



# ISAS - INTERNATIONAL SCHOOL FOR ADVANCED STUDIES

## Variational Cluster Calculation of t-J model

Thesis submitted for the degree of  
“Magister Philosophiæ”

CANDIDATE

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SUPERVISORS

Prof. Patrik Fazekas

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# 1 Introduction

## 1.1 The Hubbard model

Interactions in Fermi systems lead to a particularly complex quantum mechanical many-body problem. Even in the noninteracting case, the Pauli principle implies spatial correlations between fermions. Interactions, especially those of short range, further enhance these complications since they introduce additional subtle phase relations among the fermions in real space. That is why many problems in theoretical physics are investigated by considering mathematical models which are simplifications of the real situation. Such an approach can be very illuminating if the model incorporates the most important physical mechanisms of the real problem.

The narrow band Hamiltonian introduced by Hubbard (1963, 1964, 1965), Kanamori (1963) and Gutzwiller (1963, 1964, 1965) is an example of such a situation. The simplifying assumption made in this so-called Hubbard model may make a direct comparison with experiments difficult. The theoretical predictions and implications of the model may, however, be relevant and useful for a deeper understanding of transition metals and transition-metal oxides, of metal-nonmetal transitions and of magnetic transitions. Moreover recent developments have revealed that heavy electron systems and high- $T_c$  superconductors arise from the effect of strong correlation between electrons. For an understanding of this effect, of all the various models of electron correlation the Hubbard model is the simplest one. The problem of strongly correlations remains one of the most challenging in solid state physics.

The Hubbard Hamiltonian describes a lattice model for an electron gas with the Coulomb repulsion is completely screened out except between electrons on the

same site. It is the simplest model which contains the co-operation and competition of kinetic energy (electron hopping), Coulomb repulsion and exclusion principle, thus describing both itinerant and localized aspects.

In the simplest case only the  $s$ -band is considered

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow} . \quad (1.1)$$

The indices  $i$  and  $j$  label the lattice points, and  $\sigma$  represents the spin state.  $c_{i,\sigma}^\dagger$  and  $c_{j,\sigma}$  are the creation and annihilation operators for an electron of spin  $\sigma$  in the Wannier state centered on atom  $\mathbf{R}_i$ , and  $n_{i,\sigma} = c_{i,\sigma}^\dagger c_{i,\sigma}$  is the corresponding number operator. The model can easily be applied in the case of a degenerate band or in a system with several bands. The first term describes the tunneling (or hopping) of the electrons between nearest neighbour lattice sites, then  $t$  is the transfer integral. The second term in (1.1) represents the Coulomb repulsion between two antiparallel-spin electrons on the same lattice site.  $U$ , the strength of the on-site correlation, is the matrix element of the (screened) Coulomb interaction between Wannier functions centered on atom  $\mathbf{R}_i$ .

This model is significant in the sense that despite its simplicity it contains the crucial effect of the electron-electron interaction on lattice systems. It includes at zero temperature, three important parameters : i) dimensionality and crystal structure, ii) correlation strength  $U/t$ , and iii) electron density  $n = N_e/N$ , where  $N$  is the number of lattice sites,  $N_e$  the number of electrons.

In the case of one electron per site the ground state energy is always negative. This is evident from the fact that the expectation value of (1.1) with respect to any state, with each site singly occupied, is zero. These states are the exact groundstates in the limit of zero hopping (known as *atomic* or  $U \rightarrow \infty$  limit), where we therefore have an exclusion of doubly occupied sites and thus an insulating

behaviour. On the other hand, if  $U = 0$  (i.e., *band* limit), (1.1) can be exactly diagonalized in terms of Bloch functions by performing the Fourier transformation

$$c_{\mathbf{k},\sigma}^\dagger = N^{-1/2} \sum_i e^{-i\mathbf{k}\cdot\mathbf{R}_i} c_{i,\sigma}^\dagger, \quad (1.2)$$

$$c_{\mathbf{k},\sigma} = N^{-1/2} \sum_i e^{i\mathbf{k}\cdot\mathbf{R}_i} c_{i,\sigma}. \quad (1.3)$$

In the following, consider  $\mathbf{k}$  to be defined in the first Brillouin-zone of the reciprocal lattice. Thus (1.1) is exactly diagonal to

$$H = \sum_{\mathbf{k},\sigma} \varepsilon_{\mathbf{k}} c_{\mathbf{k},\sigma}^\dagger c_{\mathbf{k},\sigma}, \quad (1.4)$$

where the band energy  $\varepsilon_{\mathbf{k}}$  is given by the following tight-binding expression

$$\varepsilon_{\mathbf{k}} = -t \frac{1}{N} \sum_{\langle i,j \rangle} e^{-i\mathbf{k}\cdot\mathbf{R}_{ij}}, \quad (1.5)$$

and  $\mathbf{R}_{ij} = \mathbf{R}_j - \mathbf{R}_i$ . Thus, depending on the ratio  $U/t$ , there exist two limiting cases : perfectly localized moments on one hand and uncorrelated band ground state on the other. In reality one is often faced with an intermediate state.

Various many-body techniques have been applied to the problem of approximating electron-electron correlations. The significance and usefulness of these results has been critically reviewed by Cyrot (1977). Further references to previous work in this field can be found in the review articles by Bari (1975) and Ovchinnikov *et al.* (1973). In contrast to approximate theories, Lieb and Wu (1968) succeeded in exactly solving the one dimensional case using the Bethe Ansatz. Their results illustrate that for the half-filled band the system is always insulating when  $U > 0$ . In addition the ground state has no antiferromagnetic long range order. Consequently, the metal-insulator transition occurs at  $U = 0$ , and a singlet liquid state is realized for a finite value of  $U$ . On the other hand, for less than

half-filled systems, there is no energy gap for any value of  $U$  so that the system is always metallic.

Recently, the theoretical developments in new areas such as heavy electron systems, and most significantly high-temperature superconductivity have drawn great attention to the Hubbard model and have further challenged the understanding of strongly correlated fermions. But, in spite of the existence of an analytic solution in one dimension and an impressive research activity, the properties of this seemingly simple model are far from understood. With this model numerical methods have been particularly valuable and have yielded significant insight into the properties of different dimensions. But, on the other hand, this approach is confined to the study of finite samples.

### 1.2 The t-J model

After the suggestion by Anderson (1987), that the high-temperature superconductors can be understood on the basis of the strongly correlated Hubbard model, several studies have addressed this issue. Several versions of the Hubbard model have been proposed in this regard, and recently works by Gros *et al.* (1987), Bonca *et al.* (1989), and Dagotto *et al.* (1989) suggests that the closely related t-J model (i.e., the two dimensional Heisenberg antiferromagnet with hopping term) may reproduce both mobile hole disruption of long range order and superconductivity for physically reasonable parameter values.

The strongly correlated limit of the Hubbard Hamiltonian has been extensively investigated by many authors up to now : Nagaoka (1966), Roth (1966), Caron and Pratt (1968), Langer *et al.* (1969), Kaplan and Bari (1970), Visscher (1974), and Ogawa *et al.* (1975). In addition to these approaches, Klein and Seitz (1973), Cleveland and Medina (1976), Florencio and Chao (1975, 1976) all used a perturbation theory, since  $U/t \gg 1$ , the electron hopping can be treated as a

perturbation which at the second order yields an antiferromagnetic coupling due to the virtual hopping of electrons. On the other hand, one can perform canonical transformation such as the new quasiparticles have the property that although they do hop around, their hopping does not change the effective number of doubly occupied sites, as it was made by Kohn (1964), Harris and Lange (1967), Sokoloff (1970), Chao *et al.* (1977), and Hirsch (1985). The equivalent of these methods was demonstrated by Anderson (1959) in terms of the so-called kinetic exchange interaction. We will use the canonical transformation approach to obtain the effective Hamiltonian for the strongly correlated limit.

It is known that for sufficiently large  $U$  the bare energy band splits into two sub-bands. For one electron per atom, the lower sub-band is full while the upper sub-band is empty. The antiferromagnetic coupling is due to the virtual electron hopping from the lower to the upper and then back to the lower sub-band. The hopping process which change the number of doubly occupied sites are virtual ones, on account of the energy cost of  $U$ . Thus, we can carry out a canonical transformation which eliminates such processes in the lowest order. In doing this we follow the procedure used by Chao *et al.* (1977) by decomposing the Hamiltonian into projectors onto states with a given electron number. In this way we have full control of the electronic states on any atomic site  $\mathbf{R}_i$ . For this we consider, instead of (1.1), a two-site Hubbard Hamiltonian

$$\mathcal{H} = -t \sum_{i,j,\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} . \quad (1.6)$$

Where  $i = 1, 2$ ,  $j = 1, 2$ , and terms with  $i = j$  are excluded. We define the projection operators for the  $\mathbf{R}_i$ th atom through the relation

$$\prod_{\sigma} [(1 - n_{i,\sigma}) + x n_{i,\sigma}] = \sum_{m=0}^2 p(m, \mathbf{R}_i) x^m . \quad (1.7)$$

$p(m, \mathbf{R}_i)$  projects out the atomic configurations each of which contains  $m$  electrons.  $m$  can take three values : 0, 1 and 2, corresponding to empty, single, and doubly occupied site. By identifying the coefficients of  $x$  in (1.7), the projection operators can be obtained as

$$p(0, \mathbf{R}_i) = (1 - n_{i,\sigma}) (1 - n_{i,-\sigma}) , \quad (1.8)$$

$$p(1, \mathbf{R}_i) = n_{i,\sigma} (1 - n_{i,-\sigma}) + n_{i,-\sigma} (1 - n_{i,\sigma}) , \quad (1.9)$$

$$p(2, \mathbf{R}_i) = n_{i,\sigma} n_{i,-\sigma} . \quad (1.10)$$

Then

$$\sum_{m=0}^2 p(m, \mathbf{R}_i) = 1 , \quad (1.11)$$

and

$$p(m, \mathbf{R}_i) p(n, \mathbf{R}_i) = p(m, \mathbf{R}_i) \delta_{m,n} . \quad (1.12)$$

For two atoms, one at site  $\mathbf{R}_i$  and the other at site  $\mathbf{R}_j$ , we can define the following projection operators as

$$P_1 = p(1, \mathbf{R}_1) p(1, \mathbf{R}_2) + \sum_{i,j} p(1, \mathbf{R}_i) p(0, \mathbf{R}_j) + p(0, \mathbf{R}_1) p(0, \mathbf{R}_2) , \quad (1.13)$$

for all two atom configurations which contain just empty and single occupied sites,

$$P_2 = \sum_{i,j} p(2, \mathbf{R}_i) p(1, \mathbf{R}_j) + \sum_{i,j} p(2, \mathbf{R}_i) p(0, \mathbf{R}_j) + p(2, \mathbf{R}_1) p(2, \mathbf{R}_2) , \quad (1.14)$$

and for all configurations which contains at least one double occupied site. Similarly to (1.11) and (1.12) we have it for this case

$$\sum_{\mu} P_{\mu} = 1 , \quad (1.15)$$

and

$$P_{\mu} P_{\nu} = P_{\mu} \delta_{\mu,\nu} . \quad (1.16)$$

Applying  $P_\mu$  to the Hamiltonian  $\mathcal{H}$  of (1.6) from both sides, we get

$$P_1 \mathcal{H} P_1 = -t \sum_{i,j,\sigma} (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}), \quad (1.17)$$

$$P_1 \mathcal{H} P_2 = -t \sum_{i,j,\sigma} (1 - n_{i,-\sigma}) c_{i,-\sigma}^\dagger c_{j,\sigma} n_{j,-\sigma}, \quad (1.18)$$

$$P_2 \mathcal{H} P_1 = -t \sum_{i,j,\sigma} n_{i,-\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}), \quad (1.19)$$

$$P_2 \mathcal{H} P_2 = -t \sum_{i,j,\sigma} n_{i,-\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} n_{j,-\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}. \quad (1.20)$$

Deriving from Eqs. (1.17) - (1.20) we introduce the values of  $p(m, \mathbf{R}_i)$  from (1.8), (1.10) in (1.13) and (1.14) and obtain

$$P_1 = (1 - n_{1,\sigma} n_{1,-\sigma}) (1 - n_{2,\sigma} n_{2,-\sigma}), \quad (1.21)$$

and

$$P_2 = n_{1,\sigma} n_{1,-\sigma} + n_{2,\sigma} n_{2,-\sigma} - n_{1,\sigma} n_{1,-\sigma} n_{2,\sigma} n_{2,-\sigma}. \quad (1.22)$$

Using  $P_1$  and  $P_2$  from (1.21) and (1.22), respectively, and the anticommutation rules of the fermionic operators, Eqs. (1.17), (1.20) can be immediately obtained.

