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Exact sign structure of the t–J chain and the single hole ground state

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Abstract

Injecting a single hole into a one-dimensional Heisenberg spin chain is probably the simplest case of doping a Mott insulator. The motion of such a single hole will generally induce a many-body phase shift, which can be identified by an exact sign structure of the model known as the phase string. We show that the sign structure is nontrivial even in this simplest problem, which is responsible for the essential properties of Mott physics. We find that the characteristic momentum structure, the Luttinger liquid behavior, and the quantum phase interference of the hole under a periodic boundary condition can all be attributed to it. We use the density matrix renormalization group (DMRG) numerical simulation to make a comparative study of the t–J chain and a model in which the sign structure is switched off. We further show that the key DMRG results can be reproduced by a variational wave function with incorporating the correct sign structure. Physical implications of the sign structure for doped Mott insulators in general are also discussed.

1. Introduction

How a doped hole propagates in a "vacuum" that is full of quantum spins is a central question in a doped Mott system [1,2]. On general grounds, one expects a "cloud of spin excitations" to

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be generated to accompany the motion of the hole. In a more conventional/weakly correlated system, a similar "cloud" forming around a testing particle is usually finite in size, remains featureless and rigid at low energy, which dresses only the particle's effective mass. The challenge arises, however, if the spin cloud becomes neither featureless nor rigid, or in other words, the motion of the hole becomes strongly-correlated in nature. Generally speaking, a new mathematical description will be needed here. The issue of the single hole problem has attracted intense attention since the discovery of the high-T_c cuprate, which is considered to be a doped Mott insulator [3].

In literature, the one-dimensional (1D) doped Mott systems have been well studied. The exact Bethe ansatz or the Lieb–Wu solution [4] exists for the Hubbard model at an arbitrary doping concentration and ratio of the on-site Coulomb repulsion U and the nearest-neighbor hopping integral t. In particular, the 1D t–J model can be solved exactly at $t/J \to \infty$ [5–7] and $t/J = 1/2$ [8–11] (J is the superexchange coupling), both of which behave like a Luttinger liquid [12,13] at finite doping. Numerically, the phase diagram has been also given via exact diagonalization (ED) [14,15] and the density matrix renormalization group (DMRG) [16] methods. As a matter of fact, based on the 1D exact solution, Anderson proposed [17] the idea of the unrenormalizable many-body phase shift, which is argued [1,18] to be generally responsible for the Luttinger liquid behavior in the doped Mott insulator. The quantitative characterization of such phase shift was later analytically identified [19–21] in the 1D t–J model. The ground state properties of the doped Hubbard model at $U \gg t$ or the t–J model at $J \ll t$ can be also approximated by the so-called squeezed spin chain description [6,7,19,20,22–25].

Nevertheless, a simple microscopic understanding is still much needed, even for the simplest one-hole-doped 1D case. By answering the question raised at the beginning of this paper, one may gain a deeper insight into the strong correlation nature of the Mott physics, which goes beyond the specific 1D geometry. Utilizing exact analysis and numerical methods, one hopes to clearly illustrate the single-hole's motion in an antiferromagnetic spin background qualitatively and quantitatively, which are relatively easier to handle in 1D. It may then provide important insights for the problem in two dimensions (2D), which is more relevant to cuprate superconductors and other strongly correlated materials.

In this paper, we investigate the ground state of the one-hole-doped 1D Heisenberg chain using the exact analysis, DMRG, and wave function approach based on a variational Monte Carlo (VMC) method. The main results are obtained as follows. First of all, we explicitly show that a nontrivial sign structure or phase string emerges once a hole is doped into the Heisenberg spin chain, which otherwise is statistical-sign free. Since such sign structure is present for any dimension, the 1D limit provides the simplest example to show its novel consequences. The detailed analyses will be given in Sec. 2. Secondly, in contrast to a bare hole state created by annihilating an electron in the half-filled ground state, the true hole ground state differs by a fundamentally changed momentum distribution, as well as the vanishing single-particle spectral weight, obeying a power-law scaling with the length of the chain. The phase string induced by one hole doping, as the singular many-body phase shift contributed by the spins in the vacuum, is responsible for the above momentum readjustment and the Luttinger liquid behavior. These will be confirmed by the DMRG simulations in Sec. 3. Furthermore, we show that a variational wave function constructed by incorporating the correct sign structure or the phase string can reproduce the DMRG results by using the VMC calculation in Sec. 4. Finally, in the summary section (Sec. 5), we will also discuss how the phase string sign structure plays a critical role in a general doped Mott insulator beyond the 1D case examined in the present work.