博士論文 (要約)

Study of quantum criticality with strong space-time anisotropy by quantum Monte Carlo with stochastic optimization

（量子モンテカルロと確率的最適化による強い時空異方性のある量子臨界現象の研究）

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Understanding of phase transitions and critical phenomena is one of the main topics in the statistical physics. In particular, the quantum criticality, which is accompanied by the second-order quantum phase transition, has caught much attention in these days. Unlike thermal phase transitions, quantum phase transitions occur at absolute zero temperature, triggered by quantum fluctuations. Through the quantum-classical mapping, a quantum phase transition in d dimensions, if it is of second order, can be generally described by the critical theory as the temperature-driven phase transition in a $(d + z)$-dimensional classical system with the same symmetries, where z is called *the dynamical exponent*.

Finding a novel kind of universality itself has much impact on the statistical physics. To this end, it is important to judge the universality with high precision if it is new one or not, when a new phase transition is suggested. As quantitative indices of the critical phenomena, critical exponents and critical amplitudes are generally used. At criticality, physical quantities typically show power-law behavior. The exponents of the physical quantities are universal, i.e., they depend only on the dimensionality and the symmetry property of the order parameter, and are independent from detailed structure of models under consideration, e.g. shape of lattices. Such universal exponents are called the critical exponents. A critical amplitude, defined as the ratio between two physical quantities that have the same exponents, also takes its universal value at a critical point only for isotropic systems. An advantage of analyzing the critical amplitude is its precision. It generally can be obtained with higher precision than the critical exponents. On the other hand, the amplitude has a disadvantage: it depends on the aspect ratio of models. We thus always need to optimize the aspect ratio in order to investigate the critical phenomena when using the critical amplitude.

Fortunately, recent enhancement of computational power together with development of simulation algorithms have enabled us to simulate larger-scale systems with higher precision than ever before and to elucidate the novel nature of quantum phase transitions, in which many-body physics plays an essential role. In the context of studying the critical phenomena, the combination of the world-line quantum Monte Carlo (WLQMC) with the finite-size scaling method is one of the most useful numerical tools because the WLQMC method can estimate the expectation value of physical quantities without any bias or approximation within the statistical error even for interacting many-body quantum systems. In the WLQMC simulation, although we are to work on finite-size and finite-temperature systems, there is no phase transition in finite-size systems because in such systems the partition function is analytic and differentiable. By using the finite-size scaling, the thermodynamic properties of the system can be obtained from the data of finite-size systems.

However, attention should be paid for anisotropic systems. In the WLQMC method, simulation of a d-dimensional quantum system is performed by mapping it to a $(d + 1)$-dimensional classical system. As a result, even for the case where the dynamical exponent $z = 1$ and interactions are spatially isotropic, there emerges an unknown constant factor of the ratio between the imaginary-time length and the system linear length, which is called *the velocity*. This inevitably introduces space-time anisotropy. Needless to say, if the system has anisotropic interactions, there is also intrinsic real-space anisotropy. When simulating such anisotropic systems, we often encounter some problems and/or difficulties as mentioned below.

In principle, the finite-size scaling analysis works for arbitrarily anisotropic systems. In practice, however, anisotropy of a system affects greatly from various aspects in finite-size scaling analysis. For example, it was reported that the universality class seems to change from the conventional to a novel one for a quantum spin model with the special pattern of anisotropic interactions, which is called the staggered dimer model. The universality class to which a model belongs does not depend on the detailed structure of the model, which implies the critical exponents of the staggered dimer model should be the same as the classical known values. However, it was reported that it was not the case with the staggered dimer model. This problem was resolved by using the WLQMC in combination with the aspect ratio optimization by the stochastic approximation. With the optimization, it has been shown that the critical amplitude of the Binder ratio for the staggered dimer model takes the universal value that is the same as the corresponding classical model.