At this stage,  $P_1 \mathcal{H} P_2$  and  $P_2 \mathcal{H} P_1$  can be recognized to describe the hopping processes which change the number of doubly occupied sites. Such processes, we wish to eliminate in the lowest order, by applying an appropriate canonical transformation  $e^{\epsilon \mathcal{S}}$  on the

$$\mathcal{H}(\epsilon) = \mathcal{H}_0 + \epsilon \mathcal{H}_1, \quad (1.23)$$

Hamiltonian.  $\mathcal{H}_0$  and  $\mathcal{H}_1$  are chosen to be

$$\mathcal{H}_0 = P_1 \mathcal{H} P_1 + P_2 \mathcal{H} P_2, \quad (1.24)$$

$$\mathcal{H}_1 = P_1 \mathcal{H} P_2 + P_2 \mathcal{H} P_1. \quad (1.25)$$

The formal  $\epsilon$  parameter is treated as  $\leq 1$ , except at the end of the calculations, where  $\epsilon = 1$  will be assumed. In this way the transformed Hamiltonian will be

$$\begin{aligned}\tilde{\mathcal{H}}(\epsilon) &= e^{-\epsilon S} \mathcal{H}(\epsilon) e^{\epsilon S} \\ &= \mathcal{H}(\epsilon) + \epsilon [\mathcal{H}(\epsilon), S] + \frac{1}{2} \epsilon^2 [ [\mathcal{H}(\epsilon), S], S] + \dots \\ &= \mathcal{H}_0 + \epsilon(\mathcal{H}_1 + [\mathcal{H}_0, S]) + \frac{1}{2} \epsilon^2 (2[\mathcal{H}_1, S] + [[\mathcal{H}_0, S], S]) + \dots .\end{aligned}\quad (1.26)$$

The term linear in  $\epsilon$  vanishes if

$$\mathcal{H}_1 + [\mathcal{H}_0, S] = 0 .\quad (1.27)$$

Substituting (1.27) in (1.26) and let  $\epsilon=1$ , we obtain

$$\tilde{\mathcal{H}} = \mathcal{H}_0 + \frac{1}{2} [\mathcal{H}_1, S] .\quad (1.28)$$

To determine the value of S, (1.27) is projected on to the configurational subspaces by applying the operator  $P_\mu$  from both sides. Taking into account the definition of  $\mathcal{H}_0$  and  $\mathcal{H}_1$  from (1.24) and (1.25), respectively, and the property (1.16) of the two-site projection operator, four equations emerge

$$P_\mu \mathcal{H} P_\nu (1 - \delta_{\mu,\nu}) + P_\mu \mathcal{H} P_\mu P_\mu S P_\nu - P_\mu S P_\nu P_\nu \mathcal{H} P_\nu = 0 .\quad (1.29)$$

For  $\mu = \nu$ , it reduces to

$$P_\mu \mathcal{H} P_\mu P_\mu S P_\mu = P_\mu S P_\mu P_\mu \mathcal{H} P_\mu ,\quad (1.30)$$

in simple terms

$$P_\mu S P_\mu = \text{const} \times P_\mu .\quad (1.31)$$

While for  $\mu \neq \nu$ , (1.29) becomes

$$P_\mu S P_\nu P_\nu \mathcal{H} P_\nu - P_\mu \mathcal{H} P_\mu P_\mu \mathcal{H} P_\nu = P_\mu \mathcal{H} P_\nu .\quad (1.32)$$



The operators  $P_\mu \mathcal{H} P_\mu$  and  $P_\nu \mathcal{H} P_\nu$  on the left-hand-side of Eq. (1.31) will be approximated by the proper expectation values. From (1.18) and (1.19) we see that the right-hand-side of Eq. (1.32) consists of all possible single-hopping processes between the two-sites. Consequently,  $\langle P_\mu \mathcal{H} P_\mu \rangle - \langle P_\nu \mathcal{H} P_\nu \rangle$  should be the mean energy difference between the final and the initial states of the inter-site hopping. For  $U \gg t$ , this energy difference can be approximated by  $U$ . Indeed, as it can be seen from (1.17) and (1.20),  $\langle P_2 \mathcal{H} P_2 \rangle - \langle P_1 \mathcal{H} P_1 \rangle \simeq U$ . Thus from (1.32)

$$P_1 S P_2 = \frac{1}{U} P_1 \mathcal{H} P_2, \quad (1.33)$$

and

$$P_2 S P_1 = -\frac{1}{U} P_2 \mathcal{H} P_1. \quad (1.34)$$

Thus the effective Hamiltonian can now be derived explicitly from (1.28), by using (1.15), (1.24), (1.31), (1.33) and (1.34), to be

$$\tilde{\mathcal{H}} = P_1 \mathcal{H} P_1 + P_2 \mathcal{H} P_2 - \frac{1}{U} [ P_1 \mathcal{H} P_2 \mathcal{H} P_1 - P_2 \mathcal{H} P_1 \mathcal{H} P_2 ]. \quad (1.35)$$

Substituting Eqs. (1.17), (1.20) and using (1.16) the Hamiltonian for two-sited Hubbard model becomes

$$\begin{aligned} \tilde{\mathcal{H}} = & -t \sum_{i,j,\sigma} (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) \\ & -t \sum_{i,j,\sigma} n_{i,-\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} n_{j,-\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \\ & -\frac{t^2}{U} \left[ \left( \sum_{i,j,\sigma} (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} n_{j,-\sigma} \right) \left( \sum_{i,j,\sigma} n_{i,-\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) \right) \right. \\ & \left. - \left( \sum_{i,j,\sigma} n_{i,-\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) \right) \left( \sum_{i,j,\sigma} (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} n_{j,-\sigma} \right) \right] \end{aligned} \quad (1.36)$$

Eq. (1.36) in algebraic terms can be written as

$$\begin{aligned}
\tilde{\mathcal{H}} = & -t \sum_{i,j,\sigma} (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) \\
& -t \sum_{i,j,\sigma} n_{i,-\sigma} c_{i,\sigma}^\dagger c_{j,\sigma} n_{j,-\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow} \\
& -\frac{t^2}{U} \left[ \sum_{i,j,\sigma} \left( (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} - (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) \right) \right. \\
& \quad \times \sum_{i,j,\sigma} \left( c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) - (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) \right) \\
& \quad - \sum_{i,j,\sigma} \left( c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) - (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) \right) \\
& \quad \left. \times \sum_{i,j,\sigma} \left( (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} - (1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger c_{j,\sigma} (1 - n_{j,-\sigma}) \right) \right] \quad (1.37)
\end{aligned}$$

In order to give the effective Hamiltonian for the strong correlation limit of the complete Hubbard model (1.1), we completely eliminate the doubly occupied states from (1.37), i.e. the second and third term of (1.37), because they describe a high energetic sub-band. We substitute the sum over  $i$  and  $j$  to run over all nearest neighboring sites instead of just two, thus  $H_{eff} = \tilde{\mathcal{H}}$  (for all  $\langle i, j \rangle$ ). Introducing the

$$\begin{aligned}
(1 - n_{i,-\sigma}) c_{i,\sigma}^\dagger &= \tilde{c}_{i,\sigma}^\dagger, \\
\tilde{c}_{j,\sigma} &= c_{j,\sigma} (1 - n_{j,-\sigma}). \quad (1.38)
\end{aligned}$$

notations, as Hirsch (1985), the form of the effective Hamiltonian will be

$$\begin{aligned}
H_{eff} = & -t \sum_{\langle i,j \rangle, \sigma} \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} \\
& -\frac{t^2}{U} \left[ \sum_{\langle i,j \rangle, \sigma} \left( \tilde{c}_{i,\sigma}^\dagger c_{j,\sigma} - \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} \right) \times \sum_{\langle i,j \rangle, \sigma} \left( c_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} - \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} \right) \right. \\
& \quad \left. - \sum_{\langle i,j \rangle, \sigma} \left( c_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} - \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} \right) \times \sum_{\langle i,j \rangle, \sigma} \left( \tilde{c}_{i,\sigma}^\dagger c_{j,\sigma} - \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} \right) \right] \quad (1.39)
\end{aligned}$$

After performing the products in (1.39) we disregard higher order processes, and those which involve other sites than nearest neighbours. Knowing that

$$\begin{aligned}
\vec{S}_i \cdot \vec{S}_j &= S_i^x S_j^x + S_i^y S_j^y + S_i^z S_j^z \\
&= \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z \\
&= \frac{1}{2} (c_{i\uparrow}^\dagger c_{i\downarrow} c_{j\downarrow}^\dagger c_{j\uparrow} + c_{i\downarrow}^\dagger c_{i\uparrow} c_{j\uparrow}^\dagger c_{j\downarrow}) + \frac{1}{4} (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}), \quad (1.40)
\end{aligned}$$

the final form of the effective Hamiltonian will be

$$\begin{aligned}
H_{eff} &= -t \sum_{\langle i,j \rangle, \sigma} \tilde{c}_{i,\sigma}^\dagger \tilde{c}_{j,\sigma} \\
&\quad + \frac{4t^2}{U} \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j). \quad (1.41)
\end{aligned}$$

The  $N_i = \sum_\sigma n_{i,\sigma}$  notation is used. Usually the doubly occupied sites are projected from (1.41) by applying a Gutzwiller projection operator, and the charge-charge correlation effects are considered to be small. Also care must take for the counting of the sites, because the original transformation was made for a pair Hamiltonian, while in (1.39) we have a sum over the bonds. By introducing the  $J = 4t^2/U$  notation, the Hamiltonian which is gained

$$H = -t \sum_{\langle i,j \rangle, \sigma} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + J \sum_{\langle i,j \rangle} \vec{S}_i \cdot \vec{S}_j, \quad (1.42)$$

is the Heisenberg antiferromagnetic exchange with a hopping term. This is called the  $t$ - $J$  model.

The above derivation from the Hubbard model gives a  $t$ - $J$  model which makes sense only if  $J/t \sim (t/u)^2 \ll 1$ . In the current literature the  $t$ - $J$  model is used in a wider sense, where  $t/J$  is essentially arbitrary. This can be justified by starting from more complicated many-band models, such as are thought to be applicable for

the superconducting Cu-O compounds, and ending up with an effective one-band t-J model for the description of the low-lying part of the spectrum.

The search for the mechanism underlying high-temperature superconductivity has stimulated interest in the behaviour of holes in quantum antiferromagnets. Extensive research, mostly numerical, has been undertaken, in order to expose the properties of the t-J model, especially in relation to the appearance of a possible superconducting state. For a recent review on the subject, see Chen, and Schuttler (1989).

Our purpose is to give a variational description of the ground state properties of the t-J model. Our treatment is, broadly speaking, reminiscent of the Gutzwiller method for the Hubbard model, but we suggest essential improvements at both the Ansatz, and the evaluation of the expectation values. We concentrate on the properties of a normal (non-symmetry breaking) ground state, emphasizing that - just as in the case of the Hubbard model - a crude description of the normal state leads to an exaggerated tendency to ordering instabilities. In the limit of half filling, our Ansatz corresponds to a quantum paramagnetic (*RVB*) ground state of the Heisenberg model. Out of half filling, the ground state corresponds to a normal conductor.

We propose to bring essential improvement in the treatment of short range order effects. On the other hand, we introduce new variational parameters to control nearest neighbour hole-hole, and spin-spin correlations. The former, if enhancement over the Fermi sea values is found, might be signalling hole-hole binding, and possibly superconductivity. The latter characterizes the background spin fluid, and in the limit of half filling, gives variational ground states for the Heisenberg model, which should be either identifiable, or competitive with trial states known from the literature.

The other essential aspect of our method is the introduction of a cluster Gutzwiller approximation. It is known that the exchange hole effect inherited from the Fermi sea can account for a good part of antiparalel spin correlations in the  $U \rightarrow \infty$  limit low dimension. To keep this feature, we take multielectron configuration amplitudes from the Fermi sea ground state, and modify these with variational parameters. We take clusters which are sufficiently large so that there is a central pair of sites fully surrounded by cluster sites. This way we hope to describe the effect of intersite correlations on hopping, and spin-flip amplitudes.

The method is applicable in any dimension, and the results are sensitive - through the geometry of the cluster - not only to dimensionality, but also to lattice structure. Of course, increasing dimensionality means increasing complication, the number of independent cluster states being  $3^{2D}$  for a  $D$  dimensional cubic lattice. Here we consider the linear chain (four site cluster) and the square lattice (eight site cluster), as examples.

## 2 Variational approaches to the Hubbard model

### 2.1 The Gutzwiller wave function

Theoretical studies of systems with short-range, repulsive interactions face the problem of how to incorporate an interaction that is simple only in real space into a noninteracting Fermi system that is simple in momentum space. In this situation variational-type methods are especially useful. Starting with an appropriate many-body trial wave function, the energy expectation value is calculated, which then has to be minimized with respect to some variational parameters. The simplest such wave function is an antisymmetrized product of one-particle functions, the next step should be to consider also two-particle functions.

