Section 4   Surfaces and Interfaces

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

Academic and Research Staff

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1.1 Introduction

Sponsor

Our objectives are to develop, using renormalization-group theory and other methods of statistical mechanics, microscopic theories of quantum electronic systems and of semiconductor alloy systems that properly account for correlation effects. Our approach is particularly suited to systems with fluctuations due to finite temperatures, impurities, surfaces or other geometric constraints.

1.2 Renormalization-Group Approach to Electronic Systems

Project Staff

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High-T_c superconductivity, metallic magnetism, the metal-insulator transition, and heavy fermion behavior are all phenomena produced by the strong correlations of electrons in narrow energy bands. It is therefore important to study theoretical models that incorporate the strong correlation effects of electrons. The tJ model is such a system. It is defined on a lattice with one spherically symmetric orbital per site by the Hamiltonian

$$\mathcal{H}_{tJ} =$$

$$P\left[-t \sum_{<ij>,\sigma} (c_{i\sigma}^{\dagger} c_{j\sigma} + h.c.)\right.$$

$$\left. + J \sum_{<ij>} (\vec{s}_i \cdot \vec{s}_j - n_i n_j/4)\right] P,$$

where P is an operator that projects out all doubly occupied sites, $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are creation and annihilation operators for an electron in a Wannier state at site i with z-component of spin σ, n_i is the electron number operator that counts the total number of electrons at site i, and $\vec{s}_i$ is the spin operator. This Hamiltonian can be interpreted in two ways: (1) In the case of small J, the system can be thought of as the large U limit of the single-band Hubbard model of electronic systems. The antiferromagnetic exchange comes as a result of a virtual process where one electron hops onto a singly occupied nearest-neighbor site and then hops back. The energy gain for such a process is of the order of t^2/U since a doubly occupied site has energy U. (2) The system can also be thought of as an electronic system with a "super" exclusion principle where no two electrons (like or unlike spins) are allowed on the same site. The second interpretation does not put any restriction on the size of J.

There are few rigorous results available on this system: (1) At half filling, the system reduces to a Heisenberg antiferromagnet; (2) At $2t = \pm J$, the model has been solved by the Bethe-ansatz technique; and (3) In one dimension and $J = 0$, the model has been solved also by the Bethe-ansatz technique. Other attempts to study this model have focused on the ground state and the first few excited states. We have decided, instead, to focus on the thermodynamic properties of this system. Our method, the renormalization-group approach, involves solving a statistical mechanics problem by a recursive elimination of the degrees of freedom. Since the Hamiltonian involves a regular lattice, this problem is well suited for the position-space renormalization-group method. The solution is obtained in an expanded space with Hamiltonian

$$\mathcal{H} =$$

$$P \left[-t \sum_{<ij>, \sigma} (c^\dagger_{i\sigma} c_{j\sigma} + h.c.) \right.$$

$$\left. + \sum_{<ij>} (J\vec{s_i} \cdot \vec{s_j} + Vn_i n_j) + \mu \Sigma_i n_i \right] P.$$

Because of the non-commutativity of quantum operators, we had to develop new techniques of renormalization-group theory.

We have obtained the renormalization-group flows for the effective coupling constants for one-, two-, and three-dimensional systems. The flows determine the phase diagrams and all thermodynamic properties. In one dimension, we find, as expected, no finite-temperature phase transition. In two dimensions, we find a single finite-temperature critical point, as previous researchers conjectured but were unable to derive.

In three dimensions, we find a global finite-temperature phase diagram that is richly structured. Disordered, antiferromagnetic, and conducting phases are separated by first- and second-order phase boundaries, which are themselves delineated by lines of tricritical points, critical points, and critical endpoints. Complicated structures with multiple reentrances occur. We have also calculated, using our renormalization-group transformation, electronic densities and nearest-neighbor correlations as a function of electronic chemical potential. These yield a microscopic understanding of the different phases. We have also completed small-cluster calculations which cannot yield phase transitions, but which support the densities and correlations of the renormalization-group theory.

1.3 Suzuki-Trotter Approach to Electronic Systems

Project Staff

Daniel P. Aalberts, Professor A. Nihat Berker

It is possible to rigorously map d-dimensional quantum mechanical spin systems onto (d+1)-dimensional classical systems with more complicated interactions. This method, introduced by Suzuki, uses the Trotter formula and is the analog for statistical mechanics of the Feynman-path approach to particle propagators.

