8.0 Phase Transitions in Chemisorbed Systems

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8.1 Selenium Chemisorbed onto Nickel (100): Deviations from the Ashkin-Teller Model

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In view of the interpretation of electron scattering experiments, the microscopics of selenium atoms chemisorbed onto the nickel (100) surface is considered. An exact mapping onto Ashkin-Teller variables is reviewed. It is seen that the adatom-adatom interactions deviate from the Ashkin-Teller Hamiltonian. These interactions involve helicity and also otherwise violate the Ashkin-Teller symmetry. A phase diagram excluding the Ashkin-Teller topology is presented for selenium on nickel (100) from an extensive renormalization-group calculation in agreement with published finite-size scaling calculation. This phase diagram exhibits, in addition to 2x2 and $\sqrt{2}$ x$\sqrt{2}$ phases, a 2x1 phase with a disordering boundary with non-universal critical behavior.[1]

8.2 HCP versus FCC Freezing of Hard Spheres: A Variational Density Functional Study

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A density-functional calculation is used to study the crystallization transition in the three-dimensional hard-sphere fluid, determining lattice parameter, density, and real-space peak width of the ordered phase variationally for hexagonal-close-packed, face-centered-cubic, and body-centered-cubic lattices. Using the short-range Percus-Yevick approximate structure factor, it is found that the HCP and FCC lattices have very nearly the same transition properties, with HCP the slightly more stable phase at the melting point. The BCC phase is highly metastable, having a free energy higher than the isotropic liquid phase. When the more realistic and longer-ranged Waisman-Henderson-Barker structure factor is used, the degeneracy of the HCP and FCC phases is broken, HCP being the favorable structure, while the BCC phase continues to be highly metastable. Also, the effect of anharmonicity in the density functional is investigated and is seen to shift the real-space lattice peaks only slightly away from being pure Gaussians.[2]

8.3 Reentrant Behavior of an Anti-Metamagnet in Magnetic Field

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We introduce an "anti-metamagnet" model, which is an Ising cubic lattice with nearest-neighbor antiferromagnetic couplings in the x and y directions, and nearest-neighbor ferromagnetic couplings in the z direction. It is called an anti-metamagnet because it can be derived from a metamagnet by reversing the signs of all the interactions in a metamagnet. The anti-metamagnet in a uniform magnetic field is studied by an extended mean-field method. In this method, the lattice is divided into "bundles" of spins along the z direction. Each bundle is composed of four columns (lines) of spins along the z direction and each of them is imbedded in the mean field of its neighboring bundles. The interactions within the bundle and the mean field due to the neighbors are solved exactly using the transfer-matrix method along the z direction. Within this extended mean-field calculation, the system exhibits a reentrant second-order phase boundary which separates the disordered phase from the antiferromagnetic phase. In the reentrant region, the system approaches a picture of effectively one-dimensional disordered Ising models surrounded by fully magnetized lines of spins.[3]

8.4 The Hard Ellipsoid Fluid: First-Order Phase Transitions to Plastic Crystal, Liquid Crystal, and Crystal Phases using Optimized Direct Pair Correlations

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John F. Marko

The statistical mechanics of a fluid of prolate ellipsoids of revolution is addressed using density-functional methods. The direct pair correlation function of the isotropic liquid required by this method is adjusted from the Pynn-Wulf form using a variational approach, and then is used in a density-functional theory for the transitions to ordered phases. For the first time, calculations have been done with a density functional that can properly describe the narrow real-space peaks at crystallization transitions, and that can accommodate simultaneous translational and orientational ordering. As a result, transitions to the (orientationally ordered) solid, as well as to the (orientationally disordered) plastic crystal and nematic fluid phases can be described, and the resulting phase diagram is in quantitative agreement with Monte Carlo results.[4]

8.5 Exact Statistical Mechanics of a One-Dimensional Fluid of Hard Cores with Orientational and Translational Degrees of Freedom

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John F. Marko

A fluid of anisotropic hard cores with orientational as well as one-dimensional translational degrees of freedom is studied using the Ornstein-Zernicke integral equation for the direct and usual pair correlation functions. For the class of systems studied, this integral equation can be solved to yield the exact correlation functions, and thus an exact description of thermodynamic properties. Application of these results to improving approximations for direct correlation functions of three-dimensional fluids with orientational degrees of freedom is discussed.[5]

References

[1] A.N. Berker, R.G. Caflisch, and A. Aharony, preprint (1988).

[2] J.F. Marko, *Phys. Rev. Lett.*, submitted (1988).

[3] K. Hui, *Phys. Rev. B*, to be published (1988).

[4] J.F. Marko, preprint (1988).

[5] J.F. Marko, preprint (1988).

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