In the case of Hubbard model, where the pointlike on-site interaction between the electrons of opposite spin is combined with a kinetic energy on a lattice, Gutzwiller (1963, 1964, 1965) has proposed a very simple variational wave function. With this it introduces correlations into the noninteracting wave function through a local correlation factor in real space. He, then introduced a further approximation, the so-called *Gutzwiller* approximation, to calculate the ground state energy. In the Gutzwiller approximation spatial correlations are neglected. The Gutzwiller wave function is in the form of

$$\Psi_G = \prod_i [1 - (1 - g) n_{i\uparrow} n_{i\downarrow}] \Phi_F , \quad (2.1)$$

where  $g$  is the variational parameter.  $\Phi_F$  is the Fermi sea for the noninteracting electrons

$$\begin{aligned} \Phi_F &= \prod_{\mathbf{k} < \mathbf{k}_F} c_{\mathbf{k},\sigma}^\dagger |0\rangle \\ &= \sum_{\mathbf{r}_U} \sum_{\mathbf{r}_D} \det[\phi_\uparrow(\mathbf{k}, \mathbf{r})] \det[\phi_\downarrow(\mathbf{k}, \mathbf{r})] |D, U\rangle . \end{aligned} \quad (2.2)$$

$c_{\mathbf{k},\sigma}^\dagger$  is the Fourier transform of  $c_{i,\sigma}^\dagger$  defined in (1.2).  $D$  and  $U$  are set of lattice sites occupied by down- up-spin electrons. The  $(i,j)$  elements of the determinants are simply

$$\phi_\sigma(\mathbf{k}_i, \mathbf{r}_j) = \exp(i \mathbf{k}_i \cdot \mathbf{r}_{j,\sigma}) . \quad (2.3)$$

Let us consider the meaning of  $\Psi_G$ . According to the occupation, the state of each site can be classified into four states. These are : an empty site, a site with up-spin, a site with down-spin, and a doubly occupied site. In  $\Phi_F$  the number of doubly occupied sites is given by  $N_d = N_\uparrow N_\downarrow / N$ . Once the interaction term ( $U$ ) is switched on, the increase of the energy is given by  $UN_d$ . Then  $N_d$  will diminish from  $N_\uparrow N_\downarrow / N$  to lower the energy.  $\Psi_G$  assigns  $1-g$  to this reduction factor per one doubly occupied site. The variational energy is determined using

$$E = \frac{\langle \Psi_G | H | \Psi_G \rangle}{\langle \Psi_G | \Psi_G \rangle} . \quad (2.4)$$

As stated previously, with the addition of the Gutzwiller approximation the energy can be determined. The hard calculations from the original work of Gutzwiller were clarified later by Ogawa *et al.* (1975). Here we do not discuss the details of the calculation (see Vollhardt (1984)), just briefly review the results. The non-magnetic half filled case was examined by Brinkman and Rice (1970) . They found that a form of metal-insulator transition exists at  $U = U_c$ , which is often called the Brinkman-Rice transition. It takes place at  $U_c = 8|\epsilon_0|$ , where  $\epsilon_0 = 2\epsilon_\uparrow = 2\epsilon_\downarrow$  with  $\epsilon_\sigma$  as the average energy of the  $\sigma$  spins in the uncorrelated state. However, this result, cannot be correct physically, because from the perturbation theory the energy lowering is always nonzero and is proportional to  $t^2/U$  when  $U/t \gg 1$  and the electrons tend to line up antiferromagnetically. This result is quite different in that, the system undergoes a metal-insulator transition remaining paramagnetic. To overcome this situation, many researchers tried to go beyond

the Gutzwiller approximation, like Bernasconi (1972), Ogawa and Kanda (1978), Razafimandimby (1982), Hashimoto (1985), Fazekas (1989). In parallel with this, an exact analytic estimation for the Gutzwiller wave function has been developed recently for the one dimensional case by Metzner and Vollhardt (1987, 1988), and Gebhard and Vollhardt (1987, 1988). Their method is based on the observation that, the ground state expectation values in terms of the Gutzwiller variational wave function may be expressed by sums over different lattice sites. This makes possible the application of Wick's theorem and the resulting contractions can be performed. To calculate the coefficients of these contractions a diagrammatic expansion is used. In the one dimensional case these coefficients may be determined in all orders which yield an approximation free calculation of the ground state energy. However, in the case of half filling, and large  $U$  nonanalyticities are found.



## 2.2 The variational cluster approximation method

As proposed, in order to obtain physically satisfactory results, we must go beyond the Gutzwiller approximation, i.e. to use more powerful approximations. One of the possibilities is to use a cluster type expansion for the ground state combined with a variational ansatz for the wave function, as first applied by Bernasconi (1972). Let consider a trial wave function of the form of (2.1)

$$\Psi_I = \prod_{i \in I} \Psi_i, \quad (2.5)$$

where  $\Psi_i = P_i \Phi_F$ ,  $I$  represents for a set of indices which label the lattice, and the projection operator is defined as

$$P_i = 1 - \eta n_{i\uparrow} n_{i\downarrow} + \alpha (n_{i\uparrow} + n_{i\downarrow}). \quad (2.6)$$

It can be observed that in (2.6) it is included an extra term, as compared with the Gutzwiller projection, corresponding to the chemical potential. The introduction of this second parameter is necessary in order to keep the filling at a prescribed value. The projection operator  $P_i$  reduces the probability for double occupancy of site  $\mathbf{R}_i$ . In an exact treatment this would not change the number of electrons. However, in an approximate analysis it may change the average electron density on site  $\mathbf{R}_i$ . To compensate this,  $\alpha$  will be determined by the condition

$$\frac{\langle \Psi_i | n_i | \Psi_i \rangle}{\langle \Psi_i | \Psi_i \rangle} = \langle \Phi_F | n_i | \Phi_F \rangle, \quad (2.7)$$

where  $n_i = n_{i\uparrow} + n_{i\downarrow}$ . Using the  $\langle \dots \rangle$  an abbreviation for  $\langle \Phi_F | \dots | \Phi_F \rangle$ , condition (2.7), it reads

$$\frac{(1 + 2\alpha + \alpha^2) \langle n_i \rangle + (4\alpha + 6\alpha^2 - 8\alpha\eta - 4\eta + 2\eta^2) \langle n_{i\uparrow} n_{i\downarrow} \rangle}{1 + (2\alpha + \alpha^2) \langle n_i \rangle + (2\alpha^2 - 4\alpha\eta - 2\eta + \eta^2) \langle n_{i\uparrow} n_{i\downarrow} \rangle} = \langle n_i \rangle. \quad (2.8)$$

Bernasconi (1972) obtains  $\alpha = \eta/2$ , working just in the one electron per site condition, i.e.  $\langle n_i \rangle = 1$ . Accordingly,  $\eta$  remains the only variational parameter

which controls the energy minimization. The cluster expansion is performed in the following way. A splitting of the original Hubbard Hamiltonian (1.1) in manner of

$$H = H_0 + V_J, \quad (2.9)$$

where  $V_J$  is of the form

$$V_J = \sum_{j \in J} V_j. \quad (2.10)$$

$H_0$  must be chosen so that the ground state wave function is an eigenfunction of it. This means that in our particular case  $H_0$  must be equal with the kinetic energy from (1.1).  $J$  is the set of indices which label the lattice points in the crystal. For each subset  $I$  of  $J$ , i.e. for each cluster of lattice sites, Bernasconi (1972) defines a Hamiltonian

$$H_I = H_0 + V_I, \quad (2.11)$$

with

$$V_I = \sum_{i \in I} V_i, \quad (2.12)$$

and the variational wavefunction (2.5). In the Hamiltonian  $H_I$  the intrasite Coulomb repulsion is restricted to the sites within the cluster  $I$ . We denote the expectation values of  $H_I$  with respect to  $\Psi_I$ , and  $H$  with respect to  $\Psi_J$  with  $E_I$ , and  $E_J$ , respectively. The variational ground state energy of the total Hamiltonian  $H$  can be written in the form of a cluster expansion

$$E_J = \sum_{n=0}^N \left[ \sum_{\{I_n\}} W_{I_n} \right], \quad (2.13)$$

where

$$W_{I_n} = E_{I_n} - \sum_{\{I_m | I_m \subset I_n\}} W_{I_m}, \quad (2.14)$$

and

$$W_{\emptyset} = \langle \Phi_F | H_0 | \Phi_F \rangle . \quad (2.15)$$

The summation  $\{I_n\}$  applies to all clusters containing  $n$  atoms,  $N$  denotes the total number of sites, and  $\emptyset$  denotes the empty set. Thus the ground state energy in  $M$  site cluster approximation, is obtained by totaling all clusters containing  $M$  atoms or less

$$E^{(M)} = \sum_{n=0}^M \left[ \sum_{\{I_n\}} W_{I_n} \right] . \quad (2.16)$$

If we restrict ourselves to contributions from clusters containing only a very small number of lattice sites, the use of (2.16) becomes manageable without further approximations. For the case presented previously, i.e. paramagnetic ground state, the two site cluster approximation predicts a sharp transition from a non-magnetic metal to a non-magnetic insulator as  $U$  is increased. This result is in synthesis with that obtained by Brinkman and Rice (1970) on the basis of the Gutzwiller approximation, though  $U_c$  is shifted. The second problem which arises is related to the  $U \rightarrow \infty$  limit. The Gutzwiller ground state energy is 0 for  $U$  strictly infinity. Bernasconi is not able to recover this result. This feature does not appear in later versions of the cluster method.

These problems, are lifted if the cluster approximation scheme is defined with use of a decoupling approximation, as in Razafimandimby (1982). The same projection operator as (2.6) is used in Razafimandimby (1982) in a two-site variational cluster approximation with the trial wave function

$$\Psi = \prod_i P_i \Phi_F . \quad (2.17)$$

Introducing  $n$  as the number of electrons per site and per spin, the condition (2.7) which guarantees the conservation of the electron number at site  $\mathbf{R}_i$ , with use of

Eq. (2.8), in algebraic terms

$$\alpha = \frac{-1 + 2n\eta + [1 - n(1 - 2n)(2\eta + \eta^2)]^{1/2}}{1 + 2n}. \quad (2.18)$$

The Gutzwiller ground state energy is obtained by minimizing

$$E(\eta) = \frac{\langle \Psi | H | \Psi \rangle}{\langle \Psi | \Psi \rangle}, \quad (2.19)$$

where  $\Psi$  is the one from Eq. (2.17). In order to approximately calculate (2.19), the Hubbard Hamiltonian (1.1) is rewritten as

$$H = \sum_{\langle i \neq j \rangle} H_{i,j}, \quad (2.20)$$

where

$$H_{i,j} = -t c_{i,\sigma}^\dagger c_{j,\sigma} + \frac{z}{2} U (n_{i\uparrow} n_{i\downarrow} + n_{j\uparrow} n_{j\downarrow}), \quad (2.21)$$

and  $z$  is the number of nearest neighbours. The ground state energy functional (2.19) with help of (2.17) and (2.20) is

$$\begin{aligned} E(\eta) &= \sum_{\langle i \neq j \rangle} \frac{\langle \Phi_F | P_i P_j H_{i,j} P_j P_i \prod_{l \neq i,j} P_l^2 | \Phi_F \rangle}{\langle \Phi_F | P_i^2 P_j^2 \prod_{l \neq i,j} P_l^2 | \Phi_F \rangle} \\ &\simeq \sum_{\langle i \neq j \rangle} \frac{\langle \Phi_F | P_i P_j H_{i,j} P_j P_i | \Phi_F \rangle \langle \Phi_F | \prod_{l \neq i,j} P_l^2 | \Phi_F \rangle}{\langle \Phi_F | P_i^2 P_j^2 | \Phi_F \rangle \langle \Phi_F | \prod_{l \neq i,j} P_l^2 | \Phi_F \rangle} \\ &= \sum_{\langle i \neq j \rangle} \frac{\langle \Phi_F | P_i P_j H_{i,j} P_j P_i | \Phi_F \rangle}{\langle \Phi_F | P_i^2 P_j^2 | \Phi_F \rangle}. \end{aligned} \quad (2.22)$$

The physical meaning of such an approximation is that it has treated the correlation effects at two nearest neighbour sites independently of other sites. Such approximation is sufficient to cancel the large restricted Hartree-Fock Coulomb energy  $U^2 n$  for large  $U$  because the double occupancy is reduced in each site. Such an approximation is also sustained due to its consistency with the Gutzwiller

ground state energy at  $U$  infinity. Razafimandimby (1982) is using (2.22) for the linear chain, the square and the body centered cubic three dimensional lattices. However, in three dimension, spherical Fermi surface it is assumed. For half filling, the Hartree-Fock result is recovered, i.e. a metal-insulator transition at  $U_c = 8/(1 - 16F^4)$ , where  $F = (1/2)(2/\pi)^D$ , in  $D$  dimension. For  $D = 1$ , 72% of the exact value of the ground state energy, and 97% of the exact Gutzwiller value is recovered. For less than half filling and for  $n \leq 0.3$  this approximation yields 80% of the exact value.

Further improvements in the cluster expansion technique were introduced by Fazekas (1989). The method used becomes one of the most powerful variational type calculation. The observation is that the Gutzwiller correlations are, being the most simple ones, unsatisfactory on several accounts. A description of the differences of pure Gutzwiller correlations in the one dimensional Hubbard model was made by Fazekas and Penc (1988). The main ingredients missing from the original Gutzwiller Ansatz are, at least near half filling, known to be the charge-charge correlations, particularly the so-called e-d correlations, discussed originally by Kaplan, Horsch and Fulde (1982). A very good physical description of this is given by Wang (1989). That is the empty (e) and doubly (d) occupied sites are left uncorrelated by the Gutzwiller wave function. At half filling, where e and d are present in equal numbers, bound pairs tend to be formed, with a binding energy of the order of  $t^2/U$ . Because of this the e-d correlations fall exponentially with distance. The nature of the insulating ground state can be seen as *excitonic*, i.e. it contains e-d pair condensates. Away from half filling there is an excess of e over d, and so the final nature of the ground state is decided by a three-body scattering process  $e+(ed)$ . The general belief is that in this regime, the one dimensional Hubbard model becomes a marginal conductor, that is, a borderline

between a metal and an insulator. This implies that, although the ed bound state is not destroyed, its binding energy falls to zero, hence long range e-d correlations decrease only as a power law.

