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Effective Hamiltonian for a half-filled Hubbard chain with alternating on-site interactions

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Abstract

We derive an effective spin Hamiltonian for the one-dimensional half-filled alternating Hubbard model in the limit of strong on-site repulsion. We show that the effective Hamiltonian is a spin $S = 1/2$ Heisenberg chain with asymmetric next-nearest-neighbour (nnn) exchange.

1. Introduction

During the last two decades the correlation induced metal–insulator (Mott) transition has been a challenging problem in condensed matter physics [1]. In most cases the breaking of spatial symmetry is a prerequisite for a Mott insulator [2]. The undoped high-T_c copper-oxide materials are famous examples of such Mott insulators [3]. However, the one-dimensional Hubbard model [4]

$$\mathcal{H}_{\rm Hub} = t \sum_{i,j,\alpha} N_{i,j} c^{\dagger}_{i,\alpha} c_{j,\alpha} + U \sum_{i} n_{i,\uparrow} n_{i,\downarrow} \tag{1}$$

at half-filling represents a case where dynamical generation of a charge gap is not connected with the breaking of a discrete symmetry [5]. In equation (1) we have used standard notations: $n_{i,\alpha} = c^{\dagger}_{i,\alpha} c_{i,\alpha}$, U is the Hubbard on-site repulsive interaction, and $N_{i,j} = 1$ if i and j are labels for neighbouring sites and equals zero otherwise. Thus the kinetic part represents hops between neighbouring sites and the interaction part gives contributions only from electrons on the same site. At half-filling the exact solution shows a uniform ground state with exponentially suppressed density correlations [6] and gapless $SU(2)$ symmetric spin degrees of freedom [7]. This is in agreement with the large-U expansion result, that at $U \gg |t|$ the model (1) is equivalent to the effective spin $S = 1/2$ Heisenberg antiferromagnet Hamiltonian [8],

$$\mathcal{H}_{\rm Heis} = J \sum_{i} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J' \sum_{i} \mathbf{S}_i \cdot \mathbf{S}_{i+2}, \tag{2}$$

where $J = 4t^2/U(1 - 4t^2/U^2)$, $J' = 4t^4/U^3$ in the fourth-order perturbation. Several very elegant mathematical tools have been developed for calculation of the effective spin-chain Hamiltonians in higher orders [10–12]. However, in agreement with the exact solution [5], higher-order terms are irrelevant and the ground state remains featureless.

Discussions of the Mott–Hubbard transition within the framework of Hubbard type models are generally restricted to lattices of equivalent sites. However, the less common case where the spatial invariance of the system is broken via the introduction of two types of atoms, say 'anions' and 'cations', has attracted much recent interest. In the simplest case of a two-site ionic generalization of the Hubbard model we obtain a Hamiltonian of the two-band Hubbard model [13]

$$\mathcal{H} = t\sum_{i,j,\alpha} N_{i,j} c^{\dagger}_{i,\alpha} c_{j,\alpha} + \frac{\Delta}{2}\sum_{i,\alpha}\left(n_{2i,\alpha} - n_{2i+1,\alpha}\right) + U_{\mathrm{e}}\sum_{i} n_{2i,\uparrow} n_{2i,\downarrow} + U_{\mathrm{o}}\sum_{i} n_{2i+1,\uparrow} n_{2i+1,\downarrow}. \tag{3}$$

In the limit $\Delta = 0$ and $U_{\mathrm{e}} = U_{\mathrm{o}} = U$ equation (3) reduces to the ordinary Hubbard model. The limit $U_{\mathrm{e}} = U_{\mathrm{o}} = U$, $\Delta \neq 0$, is called the ionic Hubbard model (IHM) [14]. In this paper we study the alternating Hubbard model (AHM) [15] obtained from equation (3) in the limit $\Delta = 0$.

The IHM and the AHM describe two different ways in which the lattice invariance can be broken. In the IHM the broken translational symmetry is already traced by non-interacting electrons, via the *single-electron* potential energy difference between neighbouring sites (Δ). In marked contrast with the IHM the lattice unit in the AHM is doubled *dynamically*, via the different *two-electron* on-site repulsion energy on even (U_{e}) and odd (U_{o}) sites.

Current interest in the study of the Mott transition in 1D models with broken translational symmetry was triggered by the bosonization analysis of the ionic Hubbard model (IHM) by Fabrizio, Nersesyan and Gogolin (FGN) [16]. At $U = 0$ the IHM is a regular band insulator with long-range ordered charge-density wave (CDW), while in the strong-coupling limit at $U \gg t, \Delta$ it is a Mott insulator with a charge gap and gapless spin sector. The spin sector is also given by the same Heisenberg chain (2), but with slightly renormalized coupling constants [14]

$$J = \frac{4t^2}{U}\left[\frac{1}{1-\lambda^2} - \frac{4t^2}{U^2}\frac{(1+4\lambda^2-\lambda^4)}{(1-\lambda^2)^3}\right], \qquad J' = \frac{4t^4}{U^3}\frac{(1+4\lambda^2-\lambda^4)}{(1-\lambda^2)^3}, \tag{4}$$

where $\lambda = \Delta/U$.

