On the Phase Diagram of the Extended Hubbard Model

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The phase diagram of the Extended Hubbard Model in the atomic limit (zero band width) is investigated for arbitrary values of intra-site interaction $I$, inter-site repulsion $W$ and chemical potential $\mu$. First the ground states and their boundaries in the plane $(I/4W, \mu - 1/4W)$ are determined and then using the Peierls chessboard method the existence of several kinds of long range orders, corresponding to ground states, is proven. It is conjectured that the results obtained hold for finite but sufficiently small band width. Arguments in favour of this conjecture are presented.

1. Introduction

Studies of lattice fermion gas on a basis of a model which takes into account band and correlation effects have been originated by Gutzwiller [1] and Hubbard [2]. These authors were interested in properties of electron gas in a crystal. The so called Hubbard model approximates Coulomb interaction only by intra-site repulsion of particles with opposite spins. The importance of inter-site repulsion term was soon realized, especially in attempts to describe metal-insulator transitions in transition-metal oxides [3]. To our best knowledge the first work, where besides Hubbard Hamiltonian, inter-site repulsion of electrons was taken into account in calculations, was the work of Kishore and Yoshi [4]. Later, the model called the Extended Hubbard Model has been investigated by a great number of authors, who used Green's function techniques [5], functional integral methods [6], mean field [7] and cluster approximations [8], methods of effective Hamiltonian [9].

A number of works considering the Extended Hubbard Model has been inspired by the possibility of describing properties of quasi one-dimensional conductors [10] (references [5–10] constitute a very special choice from a great variety of works).

The Extended Hubbard Model Hamiltonian reads

$$H(\mu) = -t \sum_{\langle i,j \rangle} (c_i^+ \sigma_{i,a} c_{j,a} + c_{j,a}^+ \sigma_{i,a} c_{i,a}) + \mu \sum_{i \in A} n_i + W \sum_{\langle i,j \rangle} n_i n_j - \mu \sum_{i \in A} n_i,$$

where $A$ is the underlying Hilbert space.

We use the following notation: on each site $i$ of the $v$-dimensional lattice $A$ (which we assume to be the simple cubic lattice) we have a pair $\{c_i^+ \sigma, c_i \sigma\}_{\sigma=\uparrow,\downarrow}$ of creation and annihilation operators of a fermion with spin $\sigma=\uparrow,\downarrow$. $n_i=\sigma c_i \sigma, n_i=\sigma n_i + n_i \sigma, \sum_{\langle i,j \rangle}$ denotes summation over pairs of nearest neighbours sites in $A$, each pair is counted once, $t$ is the kinetic energy in a nuclear potential parameter (its sign is arbitrary), $I>0$ and $W>0$ describe respectively intra-site and inter-site Coulomb repulsion. If interaction parameters $t, I, W$ are thought of as effective parameters taking into account the interactions with phonons, then $I$ can assume negative values [7].

For $\mu = \mu_0 = zW + I/2$ ($z$ being the number of nearest neighbours on $A$) $H(\mu)$ is invariant under the unitary transformation $c_i^+ \sigma \rightarrow (-1)^{i} c_i \sigma$ (the hole-particle transformation), where for $i=(i_1, i_2, \ldots, i_v) \in A, \|i\| = |i_1| + |i_2| + \cdots + |i_v|$

This implies that $\langle \chi_{\beta} \parallel \sum_{i \in A} n_i \rangle = 1$ for all $\beta$, where

$$\langle \chi_{\beta} \rangle = z^{-1} Tr_{\mathcal{H}^i}(\chi_{\beta}) \exp(-\beta H(\mu)),$$

$$z = Tr_{\mathcal{H}^i}(-\beta H(\mu)),$$

$|A|$ is the number of sites in $A$, $\beta$ the inverse temperature and

$$\mathcal{H} = \bigotimes_{i \in A} \mathcal{H}_i, \quad \mathcal{H}_i = \mathbb{C}^2 \otimes \mathbb{C}^2,$$

is the underlying Hilbert space.
In [11] we have used the method of infrared bounds [12] to prove the existence of charge long range order in model (1) in the case $\mu = \mu_0$, $zW-I>0$, $\nu \geq 3$ i.e.