Thus Fazekas (1989) is building up the variational wave function

$$\Psi = P_G P_{ed} \Phi_F , \quad (2.23)$$

with use of two projection operators. The first is the usual Gutzwiller operator as in (2.1)

$$P_G = \prod_i [ 1 - (1 - g) n_{i\uparrow} n_{i\downarrow} ] . \quad (2.24)$$

While the second one counts the e-d correlations

$$P_{ed} = \prod_{\langle i,j \rangle} \left\{ 1 - (1 - \lambda) [ n_{i\uparrow} n_{i\downarrow} (1 - n_{j\uparrow}) (1 - n_{j\downarrow}) + n_{j\uparrow} n_{j\downarrow} (1 - n_{i\uparrow}) (1 - n_{i\downarrow}) ] \right\} , \quad (2.25)$$

i.e. gives an extra factor  $\lambda$  whenever a nearest neighboring pair is found to be in the ed configuration. It is expected that  $\lambda > 1$  in the case of  $U > 0$  corresponds to the energy minimum. The usual Gutzwiller expansion (2.2) is used with the corresponding variational parameters multiplying each term. It is known that the exact treatment of the original Gutzwiller Ansatz (2.1) is challenging. Moreover, the inclusion of another trial wave function increases the degree of difficulty. Thus, one is compelled to resort to an approximation which retains just the short range part of the exchange. This was achieved by Fazekas (1989) by choosing a finite cluster and approximating the expectation values taken with  $\Psi$  with the cluster values. But this is not meant to act as a finite size calculation. With standard procedures one must go back to the infinite lattice and make the obtained cluster calculations to be an accurate approximation for the infinite lattice. In doing this we divide the lattice in two sets : a cluster  $\Gamma$ , and the complementary set  $\tilde{\Gamma}$ . Thus

the projection operator  $P = P_G P_{ed}$  factorizes as  $P = P_\Gamma P_{\tilde{\Gamma}} P_{\Gamma\tilde{\Gamma}}$ .  $P_{\tilde{\Gamma}}$  connects the cluster with the rest of the lattice. The Hubbard Hamiltonian is decomposed in sums over nearest neighboring pair Hamiltonians as in (2.20) and (2.21). It can be argued that the cluster has a pair of inner sites, where two site processes, such as hopping, can take place in an environment which is *typical* of the bulk of the system. Thus for a  $D$  dimensional cubic lattice, the smallest meaningful cluster consists of  $2D$  sites. The ground state expectation value will be

$$\begin{aligned}
E(g, \lambda) &= \frac{\langle \Phi_F | H | \Phi_F \rangle}{\langle \Phi_F | \Phi_F \rangle} \\
&= \frac{Nz}{2} \frac{\langle \Phi_F | H_{i,j} | \Phi_F \rangle}{\langle \Phi_F | \Phi_F \rangle} \\
&= \frac{Nz}{2} \frac{\langle \Phi_F | P_{\tilde{\Gamma}} P_{\tilde{\Gamma}} P_\Gamma H_{i,j} P_\Gamma P_{\tilde{\Gamma}} P_{\tilde{\Gamma}} | \Phi_F \rangle}{\langle \Phi_F | P_\Gamma^2 P_{\tilde{\Gamma}}^2 P_{\tilde{\Gamma}}^2 | \Phi_F \rangle}. \quad (2.26)
\end{aligned}$$

The complication as compared to the previous cluster expansion (2.22) is due to the appearance of the  $P_{\tilde{\Gamma}}$  term. If a simple decoupling as in (2.22) would be performed, then this would imply the inhomogeneity of the cluster. That is, the central sites would be correlated with the full number of neighbours, while sites in the shell would be undercoordinated. This problem was tackled by Fazekas (1989) applying the standard Bethe-Peierls method to make the cluster an acceptable replacement for the bulk. Using, as before, the abbreviation  $\langle \dots \rangle$  for  $\langle \Phi_F | \dots | \Phi_F \rangle$  instead of the usual decoupling of (2.26) in

$$\begin{aligned}
E(g, \lambda) &\simeq \frac{Nz}{2} \frac{\langle P_\Gamma H_{i,j} P_\Gamma \rangle \langle P_{\tilde{\Gamma}}^2 \rangle}{\langle P_\Gamma^2 \rangle \langle P_{\tilde{\Gamma}}^2 \rangle} \\
&= \frac{Nz}{2} \frac{\langle P_\Gamma H_{i,j} P_\Gamma \rangle}{\langle P_\Gamma^2 \rangle}, \quad (2.27)
\end{aligned}$$

it becomes

$$E(g, \lambda) \simeq \frac{Nz}{2} \frac{\langle P_{BP} H_{i,j} P_{BP} \rangle}{\langle P_{BP}^2 \rangle}. \quad (2.28)$$

The Bethe-Peierls method requires that  $P_{\Gamma}$  to be replaced by the Bethe-Peierls projection  $P_{BP}$  which acts on the sites of the cluster in such a way as to make up for the neglected  $P_{\Gamma}$ . The construction of  $P_{BP}$  is a very delicate problem. In one dimensions we have a four site cluster, and we label the sites by 1,2,3 and 4. As an example, the probability of finding the cluster in configuration, e.g.  $(e d \uparrow \downarrow)$ , for non-interacting electrons is simply the product of the probabilities of the corresponding up- and down-spin configurations, i.e.  $(0 \uparrow \uparrow 0)(0 \downarrow 0 \downarrow)$ . In the interacting case, the weighting factor of the configurations has to contain the variational parameters. The cluster consists of nonequivalent sites, that is site 2 has both of its nearest neighbours inside the cluster, while the site 1 has not. This inhomogeneity, resulting from the finiteness of the cluster can be compensated by an inhomogeneous weighting procedure. This is in practically terms the Bethe-Peierls approximation. For details concerning this method, see Domb (1960). This is a standard way to deal with cluster calculations in classical statistical physics. Fazekas (1989) applied it to the present quantum mechanical problem, introducing it in the variational cluster treatment of the Hubbard Hamiltonian. Following this method, he assigned the weights  $g_c$  and  $\lambda_c$  to the central sites, and  $g_s$  and  $\lambda_s$  to the shell sites. The correspondence between the central and shell site weighting factors is obtained by fulfilling the Bethe-Peierls self consistent conditions. First, we require that the density of the doubly occupied sites be the same in the centre as in the shell. for the half filled case this means

$$n_d = \frac{1}{4} \frac{\partial \ln \langle \Psi | \Psi \rangle}{\partial \ln g_c} = \frac{1}{4} \frac{\partial \ln \langle \Psi | \Psi \rangle}{\partial \ln g_s}. \quad (2.29)$$

In the same fashion, the density of the ed pairs must also be homogeneous

$$n_{ed} = \frac{1}{2} \frac{\partial \ln \langle \Psi | \Psi \rangle}{\partial \ln \lambda_s^2} = \frac{\partial \ln \langle \Psi | \Psi \rangle}{\partial \ln \lambda_c^2}. \quad (2.30)$$



The method itself requires tedious calculations, because all the 256 configurations of the four site cluster have to be taken into account. Eventual optimization can be done only numerically, but analytic expansions can be done in the small  $U$ , and large  $U$  limits. The point of the cluster Gutzwiller approximation is that it takes into account the short range part of the exchange hole effect which is completely neglected in the single site Gutzwiller approximation. As a check on the quality of the cluster approximation he gives the  $U \rightarrow \infty$  value of the spin correlation  $\langle S_2^z S_3^z \rangle \sim -0.1324$  which is 90% of the correct value obtained by exact evaluation of the projected Fermi sea.

In the following chapter we will follow closely this method, and apply it to the one, and two dimensional t-J model for different band fillings.

### 3 Variational cluster calculation of the t-J model

The Hamiltonian model which we will deal with is the following

$$H = -t \sum_{\langle i,j \rangle} (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + J \sum_{\langle i,j \rangle} (\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j). \quad (3.1)$$

As previously stated,  $n_i = n_{i\uparrow} + n_{i\downarrow}$ . For the derivation of (3.1) see, Chap. 1. The first term is the usual nearest neighbour hopping. The second, and third term contains the two basic correlation processes within the system, namely the spin-spin, and density-density correlation. We retain all the three terms from (3.1), firstly because we aim to relate our results also to the highly correlated limit of the Hubbard Hamiltonian. Secondly, we are interested in the effect of the charge-charge correlation on the ground state. To construct our trial wave function, we act with a number of projectors onto the Fermi sea. This means looking for a non-symmetry breaking, normal ground state which, however, has various kinds of short range order. The tendency to long range order will come to be guessed from enhancement of the corresponding short range order. To map out the ground state phase diagram, one should also consider projected long range ordered states. We note that Zhang *et al.* (1988), and Yokoyama and Shiba (1987) considered projected SDW and BCS states. The approach of the present scheme lies in a more accurate characterization of the ground state, which should help to avoid predicting spurious ordering instabilities.

We consider first the generalized Gutzwiller projection, as introduced first by Bernasconi (1972) and used also by Razafimandimby (1982)

$$P_G = \prod_i [1 - n_{i\uparrow} n_{i\downarrow} + \mu n_i], \quad (3.2)$$

which includes also the chemical potential. However, the Gutzwiller variational parameter is taken to be vanishing. By this we enforce the system not to have

doubly occupied sites. The following two projection operators which will be considered are related to the two basic correlations present in the Hamiltonian (3.1). For the first projection operator, we take into account the  $S^z S^z$  correlation only

$$P_{ss} = \prod_{\langle i,j \rangle} \left[ 1 - 2(\beta - 1) (S_i^z S_j^z - \frac{1}{4}) \right], \quad (3.3)$$

i.e. we are interested in a projected antiferromagnetic state. By doing this we break the rotational invariance of the system. Ideally, we would like to construct a singlet trial state. In our formalism, this would require introducing non-commuting projectors, which would lead to tremendous technical difficulties. The best we can hope for is that the system will favour nearly isotropic spin correlations on energetical grounds. To check this, we will compute  $S^x S^x$  and  $S^y S^y$ , as well as  $S^z S^z$  which appears variationally.

The second projection operator which we will consider will be the hole-hole correlation

$$P_{hh} = \prod_{\langle i,j \rangle} [1 - \alpha (1 - n_{i\uparrow}) (1 - n_{i\downarrow}) (1 - n_{j\uparrow}) (1 - n_{j\downarrow})]. \quad (3.4)$$

This correlation is important to search for a possible superconducting instability within the system. If we find tendency for the holes to bind, this may signal the formation of a pair condensate. However, care has to be taken to differentiate it from tendency to hole segregation, which is also possible.

Thus, the trial wave function will be the following

$$\Psi = P_G P_{ss} P_{hh} \Phi_F. \quad (3.5)$$

The starting wave function into which the projection operator

$$P = P_G P_{ss} P_{hh} \quad (3.6)$$

acts is the non-interacting Fermi-sea ground state  $\Phi_F$ . The expectation values taken with  $\Phi_F$  we will denote by  $\langle \dots \rangle$ . We are dealing with two independent variational parameters  $\alpha$  and  $\beta$ , versus the energy minimization which must be performed. The third parameter entering in (3.5)  $\mu$  is the chemical potential. The value of which is determined by using a condition similar to that of Bernasconi (1972), see Eq. (2.7). The  $P_{G_i} = 1 - n_{i\uparrow}n_{i\downarrow} + \mu n_i$  part of the Gutzwiller projection excludes double occupation of a lattice site  $\mathbf{R}_i$ . The remaining two projections are counting those nearest neighbour pairs which are found to be in up-spin $\leftrightarrow$ down-spin (down-spin $\leftrightarrow$ up-spin) or hole $\leftrightarrow$ hole configuration. The effect of  $P_{G_i}$  on  $\Phi_F$  is however, is to keep the average electron density on site  $\mathbf{R}_i$  constant. Thus  $\mu$  will be determined by the condition

$$\frac{\langle \Phi_F | P_i n_i P_i | \Phi_F \rangle}{\langle \Phi_F | P_i^2 | \Phi_F \rangle} = \langle \Phi_F | n_i | \Phi_F \rangle = n . \quad (3.7)$$

In order to evaluate the cluster expectation values, we write (3.1) as a summation of pair Hamiltonians  $H_{i,j}$

$$H_{i,j} = -t (c_{i,\sigma}^\dagger c_{j,\sigma} + \text{h.c.}) + J(\vec{S}_i \cdot \vec{S}_j - \frac{1}{4} n_i n_j) , \quad (3.8)$$

than

$$H = \sum_{\langle i,j \rangle} H_{i,j} . \quad (3.9)$$

We will consider our cluster to be a set of sites  $\Gamma$  containing the nearest neighbour sites of a pair of site, i.e. of a *central* pair. This cluster approximation permits us to take into account the effect of the immediate environment on the nearest neighbour hopping process. The Bethe-Peierls condition should guarantee that the central pair is typical for the bulk. In one dimension, this is accomplished by choosing a four site cluster, while in the two dimension square lattice by eight

sites. Using (2.27) the cluster expectation value of (3.9) will be

$$\frac{2}{Nz} \langle H \rangle = \frac{\langle P_{\Gamma} H_{i,j} P_{\Gamma} \rangle}{\langle P_{\Gamma}^2 \rangle}, \quad (3.10)$$

where  $N$  is the number of lattice sites and  $z$  is the coordination number. After this stage, we can then apply the Bethe-Peierls method to replace  $P_{\Gamma}$  by the Bethe-Peierls projection  $P_{BP}$ . As the  $P_{BP}$  is dependent on the concrete cluster as well as on the trial state, it must be carefully constructed. This is why we defer specifying  $P_{BP}$  till we deal with the concrete cases.

