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Pseudofermion dynamical theory for the spin dynamical correlation functions of the half-filled 1D Hubbard model

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Abstract

A modified version of the metallic-phase pseudofermion dynamical theory (PDT) of the 1D Hubbard model is introduced for the spin dynamical correlation functions of the half-filled 1D Hubbard model Mott–Hubbard phase. The Mott–Hubbard insulator phase PDT is applied to the study of the model longitudinal and transverse spin dynamical structure factors at finite magnetic field h, focusing in particular on the singularities at excitation energies in the vicinity of the lower thresholds. The relation of our theoretical results to both condensed-matter and ultra-cold atom systems is discussed.

1. Introduction

The Hubbard model with nearest-neighbor hopping integral t and on-site repulsion U is possibly the most studied lattice system of correlated electrons. It features electrons that can hop between nearest-neighboring lattice sites due to the finite hopping integral t. When two electrons are on the same site, they have to pay the energy U due to their mutual repulsion. This introduces

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additional electronic correlations beyond those due to the Pauli principle. The model properties depend on the ratio $u \equiv U/4t$.

The calculation of dynamical correlation functions is one of the main challenges in low-dimensional theories. Some systems with spectral gap can be dealt with by the form-factor approach to quantum correlation functions [1–7]. The advantage of this method is that it is in principle not constrained to very low energies. The form-factor approach can also be implemented for spin lattice systems such as the Heisenberg *XXX* and *XXZ* chains [8–13].

The 1D Hubbard model is solvable by the Bethe ansatz (BA) [14–17]. This technique provides the exact spectrum of the energy eigenstates, yet it has been difficult to apply to the derivation of high-energy dynamical spectral and correlation functions. (In this paper we use the designation *high energy* for all energy scales larger than the model low-energy limit associated with the Tomonaga–Luttinger-liquid regime [18–21].) For instance, form factors of the 1D Hubbard model electronic creation and annihilation operators is an open problem that has not been solved. Even the eventually easier problem of determining form factors of the spin operators in the Hubbard model at finite magnetic field remains as well unsolved. For the model metallic phase, the method used in Refs. [22,23] has been the first breakthrough to address the problem of the high-energy dynamical correlation functions in the $u \rightarrow \infty$ limit. Specifically, in these references the one-electron spectral functions of the model metallic phase have been derived for the whole (k, ω) plane. That method relies on the spinless-fermion phase shifts imposed by Heisenberg spins $1/2$. Such elementary objects naturally arise from the $u \rightarrow \infty$ electron wave-function factorization [24–26].

A related pseudofermion dynamical theory (PDT) relying on a representation of the model BA solution in terms of the pseudofermions generated by a unitary transformation from the corresponding pseudoparticles considered in Ref. [27] was introduced in Refs. [28,29]. It is an extension of the $u \rightarrow \infty$ method of Refs. [22,23] to the whole finite $u > 0$ range of the metallic phase of the 1D Hubbard model. A key property is that the pseudofermions are inherently constructed to their energy spectrum having no interaction terms. This allows the expression of the dynamical correlation functions in terms of pseudofermion spectral functions. However, creation or annihilation of pseudofermions under transitions to excited states imposes phase shifts to the remaining pseudofermions. Within the PDT such phase shifts fully control the one- and two-electron spectral-weight distributions over the (k, ω) plane.

The PDT of Refs. [28,29] has been the first breakthrough for the derivation of analytical expressions of the metallic phase of the 1D Hubbard model high-energy dynamical correlation functions for the whole finite $u > 0$ range. Applications of the 1D Hubbard model metallic-phase PDT to the study of spectral features of actual condensed-matter systems are presented in Refs. [30–33].

After the PDT for the metallic phase of the 1D Hubbard model was introduced, a set of novel methods have been developed to also tackle the high-energy physics of 1D correlated quantum problems, beyond the low-energy Tomonaga–Luttinger-liquid limit [34]. In the case of the 1D Hubbard model such methods reach the same results as the PDT. For instance, the momentum, electronic density $n_e < 1$, and on-site repulsion $u = U/4t > 0$ dependence of the exponents that control the line shape of the one-electron spectral function of the model metallic phase calculated in Refs. [35,36] in the framework of a mobile impurity model using input from the BA solution is exactly the same as that obtained previously by use of the metallic-phase PDT [30–33].

However, the latter PDT as reported in Refs. [28,29] does not apply to the study of the spin dynamical correlation functions of the 1D Hubbard model Mott–Hubbard insulator phase, which for the whole $u > 0$ range corresponds to electronic density $n_e = 1$. (For that density it is usually