We are investigating the possibility of adapting this approach to electronic systems where, in more than one dimension, fermion statistics complicates the classical problem. By numerical simulation, the resulting classical models will be used to confirm the renormalization-group results mentioned above.

1.4 Phase Diagrams of Semiconductor Alloys

Project Staff

William C. Hoston, Jr., Professor A. Nihat Berker

We are conducting a study of ternary compounds on face-centered-cubic lattices. Our aim is to elucidate the phase behavior of ternary and quaternary semiconductor alloys. These alloys could exist in the zincblende, chalcopyrite, or possibly stannite structures, involving two interpenetrating fcc lattices on which up to four atomic species exist. One atomic species occupies one of the fcc lattices while three other atomic species may (chalcopyrite, stannite) or may not (zincblende) order on the other fcc lattice. At present, the chalcopyrite structure is seen experimentally in the III-V compounds. The ranges of stability of these structures are of interest.

In previous work by K.E. Newman and collaborators, the Blume-Emery-Griffiths model has been adopted for the study of the zincblende to chalcopyrite or stannite transitions. This model is a spin-1 Ising model with Hamiltonian

$$\mathcal{H} = J \sum_{<ij>} s_i s_j + K \sum_{<ij>} s_i^2 s_j^2$$

$$- \Delta \sum_i s_i^2, \quad s_i = 0, \pm 1.$$

The three spin values are each associated with a different species of atom, A, B, or C, which exist on one of the fcc lattices. The other fcc lattice is considered occupied by atomic species D. The systems under consideration have the composition $[(AB)_{1-x}C_{2x}]D_2$. The model includes interactions between the A, B, and C atoms. The parameters J and K in the Hamiltonian above are fixed as combinations of these interaction energies. They are chosen to give the chalcopyrite structure at low temperature (J < 0) and to control the phase transition between the chalcopyrite and the zincblende. Δ controls the relative densities of the species (AB) and C.

These systems contain competing, frustrated interactions, which necessitate a renormalization-group treatment. We have been able to develop a renormalization-group transformation that yields both the

ferromagnetic and, in contrast with previous work, the (fully frustrated) antiferromagnetic phase transitions on the fcc lattice in the spin-1/2 limit obtained by taking Δ to negative infinity. We are now pursuing the global phase diagram in thermodynamic field (interaction constant) space, which will be followed by a study of density space.

1.5 Renormalization-Group Theory of an Internal Critical Endpoint Structure

Project Staff

Roland R. Netz, Professor A. Nihat Berker

A prefaced renormalization-group study has been completed, indicating that all three new features of the Blume-Emery-Griffiths model with repulsive biquadratic interaction survive fluctuations in three dimensions but not in two dimensions. These features are: (1) a critical endpoint structure occurring inside the ferromagnetic phase; (2) disordered-ferromagnetic-disordered reentrance; and (3) a ferrimagnetic phase sandwiched between the ferromagnetic and antiquadrupolar phases. The renormalization-group mechanism for a critical endpoint structure inside the ordered phase is shown to be the same as that originally found for a critical endpoint structure inside the disordered phase, namely a distinct hybrid fixed point, contrary to a previous claim. This critical-endpoint structure may have been seen experimentally in the analogous alloy system of $FeBr_2$.

1.6 Phase Diagrams of the Ising Model on the Square Lattice with Crossed Diagonal Bonds

Project Staff

Professor A. Nihat Berker

The global phase diagram of the spin-1/2 Ising model with nearest- and next-nearest-neighbor interactions on the square lattice has been considered, including the fully anisotropic cases. A closed-form expression has been deduced that accurately represents the phase boundaries when the crossed next-nearest-neighbor interactions are not of opposite signs. The phase diagram includes disordered, ferromagnetic, antiferromagnetic, axially single-striped, and diagonally double-striped phases.

1.7 Publications

Berker, A.N. "Critical Behavior Induced by Quenched Disorder." *Physica A.* Forthcoming.

Berker, A.N., R.G. Caflisch, and M. Kardar. "Statistical Mechanics of Phase Transitions with a Hierarchy of Structures." In *Hierarchically Structured Materials.* Ed. I.A. Aksay. Pittsburgh: Materials Research Society, 1992.