In order to calculate  $\langle P_{\Gamma} H_{i,j} P_{\Gamma} \rangle$  and  $\langle P_{\Gamma}^2 \rangle$  we use the procedure which is applied to the Gutzwiller variational wave function, see Metzner and Vollhardt (1988). Correspondingly we proceed, firstly with the denominator, to apply Wick's theorem. This yields a sum over all contracted terms. In this sum the only nonvanishing contractions are  $\langle c_{i,\sigma}^{\dagger} c_{j,\sigma} \rangle$  and  $\langle c_{i,\sigma} c_{j,\sigma}^{\dagger} \rangle$  for all  $i,j$ . Using the Fourier transformations (1.2) and (1.3) we get

$$\begin{aligned} f_{ij} &= \langle c_{i,\sigma}^{\dagger} c_{j,\sigma} \rangle \\ &= \int d\mathbf{k} e^{-i \mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} n_{\mathbf{k},\sigma}^0, \end{aligned} \quad (3.11)$$

where  $n_{\mathbf{k},\sigma}^0 = \theta(\varepsilon_F - \varepsilon_{\mathbf{k}})$  is the momentum distribution of  $\sigma$  spins in the noninteracting system. While

$$f_{ji} = \langle c_{j,\sigma} c_{i,\sigma}^{\dagger} \rangle = \begin{cases} 1 - f_{ij}, & \text{if } i = j; \\ -f_{ij}, & \text{otherwise.} \end{cases} \quad (3.12)$$

The  $\int d\mathbf{k}$  in (3.11) is taken for the first Brillouin zone. Furthermore,  $f_{ii} = \langle c_{i,\sigma}^{\dagger} c_{i,\sigma} \rangle$  is the expectation value of the number operator ( $n_{i,\sigma} = c_{i,\sigma}^{\dagger} c_{i,\sigma}$ ). Thus, if we have, for example, a cluster built up by  $m$  sites, then  $\langle P_{\Gamma}^2 \rangle$  will be a sum over all possible configurations of expectation values of the

$$\langle \hat{O}_{1,\sigma}^g \hat{O}_{2,\sigma}^g \dots \hat{O}_{m,\sigma}^g \rangle \quad (3.13)$$

form, where

$$\hat{O}_{i,\sigma}^1 = n_{i,\sigma} , \quad (3.14)$$

if there exists one electron on site  $\mathbf{R}_i$  and

$$\hat{O}_{i,\sigma}^2 = 1 - n_{i,\sigma} , \quad (3.15)$$

if we have an empty site. Using curly brackets for the contracted terms, (3.13) then becomes

$$\langle \hat{O}_{1,\sigma}^g \hat{O}_{2,\sigma}^g \dots \hat{O}_{m,\sigma}^g \rangle = \{ \mathcal{O}_{1,\sigma}^g \mathcal{O}_{2,\sigma}^g \dots \mathcal{O}_{m,\sigma}^g \} . \quad (3.16)$$

The obtained expression can be written as a product of the probabilities of the corresponding up- and down-spin configurations

$$\{ \mathcal{O}_{1,\sigma}^g \mathcal{O}_{2,\sigma}^g \dots \mathcal{O}_{m,\sigma}^g \} = \{ \mathcal{O}_{1\uparrow}^g \mathcal{O}_{2\uparrow}^g \dots \mathcal{O}_{m\uparrow}^g \} \{ \mathcal{O}_{1\downarrow}^g \mathcal{O}_{2\downarrow}^g \dots \mathcal{O}_{m\downarrow}^g \} . \quad (3.17)$$

Subsequently we will calculate the expansion of the two terms from the right hand side of (3.17), obtaining a sum of determinants, each of them containing terms of elements  $n \leq m$  of contracted values  $c_{i,\sigma}^\dagger c_{j,\sigma}$  or  $c_{j,\sigma} c_{i,\sigma}^\dagger$ . These contractions are equal with  $f_{ij}$  or  $f_{ji}$  defined in (3.11) and (3.12). To be more explicit, let us consider a concrete example, of one dimension, in this case  $m = 4$ , and take, e.g. the configuration  $(\uparrow \downarrow 0 \uparrow)$ . That is, on the first site there is an up-spin, on the second one a down-spin, the third site is empty, and on the fourth one there is an up-spin. For this configuration we need to calculate

$$\langle \hat{O}_{1\uparrow}^1 \hat{O}_{2\downarrow}^1 \hat{O}_{3,\sigma}^2 \hat{O}_{4\uparrow}^1 \rangle . \quad (3.18)$$

Proceeding by applying in order Eqs. (3.16), (3.17), (3.14) and (3.15), we obtain

$$\begin{aligned} \langle \hat{O}_{1\uparrow}^1 \hat{O}_{2\downarrow}^1 \hat{O}_{3,\sigma}^2 \hat{O}_{4\uparrow}^1 \rangle &= \{ \mathcal{O}_{1\uparrow}^1 \mathcal{O}_{2\downarrow}^1 \mathcal{O}_{3,\sigma}^2 \mathcal{O}_{4\uparrow}^1 \} \\ &= \{ \mathcal{O}_{1\uparrow}^1 \mathcal{O}_{2\uparrow}^2 \mathcal{O}_{3\uparrow}^2 \mathcal{O}_{4\uparrow}^1 \} \{ \mathcal{O}_{1\downarrow}^2 \mathcal{O}_{2\downarrow}^1 \mathcal{O}_{3\downarrow}^2 \mathcal{O}_{4\downarrow}^2 \} \\ &= \{ n_{1\uparrow} (1 - n_{2\uparrow}) (1 - n_{3\uparrow}) n_{4\uparrow} \} \{ (1 - n_{1\downarrow}) n_{2\downarrow} (1 - n_{3\downarrow}) (1 - n_{4\downarrow}) \} . \end{aligned}$$

(3.19)

The first contraction from the right hand side of (3.19) is

$$\begin{aligned}
\{n_{1\uparrow} (1 - n_{2\uparrow}) (1 - n_{3\uparrow}) n_{4\uparrow}\} &= \{n_{1\uparrow} n_{4\uparrow}\} - \{n_{1\uparrow} n_{2\uparrow} n_{4\uparrow}\} - \{n_{1\uparrow} n_{3\uparrow} n_{4\uparrow}\} \\
&+ \{n_{1\uparrow} n_{2\uparrow} n_{3\uparrow} n_{4\uparrow}\} \\
&= \begin{vmatrix} f_{11} & f_{14} \\ f_{41} & f_{44} \end{vmatrix} \\
&- \begin{vmatrix} f_{11} & f_{12} & f_{14} \\ f_{21} & f_{22} & f_{24} \\ f_{41} & f_{42} & f_{44} \end{vmatrix} \\
&- \begin{vmatrix} f_{11} & f_{13} & f_{14} \\ f_{31} & f_{33} & f_{34} \\ f_{41} & f_{43} & f_{44} \end{vmatrix} \\
&+ \begin{vmatrix} f_{11} & f_{12} & f_{13} & f_{14} \\ f_{21} & f_{22} & f_{23} & f_{24} \\ f_{31} & f_{32} & f_{33} & f_{34} \\ f_{41} & f_{42} & f_{43} & f_{44} \end{vmatrix}. \tag{3.20}
\end{aligned}$$

While the second contraction is

$$\begin{aligned}
\{(1 - n_{1\downarrow}) n_{2\downarrow} (1 - n_{3\downarrow}) (1 - n_{4\downarrow})\} &= \{n_{2\downarrow}\} - \{n_{1\downarrow} n_{2\downarrow}\} - \{n_{2\downarrow} n_{3\downarrow}\} - \{n_{2\downarrow} n_{4\downarrow}\} \\
&+ \{n_{1\downarrow} n_{2\downarrow} n_{3\downarrow}\} + \{n_{1\downarrow} n_{2\downarrow} n_{4\downarrow}\} \\
&+ \{n_{2\downarrow} n_{3\downarrow} n_{4\downarrow}\} - \{n_{1\downarrow} n_{2\downarrow} n_{3\downarrow} n_{4\downarrow}\} \\
&= f_{22} - \begin{vmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{vmatrix} \\
&- \begin{vmatrix} f_{22} & f_{23} \\ f_{32} & f_{33} \end{vmatrix} - \begin{vmatrix} f_{22} & f_{24} \\ f_{42} & f_{44} \end{vmatrix} \\
&+ \begin{vmatrix} f_{11} & f_{12} & f_{13} \\ f_{21} & f_{22} & f_{23} \\ f_{31} & f_{32} & f_{33} \end{vmatrix} + \begin{vmatrix} f_{11} & f_{12} & f_{14} \\ f_{21} & f_{22} & f_{24} \\ f_{41} & f_{42} & f_{44} \end{vmatrix} \\
&+ \begin{vmatrix} f_{22} & f_{23} & f_{24} \\ f_{32} & f_{33} & f_{34} \\ f_{42} & f_{43} & f_{44} \end{vmatrix} - \begin{vmatrix} f_{11} & f_{12} & f_{13} & f_{14} \\ f_{21} & f_{22} & f_{23} & f_{24} \\ f_{31} & f_{32} & f_{33} & f_{34} \\ f_{41} & f_{42} & f_{43} & f_{44} \end{vmatrix}. \tag{3.21}
\end{aligned}$$

Thus the expectation value (3.18) is equal to the product of (3.20) and (3.21). The number of different configurations which must be totalled up depends on the concrete lattice which is analysed. As we noted previously, we consider our cluster to contain one central pair and all the surrounding nearest neighbour pairs. Using the Gutzwiller projection in the form of (3.2), we project out all the doubly occupied sites. Thus on each site we can have three possible situation : up-spin, down-spin and empty site. This results in, the number of configurations entering in the calculation of the nominator of (3.10) is given by  $3^m$ , where  $m$  is the number of sites within the cluster. That is, in a one dimension we have to calculate 81, and in a two dimension square lattice 6561 configurations.

Secondly, we consider the numerator of (3.10), i.e.  $\langle P_{\Gamma} H_{i,j} P_{\Gamma} \rangle$ . In this case, the same calculation technique, using Wick's theorem, is also applied as before. If we take, in order the terms appearing in  $H_{i,j}$  of (3.8), the first one is the hopping. If we continue our previous example, i.e. considering the cluster configuration  $(\uparrow \downarrow 0 \uparrow)$ , then in this concrete example, there are two possible hopping processes. Namely  $c_{3\downarrow}^{\dagger} c_{2\downarrow}$  or  $c_{3\uparrow}^{\dagger} c_{4\uparrow}$ . For the presentation of the calculation method it is enough to take one of these two possibilities. If we choose the latter, we have to calculate the expectation value of

$$\langle P_{\Gamma} c_{3\uparrow}^{\dagger} c_{4\uparrow} P_{\Gamma} \rangle, \quad (3.22)$$

in the configuration  $(\uparrow \downarrow 0 \uparrow)$ . This results in that the propagation process is the following

$$c_{3\uparrow}^{\dagger} c_{4\uparrow} | \uparrow \downarrow 0 \uparrow \rangle \longrightarrow | \uparrow \downarrow \uparrow 0 \rangle. \quad (3.23)$$

Being the expectation values taken with  $\Phi_F$  the noninteracting wave function, the amplitude factorizes according to the spin state. Thus, we can follow the sequence



presented previously. In such a way (3.22) becomes

$$\begin{aligned}
\langle \hat{O}_{1\uparrow}^1 \hat{O}_{2\downarrow}^1 c_{3\uparrow}^\dagger c_{4\uparrow} \rangle &= \{O_{1\uparrow}^1 O_{2\downarrow}^1 c_{3\uparrow}^\dagger c_{4\uparrow}\} \\
&= \{O_{1\uparrow}^1 O_{2\uparrow}^2 c_{3\uparrow}^\dagger c_{4\uparrow}\} \{O_{1\downarrow}^2 O_{2\downarrow}^1 O_{3\downarrow}^2 O_{4\downarrow}^2\} \\
&= \{n_{1\uparrow} (1 - n_{2\uparrow}) c_{3\uparrow}^\dagger c_{4\uparrow}\} \{(1 - n_{1\downarrow})n_{2\downarrow}(1 - n_{3\downarrow})(1 - n_{4\downarrow})\} \\
&= \left[ \{n_{1\uparrow} c_{3\uparrow}^\dagger c_{4\uparrow}\} - \{n_{1\uparrow} n_{2\uparrow} c_{3\uparrow}^\dagger c_{4\uparrow}\} \right] \\
&\times \left[ \{n_{2\downarrow}\} - \{n_{1\downarrow} n_{2\downarrow}\} - \{n_{2\downarrow} n_{3\downarrow}\} - \{n_{2\downarrow} n_{4\downarrow}\} \right. \\
&+ \{n_{1\downarrow} n_{2\downarrow} n_{3\downarrow}\} + \{n_{1\downarrow} n_{2\downarrow} n_{4\downarrow}\} \\
&\left. + \{n_{2\downarrow} n_{3\downarrow} n_{4\downarrow}\} - \{n_{1\downarrow} n_{2\downarrow} n_{3\downarrow} n_{4\downarrow}\} \right] \\
&= \left[ \begin{vmatrix} f_{11} & f_{14} \\ f_{31} & f_{34} \end{vmatrix} - \begin{vmatrix} f_{11} & f_{12} & f_{14} \\ f_{21} & f_{22} & f_{24} \\ f_{31} & f_{32} & f_{34} \end{vmatrix} \right] \\
&\times \left[ f_{22} - \begin{vmatrix} f_{11} & f_{12} \\ f_{21} & f_{22} \end{vmatrix} \right. \\
&- \begin{vmatrix} f_{22} & f_{23} \\ f_{32} & f_{33} \end{vmatrix} - \begin{vmatrix} f_{22} & f_{24} \\ f_{42} & f_{44} \end{vmatrix} \\
&+ \begin{vmatrix} f_{11} & f_{12} & f_{13} \\ f_{21} & f_{22} & f_{23} \\ f_{31} & f_{32} & f_{33} \end{vmatrix} + \begin{vmatrix} f_{11} & f_{12} & f_{14} \\ f_{21} & f_{22} & f_{24} \\ f_{41} & f_{42} & f_{44} \end{vmatrix} \\
&\left. + \begin{vmatrix} f_{22} & f_{23} & f_{24} \\ f_{32} & f_{33} & f_{34} \\ f_{42} & f_{43} & f_{44} \end{vmatrix} - \begin{vmatrix} f_{11} & f_{12} & f_{13} & f_{14} \\ f_{21} & f_{22} & f_{23} & f_{24} \\ f_{31} & f_{32} & f_{33} & f_{34} \\ f_{41} & f_{42} & f_{43} & f_{44} \end{vmatrix} \right]. \quad (3.24)
\end{aligned}$$

