Finite-temperature properties of extended Nagaoka ferromagnetism

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The itinerant ferromagnetism is a quantum phenomenon in which the electron correlation is essential. Microscopic origin of the itinerant ferromagnetism has been studied in the framework of the Hubbard model, which is a minimal model taking account of the electron motion and the Coulomb interaction between electrons. The Nagaoka ferromagnetism is a rigorous example of the realization of the ferromagnetic ground state in the Hubbard model. The Nagaoka ferromagnetism takes place in systems with one hole added to the half-filling and infinitely large Coulomb interaction on lattices that satisfy the so-called connectivity condition. However, the thermodynamic limit is problematic because one hole in the thermodynamic limit is not well defined. To overcome this difficulty, we have proposed an extended Nagaoka ferromagnetic model consisting of two parts: A part regarded as a main frame and a part that works as a particle bath, as illustrated in Fig. 1 [1,2]. We consider a concept of the Nagaoka ferromagnetism in the main frame. For this purpose, we set the number of electrons to that of sites in the main frame and control the distribution of electrons by the chemical potential of the particle bath, and thus we control the electron density in the main frame which is well defined in the thermodynamic limit. When there are no electrons in the particle bath, the main frame is half-filled, and the ground state is an insulating antiferromagnetic state. On the other hand, when the particle bath captures electrons, holes are introduced into the main frame, and the ground state is found to be an itinerant ferromagnetic state because of the Nagaoka mechanism in some parameter region. Thus, at zero temperature, this model shows a quantum phase transition between itinerant ferromagnetic and insulating antiferromagnetic states.

Here we note that the itinerant ferromagnetic state is induced by mobile electrons or holes travelling in the whole system. In contrast, the magnetic ordering in the localized spin system is caused by local exchange interactions between spins. Thus, we naively expect that ordering properties are different between itinerant electrons and localized spins at finite temperatures, although the ferromagnetic ground states in both cases are given by a symmetrized wavefunction with maximum total spin. To tackle this fundamental problem, we study finite-temperature properties of the model by numerical methods, such as exact diagonalization and random vector methods [3,4].

To clarify the ordering process of itinerant electron spins from a microscopic viewpoint, we measure the spin correlation function. Figure 2(a) presents the spin correlation function in the ferromagnetic ground-state regime. As the temperature increases, ferromagnetic correlations at long distances decay fast, while those in a short-range cluster persist up to relatively high temperatures. The temperature dependence of this development of ferromagnetic correlations is shown in Fig. 2(b). This kind of short-range ferromagnetic correlations at finite temperatures is observed even in the antiferromagnetic ground-state regime, as shown in Fig. 2(c). We see that the spin correlation changes its sign as a function of the temperature. That is, some neighboring spins that have antiferromagnetic correlations in the ground state show ferromagnetic correlations in a certain temperature range. Such a crossover cannot occur if we consider the antiferromagnetic Heisenberg model of localized spins. Thus, the ferromagnetic correlation originates from the motion of itinerant electrons in a short-range cluster, which is a special property of the present itinerant electron system in contrast to the localized spin system. It is an interesting future problem to study finite-temperature properties of other models for the itinerant ferromagnetism, such as a flat-band model and a Kondo-lattice model.

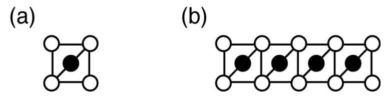

Fig. 1: (a) Unit structure of lattice, where open circles represent a main frame, and a solid circle is regarded as a particle bath. Solid lines denote the hopping connection between two sites. (b) Lattice built by arranging the units in one direction.

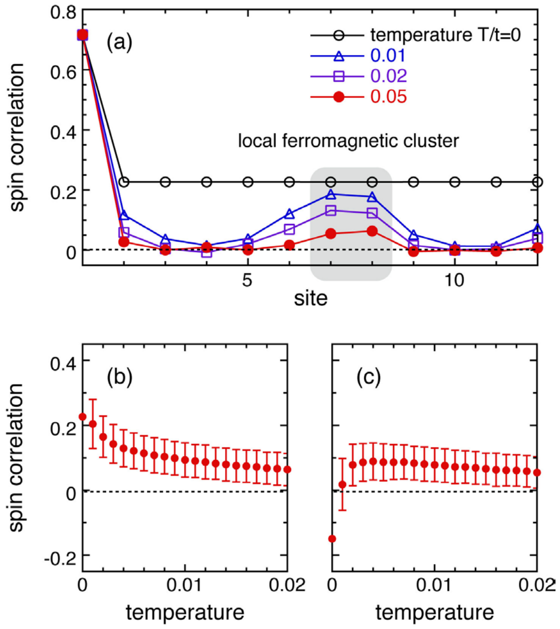

Fig. 2: (a) Spin correlation function measured at several temperatures in the ferromagnetic ground-state regime. Numerical results obtained by the random vector method for the Coulomb interaction U/t=500, the chemical potential of the particle bath μ/t=5, and the number of sites N=18. Note that the electron hopping t is taken as the energy unit. The temperature dependence of the spin correlation function between neighboring sites on the rung (b) in the ferromagnetic ground-state regime U/t=230 and μ/t=5 and (c) in the antiferromagnetic ground-state regime U/t=220 and μ/t=5. Here, N=12.

References

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