The bosonization analysis shows that the CDW–Mott insulator transition has a complicated two-step nature [16]: with increasing U there is first an *Ising type transition* from a CDW band phase into a LRO dimerized phase at $U^{\mathrm{c}}_{\mathrm{ch}}$. With further increase of the Hubbard repulsion, at $U^{\mathrm{c}}_{\mathrm{sp}} > U^{\mathrm{c}}_{\mathrm{ch}}$ a continuous *Kosterlitz–Thouless transition* takes place from the dimerized into an MI phase. The charge gap vanishes *only* at $U = U^{\mathrm{c}}_{\mathrm{ch}}$, while the spin sector is gapless for $U > U^{\mathrm{c}}_{\mathrm{sp}}$. This phase diagram was later confirmed by various numerical and analytical studies [17–21]. Moreover, these numerical studies reveal a rather complex nature of the strong-coupling, $U \gg \Delta, t$, insulating phase of the IHM. Although the spin sector of the IHM in the strong-coupling limit is qualitatively similar to that of the ordinary Hubbard model, the ground state is characterized by an LRO CDW pattern and therefore shows broken translational symmetry [18–20].

In this paper we derive the effective spin Hamiltonian in the strong-on-site-repulsion limit $U_{\mathrm{e}}, U_{\mathrm{o}} \gg t$ of the AHM. As we show below, in marked contrast with the ordinary Hubbard and the ionic Hubbard models, in the case of AHM the effective spin Hamiltonian is not translational invariant and is given by a frustrated Heisenberg chain with alternating next-nearest-neighbour

exchange

$$\mathcal{H}_{\rm eff} = J\sum_i \mathbf{S}_i \cdot \mathbf{S}_{i+1} + \sum_i (J' - (-1)^i \delta J')\mathbf{S}_i \cdot \mathbf{S}_{i+2}, \tag{5}$$

where

$$J = 2t^2\left(\frac{1}{U_{\rm o}} + \frac{1}{U_{\rm e}}\right) - 2t^4\left(\frac{3}{U_{\rm o}^3} + \frac{3}{U_{\rm e}^3} + \frac{1}{U_{\rm o}^2 U_{\rm e}} + \frac{1}{U_{\rm o} U_{\rm e}^2}\right), \tag{6}$$

$$J' = 2t^4\left(\frac{1}{U_{\rm o}^3} + \frac{1}{U_{\rm e}^3}\right), \qquad \delta J' = 2t^4 \frac{U_{\rm o} - U_{\rm e}}{U_{\rm o}^2 U_{\rm e}^2}. \tag{7}$$

The obtained effective Hamiltonian is the $S = \frac{1}{2}$ shark-tooth Hamiltonian [9], the limiting case of which ($U_{\rm e} = U_{\rm o} = U$) is a well known result for the Hubbard model.

2. The strong-coupling expansion approach

In this paper we apply the method developed by MacDonald *et al* in the case of the ordinary Hubbard chain [11] to obtain the effective spin Hamiltonian for the one-dimensional *alternating Hubbard model* given by the Hamiltonian $\mathcal{H}_{\rm AHM} = \hat{T} + \hat{V}$, where

$$\hat{T} = t\sum_{i,j,\alpha} N_{i,j} c^{\dagger}_{i,\alpha} c_{j,\alpha} \tag{8}$$

$$\hat{V} = U_{\rm e}\sum_i n_{2i,\uparrow} n_{2i,\downarrow} + U_{\rm o}\sum_i n_{2i+1,\uparrow} n_{2i+1,\downarrow}. \tag{9}$$

In what follows we consider the strong-coupling limit, assuming $U_{\rm e} > U_{\rm o} \gg |t|$. In contrast to the case of the ordinary Hubbard model where subbands can be classified by the total number of double-occupied states (doublons) $N_{\rm d}$, in the case of AHM we have to deal with a system where each band is characterized by two different numbers: the number of doubly occupied sites in even and odd sublattices, denoted by $N_{\rm de}$ and $N_{\rm do}$ respectively. The hopping term mixes states from these subbands. The 'unmixing' of the AHM subbands can be achieved by introducing suitable linear combinations of the uncorrelated basic states. The $\mathcal{S}$ matrix for this transformation, and the transformed Hamiltonian,

$$\mathcal{H}_{\rm eff} = {\rm e}^{{\rm i}\mathcal{S}} \mathcal{H}_{\rm AHM} {\rm e}^{-{\rm i}\mathcal{S}},$$

are generated by an iterative procedure, which results in an expansion in powers of the hopping integral t divided by on-site energies $U_{\rm e}$ and/or $U_{\rm o}$.

This expansion is based on a separation of the kinetic part of the Hamiltonian into three terms: T_1 which increases the number of doubly occupied sites by one, T_{-1} which decreases the number of doubly occupied sites by one and T_0 which leaves the number of doubly occupied sites unchanged. In addition, in the case of the alternating Hubbard model each of these terms splits into several different terms, depending on whether corresponding hopping process takes place from even to odd sites or vice versa.

