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Quantum critical phenomena, entanglement entropy and Hubbard model in 1d with the boundary site with a negative chemical potential $-p$ and the Hubbard coupling U positive

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ABSTRACT

Recently the ground state and some excited states of the half-filled case of the 1d Hubbard model were discussed exactly for an open chain with L sites. The case when the boundary site has the chemical potential $-p$ and the Hubbard coupling U is positive was considered. We model $CeAl_2$ nanoparticles, in which a valence of $4f$ electron number changes on surface Ce atoms, by this Hubbard model. A surface phase transition exists at some critical value p_{c3} of chemical potential (its absolute value) p in the model; when $p < p_{c3}$ all the charge excitations have the gap, while there exists a massless charge mode when $p > p_{c3}$. The aim of this Letter is to find whether this surface phase transition is of the first order or of the second order. We have found that the entanglement entropy and its derivative has a discontinuity at p_{c3} in general and thus this transition is of the first order (with exception of two points for the probability w_2 of occurrence of two electrons with opposites spins on the same site). There is a divergence in the difference of entanglement entropy for points $w_2 = 0$ and $w_2 = \frac{1}{2}$. The first point $w_2 = 0$ corresponds to ferro- (antiferro-) magnetic state at half-filled case. The second point $w_2 = \frac{1}{2}$ does not correspond to any state for halffilled case. In the first case there is present the surface phase transition of the second order type.

1. Introduction

Quantum critical phenomena are phenomena where the transition is driven by quantum effects in the system of many electrons and bosons. Quantum phase transition (QPT) with nonstandard behaviour was described in [1]. It is a phase transition and a critical behaviour deviating from the standard scheme based on the mean field theory renormalising only the mass of the critical excitations and with a perturbative scaling renormalisation of the interaction strength. Heavy fermion system $CeAl_2$ in bulk exhibits localised $4f^{(1)}$ electrons with antiferromagnetic magnetic ordering and Kondo behaviour [2] at low temperatures. The magnetic behaviour is very sensitive to the degree of electron localisation. The Ce atoms show a small amount of delocalised $4f^{(0)}$ character with Kondo behaviour [3]. As it was observed in [4] the change of valence in Ce atoms is occurring on the surface of $CeAl_2$ nanoparticles where the coordination number is changing. The $CeAl_2$ material is used in catalysis of carbon monoxide and carbon dioxide methanation f.e., see [5].

To model the change of valence of Ce atoms on the surface of $CeAl_2$ nanoparticles qualitatively we may use a simple model of a chain of atoms with $4f$ electrons described by the 1d Hubbard model with a finite number L of atoms. While this model is a simple model, it may give a qualitative description of change of valence on the surface of $CeAl_2$ nanoparticles. Surface effects may be described with a chemical potential different at the boundary site (surface) from the chemical potential on bulk sites. For simplicity we consider a chain of sites with one boundary (surface) site. The other end site of the chain in the model has the same chemical potential as sites of bulk atoms and describes an atom at the centre of the nanoparticle. Then there is a question whether changing the chemical potential on the boundary (surface) site may change quantum state on the boundary (surface) site and on the chain. The answer to this question may describe changes of valence on the surface of $CeAl_2$ nanoparticles described above.

The 1d Hubbard Hamiltonian model with open-boundary conditions, in which the first site has the local chemical potential $-p$, has the form:

$$H = -t \sum_{j=1}^{j=L-1} \sum_{\sigma=u,d} (c^*_{j,\sigma} c_{j+1,\sigma} + c^*_{j+1,\sigma} c_{j,\sigma}) + U \sum_{j=1}^{L} n_{j,u} n_{j,d} + p \sum_{\sigma} n_{1,\sigma}. \quad (1)$$

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Here $c_{j,\sigma}$, $c^*_{j,\sigma}$ and $n_{j,\sigma}$ are annihilation, creation and number operators of an electron localised at the jth site, $j = 1, \ldots, L$ with spin $\sigma = u$–up, d–down. U denotes the Hubbard interaction energy and t is the transfer energy. This system with open boundary conditions with $p \geqslant 0$ was discussed in [6].

Criticality in the 1d Hubbard model was studied recently using entanglement scaling. Entanglement entropy is a quantity which characterises nonlocal correlations in quantum systems. There is a connection between the entanglement entropy of a many particle system and the quantum critical phenomena. Discontinuity in the entanglement entropy derivative is [7–11] and [12] associated with the first order QPT, singularity with the second order. Entanglement describes how the associated nonlocal quantum correlations influence the critical behaviour of a quantum phase transition. As noted by authors [8] to what extent their results can be generalised to other quantum systems is yet to be answered. In this Letter we will discus entanglement for the 1d Hubbard model with the boundary site with a negative chemical potential $-p$ and the Hubbard energy U positive for a finite number L of atoms in the chain. The transition from the $4f^{(1)}$ magnetic state on the surface Ce atoms to the nonmagnetic $4f^{(0)}$ state in $CeAl_2$ nanoparticles has character of a 1st order surface phase transition in general (with exception of two points for the probability $w_2 = \langle n_{ju} n_{jd} \rangle \leqslant \frac{1}{2}$).

