論文の内容の要旨

論文題目

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 the phase transitions and the critical phenomena is one of the main topics in the statistical physics. When the phase transition occurs at absolute zero temperature by changing a parameter that controls the quantum fluctuation of the system, that transition is called the quantum phase transition. In the present thesis, we focus on the quantum critical phenomena, which are accompanied by the (second-order) quantum phase transitions. In the vicinity of the (quantum) critical point, various physical quantities show the power-law behavior, and their exponents, which are called the critical exponents, are useful tools to investigate the critical phenomena quantitatively. By using the sets of the critical exponents, we can classify the phase transition into some classes, each of which is called the universality class. To which universality class a critical phenomenon belongs is determined by the dimensionality and the symmetry, and does not depend on the detail structure of the system.

To discuss the universality of the phase transitions, various analytical and numerical tools have been invented so far. Especially, computer simulations have become much more important than ever before as recent growth of computing power. The combination of the quantum Monte Carlo (QMC) with the finite-size scaling method is one of the inevitable numerical tools because the QMC method can estimate the expectation value of physical quantities without any approximation within the statistical error even for the interacting many-body quantum systems. Therefore this combination enables to estimate precisely the critical exponents. In terms of this combination, it is another good idea to utilize the critical amplitude, which is defined as the ratio of the two physical quantities that diverge with the same exponent at the critical point. The critical amplitude is known to take the universal value at criticality and thus it provides information about the universality class of the phase transition. An advantage of the amplitude over the exponent is that the amplitude can be obtained more precisely than the exponent with the given computational resources in general. It however has a disadvantage of dependence on the aspect ratio of the system.

When simulating systems with anisotropic interactions, attention should be paid for the virtual aspect ratio. For example, suppose a two-dimensional system with $\xi_x \gg \xi_y$, where ξ_x (ξ_y) is the correlation length in x (y) direction. The virtual aspect ratio of this system is defined as $L_x/\xi_x : L_y/\xi_y$, where L_x (L_y) is the system linear length in x (y) direction. In this case, even if we take $L_x = L_y$, the system is not virtually isotropic. If the system is virtually isotropic, the critical amplitude of the system takes the universal value at the critical point, and we can investigate the critical phenomena much more precisely than the case where we only use the critical exponents. Moreover, there is another advantage in terms of the computational cost. The computational cost is in general a increasing function of $L_x \times L_y$. Given the condition that $L_x \times L_y$ is a constant, the optimal shape, which minimizes the systematic error, is realized if $L_x : L_y \approx \xi_x : \xi_y$. This condition is nothing but $L_x/\xi_x : L_y/\xi_y \approx 1 : 1$, virtually isotropic.

In the present thesis, the novel method is proposed that is able to optimize the size of the simulated systems automatically based on the stochastic approximation. By using this technique, it becomes possible to optimize the virtual aspect ratio without any prior knowledge. We tune the system linear length L_α to satisfy the relation $\xi_\alpha/L_\alpha = R$, where R is an α-independent constant. In our simulation, the simulation box consists of not only the real-space axis (x_1, x_2, …, x_d, where d is the space dimension) but also the imaginary-time axis (τ) because the quantum systems are mapped into the equivalent classical systems via the path integral together with introducing the imaginary-time direction. This means that the above relation should be satisfied for $\alpha = \tau, x_1, x_2, \ldots, x_d$. In our method, the optimization is performed iteratively in terms of the stochastic approximation. One first runs the short Monte Carlo simulation and measures ξ_α. Based on the result of the measurement, the system size is updated. Although the observables including ξ_α can be obtained always with the statistical errors, the stochastic approximation is robust against such kind of errors. The repetition of this procedure realizes the virtually isotropic system.

We utilized the above method and investigated the quantum critical phenomena that occur on the dimerized Heisenberg antiferromagnets on the square lattice, especially on the staggered dimer model and the columnar dimer model, that have the spatially anisotropic interactions. In the preceding study, it was reported that the staggered dimer model shows the different critical exponents from those of the columnar dimer model, and the authors claimed that the staggered dimer model belongs to the unconventional universality class. In this thesis, by precise calculations, it is shown that the critical phenomenon that the staggered dimer model shows is nothing but the conventional one. It is checked that the critical exponents and the critical amplitudes take the same value as those of other models including the columnar dimer model and the classical counterpart. It has been also demonstrated that the strong finite-size effect emerges due to the strong system-size dependence of the effective shape of the lattice (the anomalous anisotropic scaling). Our method can detect such a non-trivial size dependence of the aspect ratio and automatically recover the virtual isotropy.

The physical background that triggers the anomalous anisotropic scaling is also discussed from the viewpoint of the low energy effective field theory. Using the bond operator representation, we can see the dimerized antiferromagnets have the weakly irrelevant cubic term in the field theory in addition to the standard ϕ^4 action. It is explained in the present thesis the coefficients in one of the space dimensions (which we denote as x) and the imaginary-time directions of the standard ϕ^4 action are renormalized in the same manner but the coefficient in the other space direction (y) is left unchanged. This is the reason why the anomalous anisotropic scaling can be seen in the spatial aspect ratio L_y/L_x but not in L_τ/L_x.

The quantum critical phenomena along with the strong imaginary-time anisotropy have also been discussed. In quantum critical phenomena, the correlation length in the imaginary-time direction ξ_τ often behaves differently from that in the real space denoted as ξ even if the interactions are isotropic. The dynamical critical exponent, written as z, is used to describe such kind of anisotropy as $\xi_\tau \propto \xi^z$ at criticality. It is demonstrated that the present method successfully works for the model with $z \neq 1$. 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 $h^{\mathrm{s}} \neq 0$ 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 refer to some results obtained from application of the present method to the systems with randomness. The method is extended to simulate random systems. By changing the realization of the randomness simultaneously with updating the parameters of the system (based on the stochastic approximation procedure), the averaged properties of the random systems can be discussed. In order to demonstrate the validity of the extended method, we calculate the Heisenberg chain with the random coupling. The asymptotically exact ground state properties are already obtained by the renormalization group technique. After that the XY model in the presence of the random field is simulated with the extended procedure. 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. The value of the dynamical exponent, however, is highly controversial.

In summary, we have presented the finite-size scaling method with controlling anisotropy of the system. By using our method, which is based on the stochastic approximation, we can optimize the virtual aspect ratio of the system without any prior knowledge. We applied the method to the dimerized antiferromagnets and discussed the critical phenomena that show the non-trivial spatial anisotropy, i.e., anomalous anisotropic scaling. Additionally, our method reveals the mechanism of the extremely large corrections to scaling. The critical phenomena with the strong imaginary-time anisotropy are also investigated. We estimate the dynamical exponents of various phase transitions, which describe the anisotropy in the imaginary-time axis. The present method is extended and used as an unbiased way to determine the dynamical exponents of the systems with randomness.