In particular, we split the T_0 term into three separate hopping processes:

$$T_0 = T_0^0 + T_0^{\rm de} + T_0^{\rm do}, \tag{10}$$

where

$$T_0^0 = t\sum_{i,j,\alpha} N_{i,j} h_{i,-\alpha} c^{\dagger}_{i,\alpha} c_{j,\alpha} h_{j,-\alpha}, \tag{11}$$

is a 'hole' hopping term,

$$T_0^{\rm de} = t\sum_{i,j,\alpha} N_{2i,j} n_{2i,-\alpha} c^{\dagger}_{2i,\alpha} c_{j,\alpha} n_{j,-\alpha}, \tag{12}$$

is a 'pair' hopping term which hops a pair to an even site and

$$T_0^{\mathrm{do}} = t \sum_{i,j,\alpha} N_{2i+1,j} n_{2i+1,-\alpha} c^{\dagger}_{2i+1,\alpha} c_{j,\alpha} n_{j,-\alpha}, \tag{13}$$

is a 'pair' hopping term which hops a pair to an odd site. Here $h_{i,\alpha} = 1 - n_{i,\alpha}$.

The term which increases the number of doubly occupied sites by one is also separated into two terms, $T_1 = T_1^{\mathrm{e}} + T_1^{\mathrm{o}}$, where

$$T_1^{\mathrm{e}} = t \sum_{i,j,\alpha} N_{2i,j} n_{2i,-\alpha} c^{\dagger}_{2i,\alpha} c_{j,\alpha} h_{j,-\alpha}, \tag{14}$$

is the term which increases the number of doubly occupied sites by one on the sublattice of even sites and

$$T_1^{\mathrm{o}} = t \sum_{i,j,\alpha} N_{2i+1,j} n_{2i+1,-\alpha} c^{\dagger}_{2i+1,\alpha} c_{j,\alpha} h_{j,-\alpha}, \tag{15}$$

is the term which increases the number of doubly occupied sites by one on the sublattice of odd sites.

Similarly, the term which decreases the number of doubly occupied sites by one is also separated into two terms, $T_{-1} = T_{-1}^{\mathrm{e}} + T_{-1}^{\mathrm{o}}$, where

$$T_{-1}^{\mathrm{e}} = t \sum_{i,j,\alpha} N_{i,2j} h_{i,-\alpha} c^{\dagger}_{i,\alpha} c_{2j,\alpha} n_{2j,-\alpha} \tag{16}$$

and

$$T_{-1}^{\mathrm{o}} = t \sum_{i,j,\alpha} N_{i,2j+1} h_{i,-\alpha} c^{\dagger}_{i,\alpha} c_{2j+1,\alpha} n_{2j+1,-\alpha}, \tag{17}$$

are the terms which decrease the number of doubly occupied sites by one on the sublattices of even and odd sites, respectively.

One can easily check the following commutation relations:

$$[\hat{V}, T_m^q] = (m + \delta_{m,0}) \Lambda_q T_m^q, \tag{18}$$

where

$$\Lambda_q = \begin{cases} U_q, & q = \mathrm{e}, \mathrm{o} \\ (U_{\mathrm{e}} - U_{\mathrm{o}}), & q = \mathrm{de} \\ (U_{\mathrm{o}} - U_{\mathrm{e}}), & q = \mathrm{do} \\ 0, & q = 0. \end{cases} \tag{19}$$

We must emphasize that equation (18) is true in all cases where allowed hopping processes connect only sublattices with different on-site repulsions.

Let us now start to search for such a unitary transformation $\mathcal{S}$, which eliminates hops between states with different numbers of doubly occupied sites:

$$\mathcal{H}' = \mathrm{e}^{\mathrm{i}\mathcal{S}} \mathcal{H} \mathrm{e}^{-\mathrm{i}\mathcal{S}} = \mathcal{H} + [\mathrm{i}\mathcal{S}, \mathcal{H}] + \tfrac{1}{2}[\mathrm{i}\mathcal{S}, [\mathrm{i}\mathcal{S}, \mathcal{H}]] + \cdots. \tag{20}$$

We follow the recursive scheme [11] which allows us to determine a transformation which has the requested property to any desired order in t/U where $U = (U_{\mathrm{e}} + U_{\mathrm{o}})/2$. To proceed further we define

$$T^{(k)}[\{a\}, \{m\}] = T_{m_1}^{a_1} T_{m2}^{a_2} \cdots T_{m_k}^{a_k}. \tag{21}$$

Using equation (18) we can write

$$[\hat{V}, T^{(k)}[\{a\}, \{m\}]] = \sum_{i=1}^{k} \Lambda_{a_i} (m_i + \delta_{m_i,0}) T^{(k)}[\{a\}, \{m\}]. \tag{22}$$