2. Quantum critical phenomena and entanglement

The Hubbard model displays many features which are close to real properties of materials with strong electron–electron interactions. Some rigorous results concerning this model are described in [13]. These results and the entanglement entropy concept mentioned in the preceding section enable us to study the quantum critical phenomena in the 1d Hubbard model.

Exact solution of the Hubbard model with boundary hoppings and fields was found in [14] by the Bethe ansatz method. It was found that for certain values of the boundary hopping integrals and fields the ground state contains boundary bound states. While in [8] the authors assume periodic boundary conditions, in [14] the boundary conditions are such that periodicity is broken. The Hamiltonian in [8] is translational invariant and conserves particle number and the z component of the total spin. When the boundary fields and hoppings are present then this symmetry is broken. However boundary fields and hoppings are expected to play no role in the limit of large finite lattice, $L \to \infty$. The energy of the ground state will contain a term proportional to the number L of sites which correspond to the bulk energy, the term proportional to L^0 which corresponds to the surface energy and following terms are proportional to L^{-n} where L and n are positive integers. The reduced density matrix ρ_j for a single site j, $j = 1, \ldots, L$, is diagonal in the chosen basis for periodic boundary conditions. The single-site entanglement entropy E of the ground state for the model Hamiltonian (1) and for the site j can be written [8] in the form:

$$E = -w_0 \log_2(w_0) - w_u \log_2(w_u) - w_d \log_2(w_d) - w_2 \log_2(w_2), \tag{2}$$

where

$$w_2 \equiv \langle n_{ju} n_{jd} \rangle, \qquad w_\alpha \equiv \langle n_{j\alpha} \rangle - w_2, \qquad w_0 = 1 - w_u - w_d - w_2, \tag{3}$$

where $\alpha = u, d$ are indices for spin up and spin down respectively, and j is a site index, $j = 1, \ldots, L$. Here $\langle n_{j\alpha} \rangle$ is a mean value of the occupation number $n_{j\alpha}$ in the ground state.

We will consider the strong correlation limit of large ratio u of correlation energy U to the transfer integral t, $|u| \equiv |\frac{U}{4t}| \gg 1$. The Hellman–Feynman theorem, $\langle \frac{\partial H}{\partial u} \rangle_0 = \frac{\partial E_0}{\partial u}$ gives for the energy E_0 of the ground state of the system with a boundary atom i.e. for a system which is not translational invariant, the mean value of the quantity w_2

$$w_2 = \frac{1}{L} \sum_{j=1}^{j=L} \langle n_{ju} n_{jd} \rangle. \tag{4}$$

We will use the units in which $t = 1$ in the following. For a finite L Eq. (4) is a sum of a finite number of terms – probabilities with which are sites occupied by two electrons with opposite spins – which depends on the chemical potential $-p$. A sum of a finite number of functions of the argument $-p$ which are without a discontinuity in p cannot lead to a function with a discontinuity. If there exists at least one term with a discontinuity in p in the sum (4) then the quantity w_2 in (4) has a discontinuity, with the exception of some special cases. Then also the entanglement entropy E (2) defined through the quantity w_2 will have a discontinuity and its derivative too in general. In such a case there exists a first order phase transition in this a system.

3. Hubbard model in 1d with the boundary site with a negative chemical potential $-p$ and the Hubbard coupling U positive

The Bethe ansatz result for the ground state energy gives energy proportional to L, the number of sites in the lattice. There is present also a contribution to this energy from the surface which is of the order of L^0, and contributions of the order of L^{-1} and of the lower orders, as we mentioned above and see in [15]. The surface energy for the boundary fields was calculated exactly for the XXZ chain model by the Bethe ansatz in [16]. The energy is an analytic function of the field h, where $h = h_1 = -h_2$, for the case in which there are opposite oriented fields h_1 and $-h_2$ on boundaries. While there are identified critical fields h_{1c} and h_{2c} as fields below which and above which respectively (in absolute values) there are present 1-string boundary states in the chain, for fields with values in between h_{1c} and h_{2c} there are no boundary strings. Then using the entanglement entropy we find that there is no discontinuity or divergence in its derivative for this case. There is no quantum phase transition changing boundary fields thus. The XXZ model is related to the Hubbard model by a canonical transformation. We can then expect that at the spin sector of solutions of the Hubbard model with boundary fields and hoppings there is no surface phase transition.

Let us now concentrate on the charge sector. In [6] the Hubbard model (1) is discussed for the ground state and some excited states of the half-filled band case for an open chain with L sites. Only one of the boundary sites has a different value of the chemical potential in this case. Authors [6] considered the case when the boundary site has a negative chemical potential $-p$ and the Hubbard coupling U is positive, see (1). They have shown by an analytic method that when p is larger than some critical value some of the ground-state solutions of the Bethe ansatz equations become complex-valued. They have found, among other findings, that there is a surface phase transition at a critical value p_{3c}; when $p < p_{3c}$ all the charge excitations have the gap for this case, while there exists a massless charge mode when $p > p_{3c}$. The authors did not discuss whether the surface phase transition is of the first or of the second order in the sense discussed above for the entanglement entropy.

The surface energy of the ground state has the form