become a standard tool for ordinary critical points, considerable difficulties arise in the case of higher-order critical points. In this work, we develop and apply finite-size scaling techniques to investigate tricritical behavior. A tricritical point marks the end of a line of three-phase coexistence at which three coexisting phases simultaneously become identical. The exponents associated with the tricritical point are distinct from those of the critical point. For example, the borderline dimensionality is d=4 for ordinary critical points while for tricritical points is d=3. Tricritical points occur in multi-component fluid mixtures, metamagnets, superfluid-ordinary fluid mixtures (e.g., 3He-4He mixtures) and mixtures in which the phase behavior is determined by long-range electrostatic interactions. We have investigated the phase behavior of 1-1 electrolyte systems on simple cubic and body-centered cubic lattices by performing grand canonical Monte Carlo simulations aided with histogram reweighting and finite-size scaling techniques. In both cases we find coexistence between a disordered and an ordered phase. The structure of the ordered phase is reminiscent to that of NaCl and CsCl crystals respectively. At high temperatures the order-disorder transition is continuous but, as the temperature is lowered, the line of continuous transitions (the ƒÉ-line or Ne□Lel line) becomes discontinuous first-order coexistence via a tricritical point. We have determined the ƒÉ-line, the line of first-order transitions and the tricritical point that separates these two distinct behaviors using state-of-the art finite-size scaling techniques.