$\mathcal{H}'^{(k)}$ contains terms of order t^k, denoted by $\mathcal{H}'^{[k]}$, which couple states in different subbands. By definition $[V, \mathcal{H}'^{[k]}] \neq 0$ and $\mathcal{H}'^{[k]}$ can be expressed in the following way:

$$\mathcal{H}'^{[k]} = \sum_{\{a\}} \sum_{\{m\}} C^{(k)}_{\{a\}}(\{m\}) T^{(k)}[\{a\}, \{m\}], \qquad \sum_{i=1}^{k} m_i \neq 0. \tag{23}$$

If in each k th order step we choose $\mathcal{S}^{(k)} = \mathcal{S}^{(k-1)} + \mathcal{S}^{[k]}$, where $\mathcal{S}^{[k]}$ is the solution of the equation

$$[\mathrm{i}\mathcal{S}^{[k]}, V] = -\mathcal{H}'^{[k]} \tag{24}$$

and therefore given by

$$\mathcal{S}^{[k]} = -\mathrm{i} \sum_{a,\{m\}} \frac{C^{(k)}_{\{a\}}(\{m\})}{\sum_{i=1}^{k} \Lambda_{a_i}(m_i + \delta_{m_i,0})} T^{(k)}[\{a\}, \{m\}], \qquad \sum_{i=1}^{k} m_i \neq 0, \tag{25}$$

then the transformed Hamiltonian

$$\mathcal{H}'^{(k+1)} = \mathrm{e}^{\mathrm{i}\mathcal{S}^{(k)}} \mathcal{H} \mathrm{e}^{-\mathrm{i}\mathcal{S}^{(k)}} \tag{26}$$

contains terms of order t^k/U^{k-1} which commute with the unperturbed Hamiltonian and mix states within each subband only.

3. The Hubbard operators

To treat correlations properly, it is important to know whether at the beginning or at end of the hopping process a particular site is doubly occupied or not. The introduction of so-called Hubbard operators [22] provides us with the tool necessary for such a full description of the local environment. The X_j^{ab}-operator is determined on each site of the lattice and describes all possible transitions between the local basis states: unoccupied $|0\rangle$, singly occupied with 'up'-spin $|+\rangle$ and 'down'-spin $|-\rangle$ and doubly occupied $|2\rangle$. The original electron creation (annihilation) operators can be expressed in terms of the Hubbard operators in the following way:

$$c^{\dagger}_{i,\alpha} = X_i^{\alpha 0} + \alpha X_i^{2-\alpha} \qquad c_{i,\alpha} = X_i^{0\alpha} + \alpha X_i^{-\alpha 2}. \tag{27}$$

Correspondingly, in terms of creation (annihilation) operators the Hubbard operators have the form

$$\begin{aligned} X_i^{\alpha 0} &= c^{\dagger}_{i,\alpha}(1 - n_{i,-\alpha}), & X_i^{2\alpha} &= -\alpha c^{\dagger}_{i,-\alpha} n_{i,\alpha}, \\ X_i^{\alpha -\alpha} &= c^{\dagger}_{i,\alpha} c_{i,-\alpha}, & X_i^{20} &= -\alpha c^{\dagger}_{i,-\alpha} c^{\dagger}_{i,\alpha}, \\ X_i^{00} &= (1 - n_{i,\uparrow})(1 - n_{i,\downarrow}), & X_i^{22} &= n_{i,\uparrow} n_{i,\downarrow} \\ X_i^{\alpha\alpha} &= n_{i,\alpha}(1 - n_{i,-\alpha}). \end{aligned} \tag{28}$$

The Hubbard operators which contain even (odd) number of electron creation and annihilation operators are Bose-like (Fermi-like) operators. They obey the on-site multiplication rules $X_i^{pq} X_i^{rs} = \delta_{q,r} X_i^{ps}$ and commutation relations

$$[X_i^{pq}, X_j^{rs}]_{\pm} = \delta_{ij}(\delta_{qr} X_j^{ps} \pm \delta_{ps} X_j^{rq}), \tag{29}$$

where the upper sign corresponds to the case when both operators are Fermi-like; otherwise, the lower sign should be adopted.

It is straightforward to obtain that

$$T_0^0 = t\sum_{i,j}\sum_{\alpha} N_{i,j} X_i^{\alpha 0} X_j^{0\alpha}, \tag{30}$$

$$T_0^{\mathrm{do}} = t\sum_{i,j}\sum_{\alpha} N_{2i+1,j} X_{2i+1}^{2-\alpha} X_j^{-\alpha 2}, \qquad T_0^{\mathrm{de}} = t\sum_{i,j}\sum_{\alpha} N_{2i,j} X_{2i}^{2-\alpha} X_j^{-\alpha 2} \tag{31}$$

$$T_1^{\mathrm{o}} = t\sum_{i,j}\sum_{\alpha} \alpha N_{2i+1,j} X_{2i+1}^{2-\alpha} X_j^{0\alpha}, \qquad T_1^{\mathrm{e}} = t\sum_{i,j}\sum_{\alpha} \alpha N_{2i,j} X_{2i}^{2-\alpha} X_j^{0\alpha} \tag{32}$$

$$T_{-1}^{\mathrm{o}} = t\sum_{i,j}\sum_{\alpha} \alpha N_{i,2j+1} X_i^{\alpha 0} X_{2j+1}^{-\alpha 2}, \qquad T_{-1}^{\mathrm{e}} = t\sum_{i,j}\sum_{\alpha} \alpha N_{i,2j} X_i^{\alpha 0} X_{2j}^{-\alpha 2}. \tag{33}$$

