Section 4 Surfaces and Interfaces

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

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1.1 Introduction

Sponsor

Joint Services Electronics Program
Contract DAAL03-89-C-0001
Contract DAAL03-92-C-0001

Our objectives are to develop, using renormalization-group theory and other methods of statistical mechanics, microscopic theories of quantum spin and electronic systems. 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

Alexis Falicov, Professor A. Nihat Berker

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

$$H_{tJ} = P\left[-t\,\Sigma_{<ij>,\,\sigma}\, (c^{+}_{i\sigma}\, c_{j\sigma} + \text{h.c.}) + J\,\Sigma_{<ij>}(\vec{s}_i \vec{s}_j - n_i n_j/4)\right] P,$$

where P is an operator that projects out all doubly occupied sites, $c^{+}_{i\sigma}$ 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. (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 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

$$H = P\left[-t\,\Sigma_{<ij>,\,\sigma}\, (c^{+}_{i\sigma} c_{j\sigma} + \text{h.c.}) + \Sigma_{<ij>}\, (J\vec{s}_i\vec{s}_j + V n_i n_j) + \mu \Sigma_i n_i\right] P.$$

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

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 workers conjectured but were unable to derive. In three dimensions, our preliminary results indicate a rich finite-temperature phase diagram with novel phases, phases transition behaviors, and conductivity phenomena. Our results are also confirmed by our exact small-cluster calculations.

1.3 Phase Diagrams of Semiconductor Alloys

Project Staff

William C. Hoston, Jr., Roland R. Netz, Professor A. Nihat Berker

A study of ternary compounds on face-centered-cubic lattices has been started. The aim of the work is to elucidate the phase behavior of ternary and quaternary semiconductor alloys. These alloys have received recent attention for both fundamental and technological reasons. It has been found that these alloys can 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, not much is known about the chalcopyrite structure seen in the experimentally obtained III-V compounds. There is great interest in learning how stable this chalcopyrite phase is against other possible structures.

In recent 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

$$H = J \Sigma_{<ij>} s_i s_j + K \Sigma_{<ij>} s_i^2 s_j^2 - \Delta \Sigma_i s_i^2, \ s_i = 0, \pm 1.$$

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 so as 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.

As a preliminary study, we have completed the global phase diagram study of the Blume-Emery-Griffiths model. We found six new phase diagrams, including novel multicritical topology and two new ordered phases. Thus, we determined that the phase diagram of this simple spin system includes nine distinct topologies and three ordered phases. These results were obtained by a global mean-field theory with four independent order parameters.

It is important to note, however, that the choice of $J < 0$ makes the model on the fcc lattice frustrated, which requires analysis beyond mean-field theory. We have developed a new method, which we have called "hard-spin mean-field theory," that incorporates the hard-spin condition of local degrees of freedom and thereby conserves frustration. We have tested this method on frustrated triangular and stacked triangular lattices with the spin-1/2 Ising model, obtaining excellent results. We are now applying the method to the Blume-Emery-Griffiths model. Our future studies of semiconductor alloys will also include renormalization-group theory.

1.4 Quantum Spin Systems

Project Staff

Daniel P. Aalberts, Professor A. Nihat Berker

We are interested in calculating the thermodynamic properties of quantum mechanical systems at low temperatures, where the distinctive quantum phenomena are important. The first model we consider is the $s = 1/2$ XXZ model, with Hamiltonian

$$H = \Sigma_{<ij>} [J (s_i^x s_j^x + s_i^y s_j^y) + J_z s_i^z s_j^z].$$

This model in two dimensions is of interest in high-T_c superconductors; it is also of general interest to develop our ability to do the statistical mechanics of quantum systems and to extract, thereby, the quantitative properties of their elementary excitations.

We map this d-dimensional quantum system quantitatively onto a (d+1)-dimensional classical system with complicated interactions. For the ferromagnetic quantum system, we have been able to obtain magnon dispersion relations and magnon-magnon interactions. Eventually, we expect to apply our method to antiferromagnetic quantum systems, where even the ground state presents a many-body problem.

1.5 Publications

Alerhand, O.L., A.N. Berker, J.D. Joannopoulos, D. Vanderbilt, R.J. Hamers, and J.E. Demuth. "Finite-Temperature Phase Diagram of Vicinal Si(100) Surfaces: Alerhand et al. Reply." *Phys. Rev. Lett.* 66(7): 962 (1991).

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Netz, R.R. "Microscopic Theory of the Ripple Phase." In *Structure and Conformation of Amphiphilic Membranes.* Ed. R. Lipowsky. Berlin: Springer-Verlag, 1992.

Netz, R.R. *Frustration in Magnetic, Liquid Crystal, and Surface Systems: Monte Carlo Mean-Field Theory.* S.M. thesis, Dept. of Physics, MIT, 1991.

Meeting Papers

American Physical Society Meeting, Cincinnati, Ohio, March 18-22, 1991.

Berker, A.N. "Quenched Fluctuation Induced Second-Order Phase Transitions."

Hoston, W., and A.N. Berker. "New Multicritical Phase Diagrams from the Blume-Emery-Griffiths Model with Repulsive Biquadratic Interactions."

Netz, R.R., and A.N. Berker. "Monte Carlo Mean-Field Theory and Frustrated Systems in Two and Three Dimensions."

American Physical Society Meeting, Indianapolis, Indiana, March 16-20, 1992.

Aalberts, D.P., and A.N. Berker. "Hard-Spin Mean-Field Theory: Variational Free Energy and First-Order Phase Transitions."

Berker, A.N., and R.R. Netz. "Smectic C Order, In-Plane Domains, and Nematic Reentrance in a Frustrated Microscopic Model of Liquid Crystals."

Netz, R.R. "Symmetry-Breaking Fields in Frustrated Ising Systems on Square and Cubic Lattices."

Netz, R.R. "Multiple Reentrance and New Phases from the Blume-Emery-Griffiths Model in Three Dimensions: Monte Carlo Renormalization-Group Theory."

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Netz, R.R., and A.N. Berker. "Smectic C/A_2 Order, Domains, Reentrance in a Microscopic Model of Liquid Crystals."

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