論文内容の要旨

論文題目：Phase Transitions and Critical Phenomena in Frustrated Continuous Spin Systems with Ising-like Symmetry Breaking
（イジング的対称性破れの付随するフラストレート連続スピン系における相転移と臨界現象）

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In this thesis, we study the thermodynamic phase transitions and critical phenomena in a certain class of classical frustrated spin systems with continuous spin symmetry. The main goal is to gain a unified knowledge on this class of systems. The most important common feature of this class of systems is that the system comprises two equivalent sublattices and the symmetry of the characteristic frustrated exchange coupling precludes the inter-sublattice effective coupling of the bilinear structure. Consequently, the effect of the higher order biquadratic exchange coupling, which is usually dominated by that of the bilinear coupling in conventional systems, becomes prominent. As a result, the phase transitions in this class of systems significantly differ from those in the conventional unfrustrated systems.

In Chapter 2, by constructing an appropriate effective GLW Hamiltonian for N-component vector fields and performing the mean-field and RG analysis, we studied several generic aspects of this class of frustrated systems. The two-sublattice structure with the ferro-quadrupolar biquadratic coupling in principle allows the Ising-like intermediate phase. In this phase, only an Ising-like composite order parameter exhibits long-range ordering while the individual spins remain disordered. Because of the composite structure of the Ising-like order parameter, the Z_2 symmetry breaking transition temperature cannot be lower than that of the O(N) magnetic transition where spins exhibit long-range ordering. We then examined a mean-field theory that can account for such an intermediate phase. We found that the theory predicts a multicritical point in the vicinity of the bicritical point where the Z_2 and O(N) transition merge. While the Z_2 symmetry breaking transition is always of second order in this approximation, the O(N) transition changes itself from of second order to first order before it merges with the Z_2 transition.

In the subsequent RG treatment, we examined the stability of the conventional O(N) fixed point corresponding to decoupled sublattices using scaling analysis. The precise numerical estimation of the critical exponents available in literature allowed us to obtain an accurate conclusion on this fixed point: the XY and Heisenberg decoupled fixed points are unstable against the perturbation of the inter-sublattice quadrupolar coupling. We then reviewed the RG treatment by Aharony and we investigated the more global structure of the RG flow diagram by the one-loop approximation. No stable fixed point was found for the XY and Heisenberg spin systems. Therefore, one possibility is the fluctuation-induced first-order phase transition**.** However, this statement needs certain care because the RG flows near the O(N) decoupled fixed point obtained by the one-loop approximation contradict the results obtained by the nonperturbative scaling arguments. The latter is more reliable because higher order contribution is taken into account.

In Chapter 3, we discussed the Heisenberg model in a magnetic field on the body-centered tetragonal (BCT) lattice. The system is XY-like because of the magnetic field. A quasi-2D spin-dimer compound $BaCuSi_2O_6$ is an experimental realization of the BCT antiferromagnet when a magnetic field with strength comparable to the singlet-triplet excitation gap is applied. The main motivation of the present work is to clarify the relation between the experimental observation of the XY-like transition at $T > 0$ and the potential consequence of the previous prediction of the "bond ordering" in this compound. Using the spin-wave approximation and Monte Carlo simulation, we investigated the finite-T transition in detail. We confirmed the collinear two-sublattice state stabilized by the order-by-disorder mechanism**.** In that phase, O(2) spin symmetry and Z_2 lattice symmetry are broken. In particular, we found that the effect of the inter-sublattice bilinear coupling is completely suppressed (prohibited by symmetry) while the biquadratic coupling is allowed and present. Therefore, the system provides a realization of the effective GLW Hamiltonian with $N = 2$. Most importantly, in light of the previous RG treatment by Aharony, our observation indicated that the BCT antiferromagnet such as $BaCuSi_2O_6$ may undergo hidden crossover behavior on the verge of the XY-like ordering. This crossover is induced by the inter-sublattice biquadratic coupling. The RPA argument suggested that the two kinds of symmetry breaking (i.e. XY-like and Ising-like) take place simultaneously at a single transition in most cases of the XY spin systems. The results of Monte Carlo simulation partially succeeded in giving numerical supports for the above notions: the collinear ordered state and the single phase transition with the simultaneous Ising-like and XY-like orderings. However, we found that the scaling behavior around the transition temperature is strongly dominated by the decoupled 3D XY fixed point, which was shown to be unstable by the previous RG argument. The crossover theory can give us a reasonable account for such an observation of transient critical behavior: it is most likely due to the system size much smaller than the characteristic length for the crossover behavior. However, the crossover theory cannot provide information on the resulting true asymptotic behavior deviating from the 3D XY-like behavior on the very verge of the phase transition.