One can easily find that the spin $S = 1/2$ operators can be rewritten in terms of the X-operators in the following way:

$$S_i^+ = c_{i,\uparrow}^\dagger c_{i,\downarrow} = X_i^{+-}, \qquad S_i^- = c_{i,\downarrow}^\dagger c_{i,\uparrow} = X_i^{-+}, \qquad S_i^z = \tfrac{1}{2}(X_i^{++} - X_i^{--}). \tag{34}$$

4. Effective Hamiltonian in the half-filled band case

In what follows we focus on the case of the half-filled band. In this particular case the minimum of the interacting energy is reached in the subspace with one electron per site. Therefore, no hops are possible without increasing the number of doubly occupied sites and for any state in this subspace $|\Psi_{LS}\rangle$

$$T_{-1}^{\mathrm{e}}|\Psi_{LS}\rangle = 0 \qquad T_{-1}^{\mathrm{o}}|\Psi_{LS}\rangle = 0 \qquad T_0|\Psi_{LS}\rangle = 0. \tag{35}$$

Equation (35) may be generalized to higher orders

$$T^k[m]|\Psi_{LS}\rangle = 0, \tag{36}$$

if

$$M_n^k[m] \equiv \sum_{i=n}^{k} m_i < 0 \tag{37}$$

for at least one value of n. Equation (36) can be used to eliminate many terms from the expansion for $\mathcal{H}'$ in the minimum $\langle\hat{V}\rangle$ subspace. Thus, in the fourth order of $\hat{T}$, the perturbed Hamiltonian has the form

$$\begin{aligned}
\mathcal{H}'^{(4)} &= -\frac{1}{U_{\mathrm{o}}} T_{-1}^{\mathrm{o}} T_1^{\mathrm{o}} - \frac{1}{U_{\mathrm{e}}} T_{-1}^{\mathrm{e}} T_1^{\mathrm{e}} \\
&- \frac{1}{U_{\mathrm{o}}^3} T_{-1}^{\mathrm{o}} T_0^0 T_0^0 T_1^{\mathrm{o}} - \frac{1}{U_{\mathrm{o}}^2 U_{\mathrm{e}}} T_{-1}^{\mathrm{e}} T_0^{\mathrm{de}} T_0^0 T_1^{\mathrm{o}} - \frac{1}{U_{\mathrm{o}} U_{\mathrm{e}}^2} T_{-1}^{\mathrm{e}} T_0^0 T_0^{\mathrm{de}} T_1^{\mathrm{o}} \\
&- \frac{1}{U_{\mathrm{o}}^2 U_{\mathrm{e}}} T_{-1}^{\mathrm{o}} T_0^{\mathrm{do}} T_0^{\mathrm{de}} T_1^{\mathrm{o}} - \frac{1}{U_{\mathrm{e}}^3} T_{-1}^{\mathrm{e}} T_0^0 T_0^0 T_1^{\mathrm{e}} - \frac{1}{U_{\mathrm{o}} U_{\mathrm{e}}^2} T_{-1}^{\mathrm{o}} T_0^{\mathrm{do}} T_0^0 T_1^{\mathrm{e}} \\
&- \frac{1}{U_{\mathrm{o}}^2 U_{\mathrm{e}}} T_{-1}^{\mathrm{o}} T_0^0 T_0^{\mathrm{do}} T_1^{\mathrm{e}} - \frac{1}{U_{\mathrm{o}} U_{\mathrm{e}}^2} T_{-1}^{\mathrm{e}} T_0^{\mathrm{de}} T_0^{\mathrm{do}} T_1^{\mathrm{e}} - \frac{1}{2U_{\mathrm{o}}^3} T_{-1}^{\mathrm{o}} T_{-1}^{\mathrm{o}} T_1^{\mathrm{o}} T_1^{\mathrm{o}} \\
&+ \frac{1}{U_{\mathrm{o}}^3} T_{-1}^{\mathrm{o}} T_1^{\mathrm{o}} T_{-1}^{\mathrm{o}} T_1^{\mathrm{o}} + \left(\frac{1}{2U_{\mathrm{o}}^2 U_{\mathrm{e}}} + \frac{1}{2U_{\mathrm{e}}^2 U_{\mathrm{o}}}\right) T_{-1}^{\mathrm{o}} T_1^{\mathrm{o}} T_{-1}^{\mathrm{e}} T_1^{\mathrm{e}} + \frac{1}{U_{\mathrm{e}}^3} T_{-1}^{\mathrm{e}} T_1^{\mathrm{e}} T_{-1}^{\mathrm{e}} T_1^{\mathrm{e}} \\
&- \frac{1}{2U_{\mathrm{e}}^3} T_{-1}^{\mathrm{e}} T_{-1}^{\mathrm{e}} T_1^{\mathrm{e}} T_1^{\mathrm{e}} + \left(\frac{1}{2U_{\mathrm{o}}^2 U_{\mathrm{e}}} + \frac{1}{2U_{\mathrm{e}}^2 U_{\mathrm{o}}}\right) T_{-1}^{\mathrm{e}} T_1^{\mathrm{e}} T_{-1}^{\mathrm{o}} T_1^{\mathrm{o}} \\
&- \frac{1}{U_{\mathrm{o}} U_{\mathrm{e}} (U_{\mathrm{o}} + U_{\mathrm{e}})} T_{-1}^{\mathrm{o}} T_{-1}^{\mathrm{e}} T_1^{\mathrm{o}} T_1^{\mathrm{e}} - \frac{1}{U_{\mathrm{e}}^2 (U_{\mathrm{o}} + U_{\mathrm{e}})} T_{-1}^{\mathrm{e}} T_{-1}^{\mathrm{o}} T_1^{\mathrm{o}} T_1^{\mathrm{e}} \\
&- \frac{1}{U_{\mathrm{o}} U_{\mathrm{e}} (U_{\mathrm{o}} + U_{\mathrm{e}})} T_{-1}^{\mathrm{e}} T_{-1}^{\mathrm{o}} T_1^{\mathrm{e}} T_1^{\mathrm{o}} - \frac{1}{U_{\mathrm{o}}^2 (U_{\mathrm{o}} + U_{\mathrm{e}})} T_{-1}^{\mathrm{o}} T_{-1}^{\mathrm{e}} T_1^{\mathrm{e}} T_1^{\mathrm{o}}.
\end{aligned} \tag{38}$$