The second term in  $H_{i,j}$  is the nearest neighbour Heisenberg interaction, for this calculation we use the well-known formulas

$$S_i^x S_j^x + S_i^y S_j^y = \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+), \quad (3.25)$$

$$S_i^+ = c_{i\uparrow}^\dagger c_{i\downarrow}, \quad S_i^- = c_{i\downarrow}^\dagger c_{i\uparrow}, \quad (3.26)$$

and

$$S_i^z = n_{i\uparrow} - n_{i\downarrow}. \quad (3.27)$$

The formula obtained for  $\vec{S}_i \cdot \vec{S}_j$  is

$$\begin{aligned} \vec{S}_i \cdot \vec{S}_j &= -\frac{1}{2} (c_{i\uparrow}^\dagger c_{j\uparrow} c_{j\downarrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{j\downarrow} c_{j\uparrow}^\dagger c_{i\uparrow}) \\ &+ \frac{1}{4} (n_{i\uparrow} - n_{i\downarrow})(n_{j\uparrow} - n_{j\downarrow}). \end{aligned} \quad (3.28)$$

The first two terms from (3.27) corresponding to  $S_i^x S_j^x + S_i^y S_j^y$  are leading to spin flip processes, while the last term  $S_i^z S_j^z$  only counts the nearest neighbour spin configuration with a weight factor. In our concrete example of  $(\uparrow \downarrow 0 \uparrow)$  configuration, for

$$\langle P_\Gamma \vec{S}_i \cdot \vec{S}_j P_\Gamma \rangle, \quad (3.29)$$

will contribute  $c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger c_{1\uparrow}$  and  $n_{1\uparrow} n_{2\downarrow}$  by the processes

$$c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger c_{1\uparrow} | \uparrow \downarrow 0 \uparrow \rangle \longrightarrow | \downarrow \uparrow 0 \uparrow \rangle, \quad (3.30)$$

and

$$n_{1\uparrow} n_{2\downarrow} | \uparrow \downarrow 0 \uparrow \rangle \longrightarrow | \uparrow \downarrow 0 \uparrow \rangle. \quad (3.31)$$

Consequently, (3.29) becomes

$$-\frac{1}{2} \langle c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger c_{1\uparrow} \hat{O}_{3,\sigma}^2 \hat{O}_{4\uparrow}^1 \rangle - \frac{1}{4} \langle \hat{O}_{1,\uparrow}^1 \hat{O}_{2\downarrow}^1 \hat{O}_{3,\sigma}^2 \hat{O}_{4\uparrow}^1 \rangle. \quad (3.32)$$

It can be seen that the second expectation value from (3.31) is exactly the denominator of the corresponding configuration, i.e. Eq. (3.18). This is due to the fact that, the  $S_i^z S_j^z$  only counts the spin configurations with a weight factor  $+\frac{1}{4} \uparrow\uparrow$ ,  $-\frac{1}{4} \uparrow\downarrow$ ,  $-\frac{1}{4} \downarrow\uparrow$ , and  $+\frac{1}{4} \downarrow\downarrow$ . While the first term of (3.31) can be calculated in the

same fashion as the kinetic energy and it appeared as

$$\begin{aligned}
\langle c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger c_{1\uparrow} \hat{O}_{3,\sigma}^2 \hat{O}_{4\uparrow}^1 \rangle &= \{c_{1\downarrow}^\dagger c_{2\downarrow} c_{2\uparrow}^\dagger c_{1\uparrow} \mathcal{O}_{3,\sigma}^2 \mathcal{O}_{4\uparrow}^1\} \\
&= \{c_{2\uparrow}^\dagger c_{1\uparrow} \mathcal{O}_{3\uparrow}^2 \mathcal{O}_{4\uparrow}^1\} \{c_{1\downarrow}^\dagger c_{2\downarrow} \mathcal{O}_{3\downarrow}^2 \mathcal{O}_{4\downarrow}^2\} \\
&= \{c_{2\uparrow}^\dagger c_{1\uparrow} (1 - n_{3\uparrow}) n_{4\uparrow}\} \{c_{1\downarrow}^\dagger c_{2\downarrow} (1 - n_{3\downarrow}) (1 - n_{4\downarrow})\} \\
&= \left[ \{c_{2\uparrow}^\dagger c_{1\uparrow} n_{4\uparrow}\} - \{c_{2\uparrow}^\dagger c_{1\uparrow} n_{3\uparrow} n_{4\uparrow}\} \right] \\
&\times \left[ \{c_{1\downarrow}^\dagger c_{2\downarrow}\} - \{c_{1\downarrow}^\dagger c_{2\downarrow} n_{3\downarrow}\} \right. \\
&\quad \left. - \{c_{1\downarrow}^\dagger c_{2\downarrow} n_{4\downarrow}\} + \{c_{1\downarrow}^\dagger c_{2\downarrow} n_{3\downarrow} n_{4\downarrow}\} \right] \\
&= \left[ \begin{vmatrix} f_{21} & f_{24} \\ f_{41} & f_{44} \end{vmatrix} - \begin{vmatrix} f_{21} & f_{23} & f_{24} \\ f_{31} & f_{33} & f_{34} \\ f_{41} & f_{43} & f_{44} \end{vmatrix} \right] \\
&\times \left[ f_{12} - \begin{vmatrix} f_{12} & f_{13} \\ f_{31} & f_{33} \end{vmatrix} \right. \\
&\quad \left. - \begin{vmatrix} f_{12} & f_{14} \\ f_{41} & f_{44} \end{vmatrix} + \begin{vmatrix} f_{12} & f_{13} & f_{14} \\ f_{31} & f_{33} & f_{34} \\ f_{41} & f_{43} & f_{44} \end{vmatrix} \right]
\end{aligned} \tag{3.33}$$

The last term of  $H_{i,j}$  is the charge-charge correlation. The calculation of which is similar to the  $S_i^z S_j^z$  correlation, because it counts the nearest neighbour spin configurations, multiplying each of them with a factor of  $\frac{1}{4}$ .

In conclusion, we calculate for one configuration the corresponding average values using expressions like (3.24) and (3.33). Then, we apply the Bethe-Peierls projection, by assigning to all the pairs of the cluster a variational parameter. Then, we sum up the so obtained values for all the possible configurations of the chosen cluster. As a result the Bethe-Peierls condition must be appropriately

constructed and solved for the cluster which is analysed, and the chemical potential must be determined using Eq. (3.7), from the equation

$$\begin{aligned}
& \mu^2 [n(7A + 4B + 11C) - (A + C)(2n^2 + 1)] \\
& + 2\mu [n(2A - B + C) + 2n^2(A + 2B + 3C) - (A + C)] \\
& + n(2A + B + 2C) + n^2(A + 2B + 2C) = 0 . \tag{3.34}
\end{aligned}$$

Where  $A = (1 - 2\alpha_c + \alpha_c^2)(-\beta_c + (\beta_c - 1)^2/4)$ ,  $B = -3(\beta_c - 1)^2/2 - \alpha_c(-\beta_c + (\beta_c - 1)^2/4)$  and  $C = 3(\beta_c - 1)^2/4 + (2\alpha_c - \alpha_c^2)(-\beta_c + (\beta_c - 1)^2/4)$ .

In this introduction we presented the calculational technique of the cluster approximation. In the following chapters, we will present concrete applications to a number of systems. We are representing the one dimensional chain by a four site cluster, and the two dimensional square lattice with an eight site cluster. In both cases, we consider half filling as well as the  $n = 5/6$  filling factor. For both calculation we used the Maple algebraic manipulation program of IBM-3090 CINECA.

## 4 The linear chain

As presented in the previous chapter, for the one dimensional case the cluster will contain  $m = 4$  sites, and we will deal with 81 configurations. The band energy (1.5)

$$\varepsilon_{\mathbf{k}} = -t \frac{1}{N} \sum_{\langle i,j \rangle} e^{i \mathbf{k} \cdot \mathbf{R}_{ij}} , \quad (4.1)$$

becomes

$$\varepsilon_k = -2t \cos k . \quad (4.2)$$

We first calculate the filling dependence of the Fermi energy  $\varepsilon_F$ . We introduce an additional parameter  $0 \leq \delta \leq 1$ , in such a way that  $\varepsilon_F = -2t\delta$ , that is,  $\delta = 1$  for empty band and  $\delta = 0$  for half filled band. The momentum distribution in the noninteracting system will become

$$\begin{aligned} \theta(\varepsilon_F - \varepsilon_k) &= \theta(-2t\delta + 2t \cos k) \\ &= \theta(-\delta + \cos k) . \end{aligned} \quad (4.3)$$

Considering  $n_\uparrow = n_\downarrow = n/2$  with  $n$  being the number of electrons per site

$$\begin{aligned} \frac{n}{2} &= \frac{1}{2\pi} \int_{-\pi}^{+\pi} dk \theta(\varepsilon_F - \varepsilon_k) \\ &= \frac{1}{2\pi} \int_{-\pi}^{+\pi} dk \theta(-\delta + \cos k) \\ &= \frac{1}{\pi} \arccos \delta . \end{aligned} \quad (4.4)$$

We need the matrix elements of the one-particle density matrix  $f_{ij}$ , introduced in (3.11).

$$\begin{aligned} f_{ij} &= \frac{1}{2\pi} \int_{-\pi}^{+\pi} dk e^{-i k (R_i - R_j)} \theta(\varepsilon_F - \varepsilon_k) \\ &= \frac{1}{\pi(R_i - R_j)} \sin((R_i - R_j) \arccos \delta) \\ &= \frac{1}{\pi(R_i - R_j)} \sin \frac{\pi n (R_i - R_j)}{2} . \end{aligned} \quad (4.5)$$

Knowing the values of  $f_{ij}$ , we can calculate the expectation value  $\langle P_{\Gamma} H_{i,j} P_{\Gamma} \rangle / Z$ , where  $Z = \langle P_{\Gamma}^2 \rangle$  using the procedure presented in the previous paragraph. After these expectation values are calculated we must assign to all the configurations the desired variational parameters, i.e. we must construct the Bethe-Peierls projections. For the one dimensional case we proceed as follows : we assign to the central pair (23) the variational parameters  $\alpha_c$  and  $\beta_c$ , and to the shell sites (12) and (34) the supplementary variational parameters  $\alpha_s$  and  $\beta_s$ , which are linked to the original variational parameters through the Bethe-Peierls conditions. These are constructed by considering that the density of the hole $\leftrightarrow$ hole pairs

$$n_{hh} = \frac{1}{2} \frac{\partial \ln Z}{\partial \ln \alpha_s^2} = \frac{\partial \ln Z}{\partial \ln \alpha_c^2}, \quad (4.6)$$

and of the up-spin $\leftrightarrow$ down-spin pairs

$$n_{ss} = \frac{1}{2} \frac{\partial \ln Z}{\partial \ln \beta_s^2} = \frac{\partial \ln Z}{\partial \ln \beta_c^2}, \quad (4.7)$$

must be the same in the centre as in the shell.

