博士論文　（要約）

論文題目 Quantum Monte Carlo approach to the quantum phase transition in low-dimensional antiferromagnets in terms of the Berry phase
（量子モンテカルロ法によるベリー位相の計算と低次元磁性体の量子相転移の研究）

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Ground states and low-energy excited states of low dimensional quantum spin systems can differ from ones of classical systems in quality. One of the simplest examples is the antiferromagnetic Heisenberg (AFH) dimmer. While the ground states of the classical one are continuously degenerate and there are excited states with infinitesimal energy gap, the ground state of the quantum one is a unique singlet pair and has a finite energy gap above the ground state. Another example is the AFH chain. For the classical AFH chain, the ground states are also continuously degenerated and infinitesimal excited state occurs (Goldstone mode). On the other hand, the ground states of the integer spin AFH chains are the non-degenerate Haldane states, which are non-magnetic states, total spin is zero, and have finite energy gap above them. The valence bond picture is a good tool to give us understandings about such ground states and excited states of quantum spin systems. In this picture, each local spin with angular momentum S is divided into 2S subspins with S=1/2, and a subspin of a local spin makes singlet pair (valence bond) with a subspin of another local spin. The states where each subspin is bound to one valence bond are the basis of the Hilbert space with total spin is zero, and each state is called the valence bond solid (VBS) state or the valence bond crystal (VBC) state. The ground state of S=1 AFH chain is the VBS state where each bond has one valence bond. Moreover, the parity of the number of valence bond on one fixed bond is a topological order parameter. Two VBS states are in the different phases if one state has the odd number of valence bonds on some bond and the other state has the even one on the same bond. For example, in S=1 dimerized AFH chain, where the strengths of coupling constants are alternately strong and weak. There is two-quantum phase transition with respect to the strength of dimerization. The number of valence bonds on some bond varies from zero to one and from one to two at the quantum phase transitions.

The string order parameter and the twisted order parameter are observables to capture the parity of the number of valence bonds. These make us possible to draw phase diagrams of one-dimensional spin systems, such as a spin chain, a spin ladder, and a spin tube. These observables, however, can be defined well only in one-dimensional systems although the valence bond picture is still useful in higher dimensional systems. In higher dimensional systems, of course, VBS picture still works well as in one dimension. Therefore an alternative observation that can be used in higher dimensional systems has been desired for long time.

Recently, the local quantized Berry phase has been proposed as a new observable to catch the parity of the number of valence bond. This is a geometric phase that the state acquires when the state goes around an adiabatic cycle by some spatially local perturbation. Although this is one of the topological order parameters, this can be defined locally since it depends where the perturbation acts. Moreover, this is quantized due to the symmetry of the internal degree of freedom such as spin inversion symmetry or particle-hole symmetry, and is stable against any

small perturbations as long as the energy gap remains finite. Therefore, the spatial pattern of this value and the change of it tell us a quantum phase transition. For the spin systems, a "twist" of one bond makes the value of local quantized Berry phase 0 or π when the number of valence bond on the twisted bond is even or odd, respectively. One of the strong points of the local quantized Berry phase is that this can be defined on any lattice in any dimension. Another one is that even in finite systems this is quantized so well that catches phase transitions.

In the past numerical studies of the phase distinguishing via the local quantized Berry phase, the calculations have been done mainly by the exact diagonalization method and the tractable system size is severely limited. The local quantized Berry phase is quantized in such finite systems indeed, but of course the transition point is affected by the finite size effect. Therefore, the unbiased numerical method that can treat large systems in any dimension is required. Quantum Monte Carlo (QMC) method is one of the candidates.