Using equations (30)–(34), one can easily rewrite the products of T-terms in (38) via the Hubbard X-operators. Using the spin $S = 1/2$ operators in equation (34) one obtains

$$T^{\rm o}_{-1}T^{\rm o}_{1} = T^{\rm e}_{-1}T^{\rm e}_{1} = -2t^2\sum_i\left(\mathbf{S}_i\cdot\mathbf{S}_{i+1} - \tfrac{1}{4}\right) \tag{39}$$

$$\begin{aligned} T^{\rm o}_{-1}T^{0}_{0}T^{0}_{0}T^{\rm o}_{1} &= T^{\rm o}_{-1}T^{\rm do}_{0}T^{\rm de}_{0}T^{\rm o}_{1} = T^{\rm e}_{-1}T^{0}_{0}T^{0}_{0}T^{\rm e}_{1} = T^{\rm e}_{-1}T^{\rm de}_{0}T^{\rm do}_{0}T^{\rm e}_{1} \\ &= -2t^4\sum_i\left(\mathbf{S}_i\cdot\mathbf{S}_{i+1} - \tfrac{1}{4}\right) \end{aligned} \tag{40}$$

$$T^{\rm e}_{-1}T^{\rm de}_{0}T^{0}_{0}T^{\rm o}_{1} = T^{\rm o}_{-1}T^{0}_{0}T^{\rm do}_{0}T^{\rm e}_{1} = -2t^4\sum_i\left(\mathbf{S}_i\cdot\mathbf{S}_{i+1} - \tfrac{1}{4}\right) + 2t^4\sum_i\left(\mathbf{S}_{2i+1}\cdot\mathbf{S}_{2i+3} - \tfrac{1}{4}\right) \tag{41}$$

$$T^{\rm e}_{-1}T^{0}_{0}T^{\rm de}_{0}T^{\rm o}_{1} = T^{\rm o}_{-1}T^{\rm do}_{0}T^{0}_{0}T^{\rm e}_{1} = -2t^4\sum_i\left(\mathbf{S}_i\cdot\mathbf{S}_{i+1} - \tfrac{1}{4}\right) + 2t^4\sum_i\left(\mathbf{S}_{2i}\cdot\mathbf{S}_{2i+2} - \tfrac{1}{4}\right) \tag{42}$$

$$T^{\rm o}_{-1}T^{\rm o}_{-1}T^{\rm o}_{1}T^{\rm o}_{1} = T^{\rm e}_{-1}T^{\rm e}_{-1}T^{\rm e}_{1}T^{\rm e}_{1} = 8t^4\sum_{i,\,j\neq i-1,i,i+1}\left(\mathbf{S}_i\cdot\mathbf{S}_{i+1} - \tfrac{1}{4}\right)\left(\mathbf{S}_j\cdot\mathbf{S}_{j+1} - \tfrac{1}{4}\right) \tag{43}$$

