Title: The condensation and ordering of models of empty liquids

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Abstract: We consider a simple model consisting of particles with four bonding sites ("patches"), two of type A and two of type B, on the square lattice, and investigate its global phase behavior by simulations and theory. We set the interaction between B patches to zero and calculate the phase diagram as the ratio between the AB and the AA interactions, epsilon(AB)*, varies. In line with previous work, on three-dimensional off-lattice models, we show that the liquid-vapor phase diagram exhibits a re-entrant or "pinched" shape for the same range of epsilon(AB)*, suggesting that the ratio of the energy scales - and the corresponding empty fluid regime - is independent of the dimensionality of the system and of the lattice structure. In addition, the model exhibits an order-disorder transition that is ferromagnetic in the re-entrant regime. The use of low-dimensional lattice models allows the simulation of sufficiently large systems to establish the nature of the liquid-vapor critical points and to describe the structure of the liquid phase in the empty fluid regime, where the size of the "voids" increases as the temperature decreases. We have found that the liquid-vapor critical point is in the 2D Ising universality class, with a scaling region that decreases rapidly as the temperature decreases. The results of simulations and theoretical analysis suggest that the line of order-disorder transitions intersects the condensation line at a multi-critical point at zero temperature and density, for patchy particle models with a re-entrant, empty fluid, regime. (C) 2011 American Institute of Physics. [doi: 10.1063/1.3657406]

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