QMC is one of the most powerful numerical methods in the field of the quantum many-body physics. In the method, we can calculate the statistical expected value of some observable as follows. First, we expand the density matrix into the weighted summation of the world-line configurations by path-integral method. Next, we calculate the mean value of some observables over the world-line configurations by Markov chain Monte Carlo method. Many developments such as loop algorithm and continuous imaginary time algorithm have overcome many weak points of QMC. However, there are still some obstacles. One of them is that QMC can treat only the observables represented by the Monte Carlo expectation form. For example, the inner product of two states cannot be calculated directly by QMC. Another obstacle is the emergence of configurations with negative or complex weight for some (many, indeed) systems. This is well known as "the sign problem," which is the most difficult problem in QMC. In this case, we need to extract information of the original system from another system free from sign problem. Unfortunately, this operation makes the statistical error grow exponentially as the inverse temperature and the system size increase, and so QMC breaks down. Although some methods, the basis transformation, the meron cluster algorithm, the nested cluster algorithm, and so on, has been developed to tackle this problem, this problem can be solved or reduced at only few models or parameters. In the calculation of the Berry phase, there are the configurations with complex weight due to the local twist.

In the present thesis, we propose a QMC scheme for the gauge-fixed Berry connection and the local quantized Berry phase. More concretely, this systematic scheme teaches us how to evaluate the coefficient of the term with arbitrary power of the perturbation of the inner product between a perturbated ground state and a non-perturbated ground state by QMC. The coefficient of the linear term is nothing but the gauge-fixed Berry connection. The Berry curvature and the susceptibility of the fidelity, which are other tools to catch the quantum phase transition, are

derived from the coefficients of the quadratic terms. Moreover, the derivatives of these values are obtained from the ones of the higher order terms. The complex weight problem for the gauge-fixed Berry connection is overcome as follows. First, for some parameters such as twist angle is $\theta = \pi$ the meron cluster algorithm can be applied to solve or reduce the problem. Next, we fitted the data for discrete parameters by the series of cosine functions since the gauge-fixed Berry connection as a function of the twist angle has a period 2π and is an even function. Finally, the local quantized Berry phase was obtained by integrating the fitting function. The meron cluster algorithm teaches us that there are the twist patterns where the complex weight problem does not occur. Such twist patterns enable us to perform the large system simulations. We call such special pattern "the magic twist pattern." For the demonstration, we calculated the local quantized Berry phase of the AFH model of the staggered dimerized ladder for some system sizes, say, 10000 sites. The estimated transition point by size extrapolation was consistent with the result of the previous studies. This is the first QMC calculation of Berry phase as far as we know.

We also propose that the quantum phase transition point can be estimated efficiently by the gauge-fixed Berry connection. The curves of the gauge-fixed Berry connection of non-twisted systems for several system sizes cross at the transition point while the Berry curvature and the susceptibility of the fidelity diverge at the point. Since it is more difficult to find a peak than a crossing, the gauge-fixed Berry connection is more efficient. Furthermore, the precision of QMC calculation is higher for the gauge-fixed Berry connection than the other ones as the order of difference of the former is one less than the one of the latter.

In order to demonstrate our method in two-dimensional systems, we calculated the Berry phase of the AFH model on the columnar dimerized square lattice defined by magic twist pattern. In this model, the gapped-gapless phase transition occurs and thus the Berry phase can be quantized in only one side (VBS phase) of the transition. Even in such case, our QMC method for the Berry phase can distinguish these phases, by using the difference of the system size dependence of the first excitation energy in the gapless Neel phase and the gapped VBS phase. The estimated critical point by the present method is consistent with the results by the past studies.

Finally, we define the local quantized Berry phase for the SU(N) AFH model and apply our QMC method. First, we calculated the Berry phase defined by the magic pattern of the SU(N) AFH models on the square lattice for several N. We concluded that the ground states for $N < 5$ are the Neel state and those for $N >= 5$ are the VBS state, which is consistent with the previous work. Next, we applied the present method for the 4 columns SU(4) AFH models on the dimerized chain in order to see the N quantization of the Z_N Berry phase. The N quantization implies that the phase diagram of the SU(N) Heisenberg model can be more complex than that

of the SU(2) Heisenberg model. Finally, We calculated the gauge-fixed Berry connection of SU(3) J-Q model, which is the Heisenberg model including the nearest neighbor interaction J and many-body interaction Q and has the quantum phase transition from Neel order to VBS order as the ratio of Q and J grows. We found that the gauge-fixed Berry connection analysis is also valid in the SU(N) model. Note that the present method allows us to see the valence bonds of SU(N) AFH model directly for the first time.