$$\begin{aligned} T^{\rm o}_{-1}T^{\rm o}_{1}T^{\rm o}_{-1}T^{\rm o}_{1} &= T^{\rm e}_{-1}T^{\rm e}_{1}T^{\rm e}_{-1}T^{\rm e}_{1} = T^{\rm o}_{-1}T^{\rm o}_{1}T^{\rm e}_{-1}T^{\rm e}_{1} = T^{\rm e}_{-1}T^{\rm e}_{1}T^{\rm o}_{-1}T^{\rm o}_{1} \\ &= 4t^4\sum_{i,j}\left(\mathbf{S}_i\cdot\mathbf{S}_{i+1} - \tfrac{1}{4}\right)\left(\mathbf{S}_j\cdot\mathbf{S}_{j+1} - \tfrac{1}{4}\right) \end{aligned} \tag{44}$$

$$\begin{aligned} T^{\rm o}_{-1}T^{\rm e}_{-1}T^{\rm o}_{1}T^{\rm e}_{1} &= T^{\rm e}_{-1}T^{\rm o}_{-1}T^{\rm o}_{1}T^{\rm e}_{1} = T^{\rm e}_{-1}T^{\rm o}_{-1}T^{\rm e}_{1}T^{\rm o}_{1} = T^{\rm o}_{-1}T^{\rm e}_{-1}T^{\rm e}_{1}T^{\rm o}_{1} \\ &= 4t^4\sum_{i,\,j\neq i-1,i,i+1}\left(\mathbf{S}_i\cdot\mathbf{S}_{i+1} - \tfrac{1}{4}\right)\left(\mathbf{S}_j\cdot\mathbf{S}_{j+1} - \tfrac{1}{4}\right). \end{aligned} \tag{45}$$

Therefore we find that in the fourth-order approximation the strong-coupling effective spin Hamiltonian for the alternating Hubbard model is given by

$$\mathcal{H}_{\rm eff} = J\sum_i\left(\mathbf{S}_i\cdot\mathbf{S}_{i+1} - \tfrac{1}{4}\right) + J_1\sum_i\left(\mathbf{S}_{2i+1}\cdot\mathbf{S}_{2i+3} - \tfrac{1}{4}\right) + J_2\sum_i\left(\mathbf{S}_{2i}\cdot\mathbf{S}_{2i+2} - \tfrac{1}{4}\right), \tag{46}$$

where

$$J = 2t^2\left(\frac{1}{U_{\rm o}} + \frac{1}{U_{\rm e}}\right) - 2t^4\left(\frac{3}{U_{\rm o}^3} + \frac{3}{U_{\rm e}^3} + \frac{1}{U_{\rm o}^2U_{\rm e}} + \frac{1}{U_{\rm o}U_{\rm e}^2}\right), \tag{47}$$

$$J_1 = 2t^4\left(\frac{1}{U_{\rm o}^3} + \frac{1}{U_{\rm e}^3} + \frac{U_{\rm o} - U_{\rm e}}{U_{\rm o}^2U_{\rm e}^2}\right), \tag{48}$$

$$J_2 = 2t^4\left(\frac{1}{U_{\rm o}^3} + \frac{1}{U_{\rm e}^3} - \frac{U_{\rm o} - U_{\rm e}}{U_{\rm o}^2U_{\rm e}^2}\right). \tag{49}$$

The effective Hamiltonian thus obtained is that of a frustrated Heisenberg chain with alternating next-nearest-neighbour exchange [23]. Note that the nnn exchange is larger for two spins separated by a site with low on-site repulsion than for spins separated by a site with high on-site repulsion.

5. Conclusion

In this paper we have derived the effective spin Hamiltonian which describes the low-energy sector of the one-dimensional half-filled alternating Hubbard model in the limit of strong on-site repulsion. The effective spin model is given by the Hamiltonian of the Heisenberg chain with alternating next-nearest-neighbour exchange. This model has been intensively studied in the last few years [23–27]. Unfortunately, conflicting results have been reported in these studies regarding the relevance of the alternating nnn exchange. In some studies [23, 25, 27] it was claimed that in the limit of small frustration, $J'/J < 0.5$, the asymmetry of the nnn exchange destabilizes the isotropic Heisenberg fixed point and leads to a new phase with

gapless excitation spectrum and vanishing spin-wave velocity. However, other studies [24, 26] claim that the alternating nnn exchange is an *irrelevant* perturbation. We believe that detailed numerical studies of the phase diagram of the alternating Hubbard model may shed more light on this topic. The weak-coupling bosonization analysis of the same model is in progress and will be published separately.

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Appendix

Using the technique developed above it is straightforward to derive the strong-coupling effective Hamiltonian in the case of the alternating ionic Hubbard model, equation (3), in the limit $\Delta \neq 0$ and $U_e \neq U_o \gg \Delta, t$.