For the half filled case, i.e  $n = 1$ , the kinetic energy gives no contribution. The denominator contains six independent terms, with the following coefficients

$$z_1 = 0.7568151446 \times 10^{-5},$$

$$z_2 = 0.001889388141,$$

$$z_3 = 0.01783035890,$$

$$z_4 = 0.006782587712,$$

$$z_5 = 0.059091623434,$$

and

$$z_6 = 0.02132792092.$$

The analytical value of this six independent coefficient result as

$$z_1 = 2 \left( \frac{1}{16} - \frac{7}{9} \frac{1}{\pi^2} + \frac{16}{9} \frac{1}{\pi^4} \right)^2 ,$$

$$z_2 = 4 \left( \frac{1}{16} - \frac{2}{9} \frac{1}{\pi^2} - \frac{16}{9} \frac{1}{\pi^4} \right)^2 ,$$

$$z_3 = 4 \left( \frac{1}{16} + \frac{2}{9} \frac{1}{\pi^2} - \frac{16}{9} \frac{1}{\pi^4} \right)^2 ,$$

$$z_4 = 2 \left( \frac{1}{16} - \frac{2}{9} \frac{1}{\pi^2} + \frac{16}{9} \frac{1}{\pi^4} \right)^2 ,$$

$$z_5 = 2 \left( \frac{1}{16} + \frac{7}{9} \frac{1}{\pi^2} + \frac{16}{9} \frac{1}{\pi^4} \right)^2 ,$$

and

$$z_6 = 2 \left( \frac{1}{16} + \frac{2}{9} \frac{1}{\pi^2} + \frac{16}{9} \frac{1}{\pi^4} \right)^2 .$$

The denominator is

$$Z = z_1 + z_2 \beta_s^2 + z_3 \beta_s^2 \beta_c^2 + z_4 \beta_c^2 + z_5 \beta_s^4 \beta_c^2 + z_6 \beta_s^4 . \quad (4.8)$$

With the same coefficients we can also express, the average value over the whole cluster of  $S^z S^z$

$$\sum_{\langle i,j \rangle} \langle S_i^z S_j^z \rangle = \frac{3}{4} z_1 + \frac{1}{4} z_2 \beta_s^2 - \frac{1}{4} z_3 \beta_s^2 \beta_c^2 + \frac{1}{4} z_4 \beta_c^2 - \frac{3}{4} z_5 \beta_s^4 \beta_c^2 - \frac{1}{4} z_6 \beta_s^4 . \quad (4.9)$$

Only four independent terms contain the average value taken over the cluster of  $S^x S^x$  or  $S^y S^y$

$$\sum_{\langle i,j \rangle} \langle S_i^x S_j^x \rangle = \sum_{\langle i,j \rangle} \langle S_i^y S_j^y \rangle = s_1 \beta_s^2 + s_2 \beta_s^2 \beta_c^2 + s_3 \beta_s^4 \beta_c^2 + s_4 \beta_s^4 . \quad (4.10)$$

The exact values of the coefficients are

$$s_1 = -0.001337761761 ,$$

$$s_2 = -0.005594470342 ,$$

$$s_3 = -0.038870843354 ,$$

and

$$s_4 = -0.03005147618 .$$

That is

$$\begin{aligned} s_1 &= -\frac{1}{2} \left( \frac{1}{4} \frac{1}{\pi} - \frac{4}{3} \frac{1}{\pi^3} \right)^2 , \\ s_2 &= -\frac{1}{2} \left[ \left( \frac{1}{4} \frac{1}{\pi} - \frac{4}{3} \frac{1}{\pi^3} \right)^2 + \left( \frac{1}{4} \frac{1}{\pi} - \frac{4}{9} \frac{1}{\pi^3} \right)^2 \right] , \\ s_3 &= -\frac{1}{2} \left[ 2 \left( \frac{1}{4} \frac{1}{\pi} + \frac{4}{3} \frac{1}{\pi^3} \right)^2 + \left( \frac{1}{4} \frac{1}{\pi} + \frac{4}{9} \frac{1}{\pi^3} \right)^2 \right] , \\ s_4 &= -\left( \frac{1}{4} \frac{1}{\pi} + \frac{4}{3} \frac{1}{\pi^3} \right)^2 . \end{aligned}$$

It should be noted that homogeneity of the cluster for  $S^z S^z$  does not guarantee that, e.g.  $S_2^z S_3^z = S_1^z S_2^z$ . We may argue that the two Bethe-Peierls conditions are the most one can do for the central pair being representative of the bulk of the system, and calculate all other quantities for the central pair. We may, however, also say that averaging over the cluster is the best way to average out remaining inhomogeneities. However, by using this procedure the computational time and memory increases considerably, that is why we will only apply it in the one dimensional case.

As such, the last term of the Hamiltonian is obtained to be

$$\sum_{\langle i,j \rangle} \langle n_i n_j \rangle = 3 [z_1 + z_2 \beta_s^2 + z_3 \beta_s^2 \beta_c^2 + z_4 \beta_c^2 + z_5 \beta_s^4 \beta_c^2 + z_6 \beta_s^4] . \quad (4.11)$$

This should of course, be just three. Equation (4.11) is used to eliminate programming errors.



In this simple case the Bethe-Peierls condition (4.7) reads

$$\beta_c^2 = \frac{z_2 \beta_s^2 + z_6 \beta_s^4}{2z_4 + z_3 \beta_s^2}. \quad (4.12)$$

The half filled case being equivalent to the Heisenberg Hamiltonian, we minimize the expectation value of  $\vec{S}_i \cdot \vec{S}_j$ , obtaining

$$\beta_s = 0.8728, \quad \text{and} \quad \beta_c = 1.0389. \quad (4.13)$$

The energy becomes -0.442416, which is 1.3 percent higher than the exact value of Bethe and Hulthen of -0.443. The spin-spin correlation is somewhat anisotropic, with  $\langle S_2^x S_3^x \rangle = -0.145066$ , and  $\langle S_2^z S_3^z \rangle = -0.152284$ . As a verification, we have also calculated the  $\sum_{\langle i,j \rangle} \langle n_i n_j \rangle$  which gives the expected value of three, i.e. the number of the bonds which we sum up. The spin-spin correlation for nearest neighbour pair is probably anisotropic due to the initial projection operator, which was not a true singlet state. Due to the Bethe-Peierls condition, we know that the obtained values for the central pair approximates well the pair correlation in the infinite system. That is, the nearest neighbour spin-spin correlation function for the linear chain it is obtained to be  $\vec{S}_i \cdot \vec{S}_j \simeq -0.442$ . This is higher than the Neel state value of -0.75, which corresponds to antiferromagnetically ordered nearest neighbour spins. The obtained value for the spin-spin correlation is 98.7 per cent of the correct value. It is in remarkable agreement with the variational Monte Carlo result of Yokoyama and Shiba (1987) of -0.442. The quality of the result is satisfying considering how simple the calculation is.

The following case calculated in one dimension is for  $n = 5/6$ . The denominator reads as

$$\begin{aligned} Z = & z_1 \beta_c^2 \beta_s^4 \mu^8 + z_2 \beta_s^4 \mu^8 + z_3 \beta_c^2 \beta_s^2 \mu^6 \\ & + z_4 \beta_s^2 \mu^8 + z_5 \alpha_s^2 \beta_s^2 \mu^4 + z_6 \beta_c^2 \beta_s^2 \mu^8 \end{aligned}$$

$$\begin{aligned}
& + z_7 \beta_s^2 \mu^6 + z_8 \mu^8 + z_9 \alpha_s^2 \mu^2 \\
& + z_{10} \mu^6 + z_{11} \alpha_s^2 \mu^4 + z_{12} \mu^4 \\
& + z_{13} \beta_c^2 \mu^6 + z_{14} \alpha_c^2 \alpha_s^2 \mu^2 + z_{15} \alpha_s^4 \alpha_c^2 \\
& + z_{16} \alpha_c^2 \mu^4 + z_{17} \beta_c^2 \mu^8 + z_{18} \beta_c^2 \mu^8 .
\end{aligned} \tag{4.14}$$

The coefficients are

$$\begin{aligned}
z_1 &= 0.03764240474 , \\
z_2 &= 0.01609753041 , \\
z_3 &= 0.06985109096 , \\
z_4 &= 0.001314473487 , \\
z_5 &= 0.02887437144 , \\
z_6 &= 0.01228157140 , \\
z_7 &= 0.1072687078 , \\
z_8 &= 0.4387270970 \times 10^{-5} , \\
z_9 &= 0.006494657560 , \\
z_{10} &= 0.01263916930 , \\
z_{11} &= 0.002499570559 , \\
z_{12} &= 0.03759157975 , \\
z_{13} &= 0.02494297061 , \\
z_{14} &= 0.002893541828 , \\
z_{15} &= 0.0001627097178 ,
\end{aligned}$$

$$z_{16} = 0.009482491476 ,$$

$$z_{17} = 0.004799846212 ,$$

and

$$z_{18} = 0.03240477690 .$$

As an example \* the analytic expression of  $z_1$  is

$$2 \left[ \frac{1225}{20736} + \frac{1}{\pi^2} \left( \frac{3587}{10368} + \frac{35}{192} \sqrt{3} \right) - \frac{1}{\pi^3} \left( \frac{5}{144} + \frac{1}{72} \sqrt{3} \right) + \frac{1}{\pi^4} \left( \frac{1441}{2304} + \frac{53}{144} \sqrt{3} \right) \right]^2 .$$

However, due to space problems, we do not give here the analytical expressions for the rest of the coefficients.

The average value of the Hamiltonian (3.1) by terms, is the following

$$\begin{aligned} \sum_{\langle i,j \rangle, \sigma} \langle c_{i,\sigma}^\dagger c_{j,\sigma} \rangle &= k_1 \alpha_c \alpha_s^2 \mu^2 + k_2 \alpha_s^2 \mu^2 + k_3 \alpha_s \mu^4 \\ &+ k_4 \alpha_s \beta_s \mu^4 + k_5 \mu^4 + k_6 \alpha_c \mu^4 \\ &+ k_7 \beta_c \mu^4 + k_8 \mu^6 + k_9 \beta_s^2 \mu^6 \\ &+ k_{10} \beta_s^2 \beta_c \mu^6 + k_{11} \beta_c \mu^6 + k_{12} \beta_s \mu^6 , \end{aligned} \quad (4.15)$$

where the coefficients are

$$k_1 = 0.008286312968 ,$$

$$k_2 = 0.006320218756 ,$$

$$k_3 = 0.01518342964 ,$$

$$k_4 = 0.04917297009 ,$$

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\* To give all the analytic expressions would be of no real consequence to the final result obtained. They are available from the author on request.

$$k_5 = 0.01974284254 ,$$

$$k_6 = 0.04935267386 ,$$

$$k_7 = 0.07235226964 ,$$

$$k_8 = 0.002378348615 ,$$

$$k_9 = 0.1010644197 ,$$

$$k_{10} = 0.1248644505 ,$$

$$k_{11} = 0.03182388890 ,$$

and

$$k_{12} = 0.03627256690 .$$

As for the denominator, we give the analytic value of the first coefficient

$$8 \left[ \frac{2401}{20736} - \left( \frac{5929}{10308} + \frac{49}{192} \sqrt{3} \right) \frac{1}{\pi^2} - \left( \frac{35}{144} + \frac{7}{72} \sqrt{3} \right) \frac{1}{\pi^3} + \left( \frac{1441}{2304} + \frac{53}{144} \sqrt{3} \right) \frac{1}{\pi^4} \right] \\ \times \left[ \frac{49}{576} \sqrt{2}(1 + \sqrt{3}) \frac{1}{\pi} + \left( \frac{7}{576} \sqrt{2} + \frac{7}{192} \sqrt{6} \right) \frac{1}{\pi^2} - \frac{3\sqrt{2}}{576} (73 + 41\sqrt{3}) \frac{1}{\pi^3} \right] .$$

The average value over the cluster of  $S^x S^x$  will contain only seven independent terms, which are

$$\sum_{\langle i,j \rangle} \langle S_i^x S_j^x \rangle = s_1 \alpha_s^2 \beta_s^2 \mu^4 + s_2 \beta_s^2 \mu^6 + s_3 \beta_s^2 \beta_c^2 \mu^6 + s_4 \beta_s^2 \mu^8 \\ + s_5 \beta_s^2 \beta_c^2 \mu^8 + s_6 \beta_s^4 \beta_c^2 \mu^8 + s_7 \beta_s^4 \mu^8 , \quad (4.16)$$

the coefficients equalize

$$s_1 = -\frac{1}{2} \left[ \frac{49}{576} \sqrt{2}(1 + \sqrt{3}) \frac{1}{\pi} + \left( \frac{7}{576} \sqrt{2} + \frac{7}{192} \sqrt{6} \right) \frac{1}{\pi^2} - \frac{3\sqrt{2}}{576} (73 + 41\sqrt{3}) \frac{1}{\pi^3} \right]^2 \\ = -0.003296850112 ,$$

$$s_2 = -0.01369955091 ,$$

$$s_3 = -0.006938757925 ,$$

$$s_4 = -0.0004653203693 ,$$

$$s_5 = -0.0007459628030 ,$$

$$s_6 = -0.1449938614 ,$$

and

$$s_7 = -0.01316940501 .$$

For the  $z$  component we obtain

$$\begin{aligned} \sum_{\langle i,j \rangle} \langle S_i^z S_j^z \rangle &= s_8 \beta_c^2 \beta_s^4 \mu^8 + s_9 \beta_s^4 \mu^8 + s_{10} \beta_c^2 \beta_s^2 \mu^6 \\ &+ s_{11} \beta_s^2 \mu^8 + s_{12} \alpha_s^2 \beta_s^2 \mu^4 + s_{13} \beta_c^2 \beta_s^2 \mu^8 \\ &+ s_{14} \beta_s^2 \mu^6 + s_{15} \mu^8 + s_{16} \mu^6 \\ &+ s_{17} \mu^4 + s_{18} \alpha_s^2 \mu^4 + s_{19} \beta_c^2 \mu^8 + s_{20} \beta_c^2 \mu^4 . \end{aligned} \quad (4.17)$$

Resulting with

$$s_8 = -0.02823180356 ,$$

$$s_9 = -0.004024382603 ,$$

$$s_{10} = -0.03492554548 ,$$

$$s_{11} = 0.0003286183717 ,$$

$$s_{12} = -0.007218592861 ,$$

$$s_{13} = -0.003070392851 ,$$

$$s_{14} = 0.02299966567 ,$$

$$s_{15} = 0.3290453228 \times 10^{-5} ,$$

$$s_{16} = 0.003233707831 ,$$

$$s_{17} = 0.0004293327839 ,$$

$$s_{18} = 0.0006248926398 ,$$

$$s_{19} = 0.001199961553 ,$$

and

$$s_{20} = -0.008101194225 .$$

Where, for example, the analytic expression of  $s_8$  is

$$\begin{aligned} & -\frac{1}{2} \left[ \frac{1225}{20736} + \frac{1}{\pi^2} \left( \frac{1739}{10368} + \frac{5}{64} \sqrt{3} \right) + \frac{1}{\pi^3} \left( \frac{37}{144} + \frac{11}{72} \sqrt{3} \right) + \frac{1}{\pi^4} \left( \frac{1441}{2304} + \frac{53}{144} \sqrt{3} \right) \right] \\ & \times \left[ \frac{1225}{20736} + \frac{1}{\pi^2} \left( \frac{971}{10368} + \frac{7}{192} \sqrt{3} \right) - \frac{1}{\pi^3} \left( \frac{47}{144} + \frac{13}{72} \sqrt{3} \right) + \frac{1}{\pi^4} \left( \frac{1441}{2304} + \frac{55}{144} \sqrt{3} \right) \right] . \end{aligned}$$

