Section 3 Surfaces and Intersurfaces

Chapter 1 Statistical Mechanics of Surface Systems and Quantum-Correlated Systems.

Chapter 2 X-Ray Diffuse Scattering.

Chapter 3 Semiconductor Surface Studies.

Chapter 4 Ultralow Temperature Studies of Nanometer Size Semiconductor Devices.

Chapter 5 Columb Repulsion and Resonant Tunnelling.

Chapter 6 Graphoepitaxy of Colloidal Crystals.

Chapter 7 Step Structures on Semiconductor Surfaces.

Chapter 1. Statistical Mechanics of Surface Systems and Quantum-Correlated Systems

Sponsor

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1.1 Finite-Temperature Properties of Correlated Systems

Project Staff

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Our objective is to produce microscopic quantitative theories of surface systems and of systems in which quantum-mechanical many-body correlations are preeminent. The ability to predict the finite-temperature properties of materials lies in statistical mechanics. The renormalization-group ideas have made it conceptually possible to contemplate the statistical mechanics of systems in which many-body correlations are important. Actual performance of realistic statistical mechanics, however, requires: 1) the ability to deal with arbitrary local interactions which the renormalization-group invariably generates, 2) the ability to show the convergence of calculations via systematically improvable procedures, and 3) the ability to deal with the dynamics of quantum operators. In our recent work, we have established the first requirement for realistic systems. Furthermore, at this time we are developing Monte-Carlo procedures for implementing the renormalization-group, thereby enabling our achieving the second requirement. Finally, we think that quantum systems could be treated by these methods, by the application of Feynman-path methods to transform them into (d+1)-dimensional classical systems.

1.2 Random-Field Mechanism in Random-Bond Multicritical Systems

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Professor A. Nihat Berker, Kenneth Hui

It is argued on general grounds that bond randomness drastically alters multicritical phase diagrams via a random-field mechanism. For example, tricritical points and critical endpoints are entirely eliminated (in dimension $d \leq 2$) or depressed in temperature ($d>2$). These predictions are confirmed by a renormalization-group calculation. Another consequence of this phenomenon is that, under bond randomness, the phase transitions of the general q-state Potts models are second-order for all q at dimensionality $d \leq 2$ and for higher q at $d>2$.

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1.3 Exact Pair Correlations in a One-Dimensional Fluid of Hard Cores with Orientational and Translational Degrees of Freedom

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John F. Marko

Exact direct and usual pair correlations for a fluid of anisotropic hard cores with orientational as well as one-dimensional translational degrees of freedom are obtained. These results indicate that previous approximations for the direct correlations in anisotropic hard-core fluids have overlooked the effect of orientational configurations for which the hard-core overlap is not a smooth function of particle separation beyond the point of hard-core contact.

Publications

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