In this case the effective Hamiltonian is also given by the Heisenberg Hamiltonian with alternating next-nearest-neighbour exchange, equation (46), but with the following exchange coupling constants:

$$J = 2t^2\left(\frac{1}{U_o-\Delta}+\frac{1}{U_e+\Delta}\right)$$
$$-2t^4\left[\frac{4}{(U_e+\Delta)^3}+\frac{4}{(U_o-\Delta)^3}-\frac{1}{U_e(U_e+\Delta)^2}-\frac{1}{(U_o-\Delta)^2U_o}\right.$$
$$+\frac{4(U_e+U_o)}{(U_e+\Delta)^2(U_o-\Delta)^2}-\frac{1}{(U_e+\Delta)^2U_o}-\frac{1}{U_e(U_o-\Delta)^2}$$
$$\left.-\frac{2}{(\Delta+U_e)(U_o-\Delta)U_o}-\frac{2}{U_e(\Delta+U_e)(U_o-\Delta)}\right], \tag{50}$$

$$J_1 = 2t^4\left[\frac{1}{(U_e+\Delta)^3}+\frac{1}{(U_o-\Delta)^3}+\frac{U_e+U_o}{(U_e+\Delta)^2(U_o-\Delta)^2}-\frac{2}{U_o(U_e+\Delta)(U_o-\Delta)}\right], \tag{51}$$

$$J_2 = 2t^4\left[\frac{1}{(U_e+\Delta)^3}+\frac{1}{(U_o-\Delta)^3}+\frac{U_e+U_o}{(U_e+\Delta)^2(U_o-\Delta)^2}-\frac{2}{U_e(U_e+\Delta)(U_o-\Delta)}\right]. \tag{52}$$

Note that in the case when the ionic term is large on the site with larger on-site repulsion, i.e. $U_e > U_o$ and $\Delta > 0$, the asymmetry in the nnn exchange in the case of AIHM

$$\delta J'(\Delta \neq 0) = 2t^4\frac{(U_e-U_o)}{U_eU_o(U_e+\Delta)(U_o-\Delta)} \tag{53}$$

is larger than it is in the case of AHM

$$\delta J'(\Delta = 0) = 2t^4\frac{(U_e-U_o)}{U_e^2U_o^2} \tag{54}$$

for $\Delta > 0$ ($\Delta \ll U_o, U_e$).

References

[1] Mott N F 1990 *Metal–Insulator Transitions* 2nd edn (London: Taylor and Francis)
Gebhard F 1997 *The Mott Metal–Insulator Transitions* (Berlin: Springer)
[2] Lee D H and Shankar R 1990 *Phys. Rev. Lett.* **65** 1490
[3] Dagotto E 1994 *Rev. Mod. Phys.* **66** 763
[4] Hubbard J 1963 *Proc. R. Soc.* A **276** 238
[5] Lieb E and Wu F W 1968 *Phys. Rev. Lett.* **20** 1445
[6] Essler F H L and Frahm H 1999 *Phys. Rev.* B **60** 8540
[7] Frahm H and Korepin V E 1990 *Phys. Rev.* B **42** 10553
[8] Anderson P W 1959 *Phys. Rev.* **115** 2
[9] Nakamura T and Kubo K 1996 *Phys. Rev.* B **53** 6393
Sen D, Shastry B S, Walstedt R E and Cava R 1996 *Phys. Rev.* B **53** 6401
[10] Takahashi M 1977 *J. Phys. C: Solid State Phys.* **10** 1289
[11] MacDonald A H, Girvin S M and Yoshioka D 1988 *Phys. Rev.* B **37** 9753
[12] Datta N, Fernández R and Frölich J 1999 *J. Stat. Phys.* **96** 545
[13] Emery V J 1987 *Phys. Rev. Lett.* **58** 2794
[14] Nagaosa N and Takimoto J 1986 *J. Phys. Soc. Japan* **55** 2735
Nagaosa N 1986 *J. Phys. Soc. Japan* **55** 2754
[15] Japaridze G I, Khomskii D and Müller-Hartmann E 1993 *Ann. Phys., Lpz.* **2** 38
[16] Fabrizio M, Gogolin A O and Nersesyan A A 1999 *Phys. Rev. Lett.* **83** 2014
Fabrizio M, Gogolin A O and Nersesyan A A 2000 *Nucl. Phys.* B **580** 647
[17] Torio M E, Aligia A A and Ceccatto H A 2001 *Phys. Rev.* B **64** 121105
Aligia A A 2004 *Phys. Rev.* B **69** 041101
[18] Kampf A P, Sekania M, Japaridze G I and Brune P 2003 *J. Phys.: Condens. Matter* **15** 5895
[19] Požgajčić K and Gros C 2003 *Phys. Rev.* B **68** 085106
[20] Manmana S R, Meden V, Noack R M and Schoenhammer K 2003 *Preprint* cond-mat/0307741
[21] Otsuka T and Nakamura M 2004 *Preprint* cond-mat/0403630
[22] Hubbard J 1965 *Proc. R. Soc.* A **285** 542
Hubbard J 1967 *Proc. R. Soc.* A **296** 82
[23] Chen S, Büttner H and Voit J 2001 *Phys. Rev. Lett.* **87** 087205
[24] Capriotti L, Becca F, Sorella S and Parola A 2002 *Phys. Rev. Lett.* **89** 149701
[25] Chen S, Büttner H and Voit J 2002 *Phys. Rev. Lett.* **89** 149702
[26] Sen D and Sarkar S 2002 *Phys. Rev.* B **65** 172408
[27] Chen S, Büttner H and Voit J 2003 *Phys. Rev.* B **67** 054412