In the present thesis, we have clarified the physical background that triggers the anomalous large corrections to scaling from the viewpoint of the low energy effective field theory. Using the bond operator representation, we can see the staggered dimer model has the weakly irrelevant cubic term in addition to the standard ϕ^4 action. The coefficients in one of the space dimensions (which we denote as x) and the imaginary-time directions of the action are renormalized in the same manner but the coefficient in the other space direction (y) is left unchanged. We have concluded that this renormalization of the coefficients triggers the system size dependence of the effective spatial aspect ratio between the x and y directions, which can be observed as the large corrections to scaling in the conventional finite-size scaling analysis.

It has also been demonstrated that we can estimate the dynamical exponent by using the aspect ratio optimization method. As mentioned, a quantum critical phenomenon in d space dimensions shares the same critical properties with the temperature-driven phase transition in a $(d + z)$-dimensional classical system with the same symmetries. This originates from the fact that the correlation length in the imaginary-time direction (denoted as ξ_τ) behaves as $\xi_\tau \propto \xi^z$ at a critical point, where ξ is the correlation length in the real space. It is difficult to know the dynamical exponent a priori, z is often assumed to be some value in advance of a simulation.

However, if the assumption is underestimated, the temperature becomes relatively higher as the system size grows. As a result, the system cannot reach its ground state. Although it is very important to know the dynamical exponent precisely, the way to estimate it has not been established. The system size including the imaginary-time direction is optimized based on the correlation length by using the above aspect ratio optimization, and thus it becomes possible to estimate the dynamical exponent unbiased.

As an example, we investigate the quantum phase transition of the quantum XY model in the presence of both the uniform magnetic field and the staggered magnetic field, whose amplitudes are denoted as h^{u} and h^{s}, respectively. If $h^{\mathrm{u}} = 0$, the particle-hole symmetry yields $z = 1$, whereas it is expected that z changes by applying $h^{\mathrm{u}} \neq 0$ due to vanishing of the symmetry. In fact, our method successfully detects the change of the dynamical exponent, and from the system-size dependence of the optimized imaginary-time length, we can conclude the dynamical exponent becomes two by imposing the uniform field.

Additionally, we extend the stochastic approximation method for random systems. By changing the realization of the randomness simultaneously with updating the parameters of the system, the averaged properties of the random systems can be obtained. In order to demonstrate the validity of the extended method, we have calculated the antiferromagnetic Heisenberg chains with random couplings. It is known that a random Heisenberg chain has a non-universal dynamical exponent that depends on the detail of the distribution function of the coupling constant. We have successfully estimated the dynamical exponents and have presented that we can judge a random system is critical or not by using the winding number squared.

In the last part of the present thesis, we applied the extended method to the XY model in the presence of random fields. This system is known to exhibit the quantum phase transition from the transverse ferromagnetic state to the so-called Bose-glass phase by changing the amplitude of the random field. There is a theoretical prediction that the dynamical exponent takes exactly the same value as the spatial dimension, namely $z = d$. For $d = 1$ and 3, this prediction is considered to be correct, however, according to the recent numerical simulations, the validity of the prediction for $d = 2$ was highly controversial. We employed the extended method as an unbiased way to estimate the dynamical exponent of the phase transition, and we have concluded that the dynamical exponent is estimated as $z = 1.91(1)$, which excludes the possibility of $z = d$ from the theoretical prediction for $d = 2$.

In summary, we have clarified the mechanism of non-trivial system size dependence of the effective aspect ratio in real space. We have also demonstrated that the aspect ratio optimization method can also be used for estimation of the dynamical exponent by simulation of the two-dimensional XY model in the presence of the magnetic fields. The optimization method has been extended for random systems and it has been demonstrated that the extended method works for the random bond Heisenberg chains. By using that extended method, the phase transition on the two-dimensional XY model in the presence of the random field has been discussed. We have ruled out that the possibility of $z = d$ from the theoretical prediction for $d = 2$. The extended method is a very efficient and unbiased way to estimate the critical properties especially for random systems. By using our method, we no longer need to scan high-dimensional parameter space or suffer from the problem that the number of disorder realization is enough. We believe our method helps to understand quantum critical phenomena more deeply than ever before and even to find novel criticalities.