The unsettled problem of the crossover from the decoupled 3D XY model was re-investigated in

Chapter 4. We explored the true asymptotic behavior resulting from the crossover from the 3D XY decoupled fixed point by introducing another effective lattice model suitable for large-scale simulation and performing systematic finite-size scaling analysis, referred to as the Monte Carlo renormalization group**.** The effective model that we introduced has the same symmetry structure as the frustrated systems but it is unfrustrated in itself allowing us to employ a variant of the efficient cluster algorithm. Using the Monte Carlo renormalization group analysis, we found that the RG flow near the 3D XY fixed point shows systematic deviations from this fixed point and reaches the region where we confirmed the first-order transition. Because we did not find any sign of a stable fixed point or a separatrix, we concluded that our observations provide a strong numerical evidence of the first-order transition in the frustrated XY spin systems. The absence of stable fixed point is qualitatively consistent with the one-loop treatment of the corresponding effective GLW Hamiltonian**.** Therefore, our numerical results in tern suggest that in spite of the incorrect features contradictory to the results of the non-perturbative scaling arguments, the one-loop approximation nevertheless captures the correct physical picture, namely the fluctuation-induced first-order transition.

The crossover region where the true weak discontinuous nature appears is tiny as long as the frustrated inter-layer coupling is small in comparison with the intra-layer exchange. This is indeed the case of the quasi-2D compound $BaCuSi_2O_6$. Therefore, the thermodynamic behavior will be dominated by the 3D XY decoupled fixed point in a broad region near the transition and the true discontinuous nature of the transition could easily be beyond the experimental precision in most cases. This is our conclusion as to the relation between the potential effect of the bond ordering and the experimental observation of the 3D XY-like criticality.

In Chapter 5, we investigated the Heisenberg spin systems. Among the same class of frustrated systems, the discovery of the high-T_c superconductivity in ferropnictides has given rise to a recurring interest on the stacked J_1-J_2 Heisenberg model because it has provided a simple understanding of the structural and spin-density-wave (SDW) order in these compounds. In particular, as argued by Xu *et al.*, the J_1-J_2 Heisenberg model can naturally explain the experimental observation that the structural transition temperature in ferropnictides is commonly either the same as the Neel temperature, as in the 3D 122-type undoped compounds, or higher than the Neel temperature as in the quasi-2D 1111-type compounds. By means of Monte Carlo simulation on an effective model called the Ising-O(3) model we found that this class of Heisenberg spin systems in $d = 3$ has the Ising ordered phase where the Heisenberg spins remain disordered in a moderate quasi-2D region. The region where the O(3)-symmetric Ising ordered phase exists was quantitatively clarified. The important difference from the XY spin systems, where we concluded such an intermediate phase is almost unlikely in d = 3, is related to the fragileness of spin ordering of the Heisenberg spin systems. Compared to the Ising-like ordering, the ordering of the Heisenberg spins is more sensitive to the magnitude of the inter-layer coupling. Our finite-size scaling analysis suggests that the transitions are of second order and in the Ising and Heisenberg universality classes. So far, the other subtle features discussed using the mean-field theory have not been reproduced but need further investigation. In the 3D region with sufficiently large inter-layer coupling the first-order transition directly bridges the paramagnetic and lowest-T ordered phases, in agreement with the absence of stable fixed points in the one-loop RG flow diagram obtained by Aharony. Finally, in d = 2 the system undergoes a finite-temperature transition in the Ising universality class where the O(3) spins remain disordered, as expected from its symmetry, range of interaction and the dimensionality.

By comparing the results of the Ising-O(3) model with experiments on ferropnictides, we found that our results provide a qualitative explanation on the experimental observations, namely the observed sequence and the orders of transitions, in terms of the magnitude of the inter-layer coupling. Firstly, the separate second-order or weakly first-order structural and SDW transitions in the 1111 systems, for which density functional calculation suggest the strong two dimensionality, may be understood in terms of the Ising-O(3) model in the quasi-2D region where the transitions are separate and of second order. Also, the first-order transition in the more 3D 122 parent systems, where the lattice distortion and the SDW ordering simultaneously occur, may be understood in terms of the Ising-O(3) model in the region where the inter-layer coupling is sufficiently large. Although the local-moment model is most likely inadequate for microscopic description of the metallic ferropnictides, the phase diagram that qualitatively reproduces the experiments leads us to expect that the J_1-J_2 Heisenberg model and the related systems serve as a good starting point for describing the universal properties of ferropnictides.