$$
\lim_{|t| \to \infty} \lim_{A \to \infty} \langle (-1)^{|i-j|}(n_i-1)(n_j-1) \rangle \geq 1 - e(|t|) - K(\beta)
$$

if $t$ is sufficiently small and $\beta$ sufficiently large, where $\lim$ stands for the thermodynamic limit,

$$
\lim_{t \to 0} e(|t|) = 0, \quad \lim_{A \to \infty} K(\beta) = 0.
$$

This inequality means that at low enough temperatures, if $i$ belongs to say even sublattice and is doubly occupied, then with probability close to one a far distant site $j$ is also doubly occupied, if it belongs to the same sublattice and is empty, if it belongs to odd sublattice. This phase transition has been predicted using Hartree-Fock approximation in [7]. The result of [11] can be extended to $\nu = 2$ by the Peierls chessboard method as was done for the Spinless Fermion Model in [13].

The condition $\mu = \mu_0$ in [11] and [13] was imposed by applied methods, which are based on the reflection positivity property. Obtained results are of perturbative nature, i.e. the situation observed in the case $t=0$ (so called atomic limit) is stable against perturbation by the band term. Therefore, it is quite plausible that the following proposition should be true:

If for $t=0$ and some $\mu$ exists a sort of long range order, then it persists for $|t|$ sufficiently small.

The above conjecture motivated our investigation of model (1) for arbitrary values of chemical potential in the atomic limit.

In Sect. 2 we describe the ground state phase diagram and in Sect. 3, using the Peierls chessboard method [12, 14, 15], we prove the existence of several kinds of long range orders in the model. Simultaneously we obtain equations for lower bounds of critical temperatures, below which the system undergoes a 1st order phase transition and there are at least two equilibrium states. We carry on our estimates in the case $\nu = 2$, however qualitatively results hold for $\nu \geq 2$. In Sect. 4 we discuss our results.

### 2. Ground State Phase Diagram

It is convenient to write down the Hamiltonian (1) in the atomic limit as follows:

$$
H^0(\mu) = \frac{1}{2} W \sum_{\langle i,j \rangle} (Q_i + Q_j)^2 - a \sum_{i \in A} Q_i^2 - (\mu - \mu_0) \sum_i Q_i + \text{constant},
$$

where $Q_i = n_i - 1$, $a = 2W-I/2$. We assume here, for simplicity, that $A$ is 2-dimensional square lattice wrapped on a torus. Since $W>0$, the finite volume Gibbs state $\langle \ldots \rangle$ has the reflection positivity property with respect to reflections in lattice planes [12]. Our investigation of the ground state is based on the following consequence of chessboard estimates with respect to lattice planes [15]:

(i) Among the ground states must be one of the states obtained by picking a configuration of a $2 \times 2$ block of lattice sites and extending it to be periodic with period 2.

(ii) Any other ground state must have the property that each of its $2 \times 2$ blocks is among those that yield a minimal energy when extended periodically as in (i).

There are $4^4$ configurations of $2 \times 2$ block. Invariance of $H^0(\mu)$ under global rotations by multiples of $\pi/2$ and under local spin flips groups possible configurations into 21 energetically different types. Moreover some configurations form hole-particle pairs, i.e. members of such a pair are related by hole-particle transformation ($n_i \to 2 - n_i$). In that way $4^4$ configurations fall into 13 groups which are enumerated in Table 1, $e(n \pm)$ stands for the energy per site of periodic configuration obtained from displayed $2 \times 2$ block configuration number $n \pm$ accord-

<table>
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<th>$n$</th>
<th>typical block configuration</th>
<th>$e(n \pm)$</th>
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