Berker, A.N., and K. Hui. "Phase Diagram of the Ising Model on the Square Lattice with Crossed Diagonal Bonds." Submitted to *Phys. Rev. B.*

Netz, R.R. "Microscopic Theory of the Ripple Phase." In *The Structure and Conformation of Amphiphilic Membranes.* Eds. R. Lipowsky, D. Richter, and K. Kremer. Berlin: Springer-Verlag, 1992.

Netz, R.R. "New Phases and Multiple Reentrance of the Blume-Emery-Griffiths Model with Repulsive Biquadratic Coupling: Monte Carlo Renormalization-Group Theory." *Europhys. Lett.* 17(4): 373-377 (1992).

Netz, R.R. "Symmetry-Breaking Fields in Frustrated Ising Systems on Square and Cubic Lattices." *Phys. Rev. B* 46(2): 61-64 (1992).

Netz, R.R., and A.N. Berker. "Microscopic Liquid Crystal Theory of Nematic Reentrance, Smectic C Ordering, and In-Plane Domain Formation." In *Phase Transitions in Liquid Crystals.* Eds. S. Martellucci and A.N. Chester. New York: Plenum Press, 1992.

Netz, R.R., and A.N. Berker. "Renormalization-Group Theory of an Internal Critical Endpoint Structure: The Blume-Emery-Griffiths Model with Biquadratic Repulsion." *Phys. Rev. B.* Forthcoming.

Netz, R.R., and A.N. Berker. "Smectic C Order, In-Plane Domains, and Nematic Reentrance in a Microscopic Model of Liquid Crystals." *Phys. Rev. Lett.* 68(3): 333-336 (1992).

Meeting Papers

Aalberts, D.P., and A.N. Berker. "Hard-Spin Mean-Field Theory: Variational Free Energy and First-Order Phase Transitions." Paper presented at the American Physical Society Meeting, Indianapolis, Indiana, March 16-20, 1992.

Berker, A.N. "Critical Behavior Induced by

Quenched Disorder." Paper presented at the International Conference on Thermodynamics and Statistical Mechanics, Berlin, Germany, August 2-8, 1992.

Berker, A.N. "Phase Transitions in Disordered Systems." Paper presented at the Summer School on Recent Developments in Statistical Physics, Istanbul, Turkey, July 26-August 6, 1993.

Berker, A.N., and K. Hui. "Closed-Form Expression for the Global Phase Diagram of the Ising Model on the Square Lattice with Crossed Diagonal Bonds." Paper presented at the American Physical Society Meeting, Seattle, Washington, March 22-26, 1993.

Berker, A.N., and R.R. Netz. "Smectic C Order, In-Plane Domains, and Nematic Reentrance in a Frustrated Microscopic Model of Liquid Crystals." Paper presented at the American Physical Society Meeting, Indianapolis, Indiana, March 16-20, 1992.

Netz, R.R. "Multiple Reentrance and New Phases from the Blume-Emery-Griffiths Model in Three Dimensions: Monte Carlo Renormalization-Group Theory." Paper presented at the American Physical Society Meeting, Indianapolis, Indiana, March 16-20, 1992.

Netz, R.R. "Symmetry-Breaking Fields in Frustrated Ising Systems on Square and Cubic Lattices." Paper presented at the American Physical Society Meeting, Indianapolis, Indiana, March 16-20, 1992.

Netz, R.R., and A.N. Berker. "Renormalization-Group Theory of the Blume-Emery-Griffiths Model with Repulsive Biquadratic Coupling." Paper presented at the General Conference of the Condensed Matter Division of the European Physical Society, 13th, Regensburg, Germany, March 29-April 2, 1993.

Netz, R.R., and A.N. Berker. "Renormalization-Group Theory of an Internal Critical Endpoint Structure: The Blume-Emery-Griffiths Model with Biquadratic Repulsion." Paper presented at the American Physical Society Meeting, Seattle, Washington, March 22-26, 1993.

Netz, R.R., and A.N. Berker. "Smectic C/A_2 Order, Domains, Reentrance in a Microscopic Model of Liquid Crystals." Paper presented at the International Conference on Thermodynamics and Statistical Mechanics, Berlin, Germany, August 2-8, 1992.