The last term of the Hamiltonian is

$$\begin{aligned} -\frac{1}{4} \sum_{\langle i,j \rangle} \langle n_i n_j \rangle &= s_8 \beta_c^2 \beta_s^4 \mu^8 + 3 s_9 \beta_s^4 \mu^8 + s_{10} \beta_c^2 \beta_s^2 \mu^6 \\ & - 3 s_{11} \beta_s^2 \mu^8 + s_{12} \alpha_s^2 \beta_s^2 \mu^4 + 3 s_{13} \beta_c^2 \beta_s^2 \mu^8 \\ & + s_{21} \beta_s^2 \mu^6 - s_{15} \mu^8 - s_{16} \mu^6 \\ & - s_{17} \mu^4 - s_{18} \alpha_s^2 \mu^4 - 3 s_{19} \beta_c^2 \mu^8 \\ & + s_{20} \beta_c^2 \mu^4 + s_{22} \beta_c^2 \mu^6 . \end{aligned} \tag{4.18}$$

The two supplementary terms are

$$s_{21} = -0.03063468824 ,$$

and

$$s_{22} = -0.01247148530 .$$

The Bethe-Peierls conditions (4.6) and (4.7) are then read

$$\alpha_c^2 = \frac{1}{2} \frac{z_5 \alpha_s^2 \beta_s^2 \mu^4 + z_{11} \alpha_s^2 \mu^4 + z_{14} \alpha_s^4 \mu^2}{z_{14} \alpha_s^2 \mu^2 + z_{16} \mu^4}, \quad (4.19)$$

and

$$\beta_c^2 = \frac{2z_2 \beta_s^4 \mu^8 + z_4 \beta_s^2 \mu^8 + z_5 \beta_s^2 \alpha_s^2 \mu^4 + z_7 \beta_s^2 \mu^6}{z_3 \beta_s^2 \mu^6 + z_6 \beta_s^2 \mu^8 + 2z_{17} \mu^8 + 2z_{18} \mu^8}. \quad (4.20)$$

For the conservation of the average electron density for  $n = 5/6$ , it requires from Eq. (3.34)

$$\mu = \frac{\frac{35}{6} \alpha_c \beta_c \left( \frac{\alpha_c \beta_c}{6} + \frac{\beta_c}{6} - \alpha_c + 1 \right) + \frac{35}{36} \alpha_c (\alpha_c - 1) - \frac{43}{36} (\beta_c^2 + 1) + \frac{13}{2} \beta_c - \frac{1}{36} \sqrt{\Delta}}{\frac{17}{18} (\beta_c^2 + 1) - \frac{16}{3} \beta_c + 5 \alpha_c \beta_c \left( \frac{\alpha_c \beta_c}{6} - \frac{\beta_c}{6} - \alpha_c - 1 \right) - \frac{5}{6} \alpha_c (\alpha_c - 1)} \quad (4.21)$$

Where  $\Delta = 4059\beta_c^4 + 475\beta_c^4\alpha_c^4 - 2600\beta_c^4\alpha_c^3 - 1985\beta_c^4\alpha_c^2 + 5980\beta_c^4\alpha_c - 25464\beta_c^3 - 5700\beta_c^3\alpha_c^4 + 31200\beta_c^3\alpha_c^3 + 4440\beta_c^3\alpha_c^2 - 51720\beta_c^3\alpha_c + 22554\beta_c^2 + 18050\beta_c^2\alpha_c^4 - 98800\beta_c^2\alpha_c^3 + 40850\beta_c^2\alpha_c^2 + 107000\beta_c^2\alpha_c - 25464\beta_c - 5700\beta_c\alpha_c^4 + 31200\beta_c\alpha_c^3 + 4440\beta_c\alpha_c^2 - 51720\beta_c\alpha_c + 475\alpha_c^4 - 2600\alpha_c^3 - 1985\alpha_c^2 + 5980\alpha_c + 4059$ . The minimum energy for  $J/t = 1$  it is obtained -0.82604. The variational parameters are obtained as

$$\alpha_s = 0.8519, \quad \text{and} \quad \alpha_c = 0.9349. \quad (4.22)$$

While for the spin-spin correlation

$$\beta_s = 0.8370, \quad \text{and} \quad \beta_c = 1.0609. \quad (4.23)$$

The chemical potential from (4.21) is obtained  $\sim 0.24$ , i.e.  $6/25$ . The different energy contributions result as

$$\sum_{\langle i,j \rangle, \sigma} (\langle c_{i,\sigma}^\dagger c_{j,\sigma} \rangle + \text{h.c.}) = -0.381311, \quad (4.24)$$

$$\sum_{\langle i,j \rangle} \langle S_i^x S_j^x \rangle = -0.118418 , \quad (4.25)$$

$$\sum_{\langle i,j \rangle} \langle S_i^z S_j^z \rangle = -0.111060 , \quad (4.26)$$

and

$$\sum_{\langle i,j \rangle} \langle n_i n_j \rangle = 0.38736 . \quad (4.27)$$

As it can be seen, the kinetic energy will contribute to the ground state with a partition which is slightly more than fifty per cent. The kinetic energy and  $\langle \vec{S}_i \cdot \vec{S}_j \rangle$  are within 90 per cent accuracy with the variational Monte Carlo result of Yokoyama and Shiba (1987), of  $\sim -0.34$ , and  $\sim -0.35$ . The values which are obtained for the central pair are mostly equal with the calculated energy values, this suggests that for the further calculations it is enough to consider only the central pair.

In the following table we are summarizing the obtained results for the one dimensional case.

Expectation Values	Band Filling	Results
$E_{kin}/N t$	$n = 1$	0
$S_2^x S_3^x$	$n = 1$	-0.14506
$S_2^z S_3^z$	$n = 1$	-0.15228
$\mathbf{S}_2 \cdot \mathbf{S}_3$	$n = 1$	-0.442416
$n_2 n_3$	$n = 1$	1
$E_{pot}/N J$	$n = 1$	-0.69241
$E_{kin}/N t$	$n = 5/6$	-0.38131
$S_2^x S_3^x$	$n = 5/6$	-0.11841
$S_2^z S_3^z$	$n = 5/6$	-0.11106
$\mathbf{S}_2 \cdot \mathbf{S}_3$	$n = 5/6$	-0.34789
$n_2 n_3$	$n = 5/6$	0.12912
$E_{pot}/N J$	$n = 5/6$	-0.44473

As it can be seen the spin-spin correlation is decreasing with doping, result which was expected. This will lead to the increase of the potential energy.



## 5 The square lattice

Here, we move on to discuss the simplest two dimensional lattice, namely the square lattice.

It is widely accepted that in two dimension non-frustrated lattice antiferromagnetism and long-range Neel ordering will prevail in the neighbourhood of half filling. In this calculations, however, we have made no explicit provision for that, since our uncorrelated state is just the paramagnetic Fermi sea. Energetically, this should not make a large difference. The true long range ordering will be replaced by short range ordering, but the two will look similar at short distances, which is the region of energetic importance. Correlations will, of course, differ very vitally, but that is discounted in the present calculations, because we can analyse only nearest neighbour correlations.

The two dimensional square lattice represents the largest cluster analysed with the use of a variational cluster method. To ensure the desired property for the cluster, i.e. to consider all the nearest neighbour correlations of a pair of sites, we must work with eight sites, that is 6561 configurations. The band energy (1.5), for the square lattice reads as

$$\varepsilon_{\mathbf{k}} = -2t (\cos k_x + \cos k_y) . \quad (5.1)$$

The Fermi energy is  $\varepsilon_F = -4t$  for empty band and  $\varepsilon_F = 0$  for half filled band. As previously, we introduce also in this case an additional parameter  $0 \leq \delta \leq 2$ , in such a way that  $\varepsilon_F = -2t\delta$ . The momentum distribution for the noninteracting system is

$$\begin{aligned} \theta(\varepsilon_F - \varepsilon_{\mathbf{k}}) &= \theta(-2t\delta + 2t(\cos k_x + \cos k_y)) \\ &= \theta(-\delta + \cos k_x + \cos k_y) . \end{aligned} \quad (5.2)$$

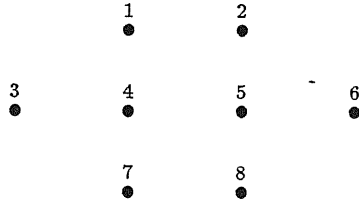
In this way, for the number of electron per site and per spin  $n$ , we can write  $n/2 = n_{\uparrow} = n_{\downarrow}$ , that is

$$\begin{aligned} \frac{n}{2} &= \frac{1}{(2\pi)^2} \int_{-\pi}^{+\pi} dk_x \int_{-\pi}^{+\pi} dk_y \theta(\varepsilon_F - \varepsilon_{\mathbf{k}}) \\ &= \frac{1}{\pi^2} \int_0^{\arccos(\delta-1)} d\xi \arccos(\delta - \cos \xi). \end{aligned} \quad (5.3)$$

For empty band, i.e.  $\delta = 2$ , Eq. (5.3) gives  $n = 0$ . Contrastingly, in the half filled band case,  $\delta = 0$ , thus  $n = 1$  it is obtained. In this particular half filled case the  $f_{ij}$  parameters from (3.11) can also be calculated analytically

$$\begin{aligned} f_{ij} &= \frac{1}{(2\pi^2)^2} \int_{-\pi}^{+\pi} dk_x \int_{-\pi}^{+\pi} dk_y e^{-i \mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \theta(\varepsilon_F - \varepsilon_{\mathbf{k}}) \\ &= \frac{1}{(2\pi^2)^2} \int_{-\pi}^{+\pi} dk_x \int_{-\pi}^{+\pi} dk_y e^{-i k_x (X_i - X_j)} e^{-i k_y (Y_i - Y_j)} \theta(\cos k_x + \cos k_y) \\ &= \frac{1}{\pi^2} \frac{\cos[\pi(X_i - X_j)] - \cos[\pi(Y_i - Y_j)]}{[(Y_i - Y_j) - (X_i - X_j)][(Y_i - Y_j) + (X_i - X_j)]}. \end{aligned} \quad (5.4)$$

Where we used the notation  $\mathbf{R}_i = X_i \mathbf{i} + Y_i \mathbf{j}$ . However, attention must be taken when constructing the  $X_i - X_j$  and  $Y_i - Y_j$  values. The cluster is the following



That is, e.g.  $X_4 - X_5 = -1$ ,  $X_4 - X_3 = 1$ ,  $Y_1 - Y_4 = 1$  and  $Y_4 - Y_7 = 1$ . In the case of  $X_i = X_j$ , or  $Y_i = Y_j$ ,  $f_{ij}$  is equal to  $2[1/(\pi(Y_i - Y_j)^2)] \sin^2[\pi(Y_i - Y_j)/2]$ , or  $2[1/(\pi(X_i - X_j)^2)] \sin^2[\pi(X_i - X_j)/2]$ , respectively.

For less than half filling,  $f_{ij}$  cannot be given in such a compact form as in (5.4), only using an integral representation

$$\begin{aligned}
f_{ij} &= \frac{1}{(2\pi)^2} \int_{-\pi}^{+\pi} dk_x \int_{-\pi}^{+\pi} dk_y e^{-i \mathbf{k} \cdot (\mathbf{R}_i - \mathbf{R}_j)} \theta(\varepsilon_F - \varepsilon_{\mathbf{k}}) \\
&= \frac{1}{\pi^2} \frac{1}{Y_i - Y_j} \int_0^{\arccos(\delta-1)} d\xi \cos[(X_i - X_j)\xi] \sin[(Y_i - Y_j) \arccos(\delta - \cos \xi)] .
\end{aligned} \tag{5.5}$$

The procedure which is used is known from the previous chapter. First, we calculate the expectation values  $\langle P_{\Gamma} H_{i,j} P_{\Gamma} \rangle / Z$ . Secondly, we assign to each configuration the appropriate variational parameters, by using the Bethe-Peierls projection. This, for the square lattice, applies in the following, we assign to the central pair (45) the variational parameters  $\alpha_c$  and  $\beta_c$ , while to the shell pairs, i.e. (12), (14), (25), (34), (56), (47), (58), and (78) the  $\alpha_s$  and  $\beta_s$  parameters. These are linked together due to the Bethe-Peierls conditions, which in this case, becomes

$$\frac{1}{8} \frac{\partial \ln Z}{\partial \ln \alpha_s^2} = \frac{\partial \ln Z}{\partial \ln \alpha_c^2} , \tag{5.6}$$

and

$$\frac{1}{8} \frac{\partial \ln Z}{\partial \ln \beta_s^2} = \frac{\partial \ln Z}{\partial \ln \beta_c^2} , \tag{5.7}$$

For the half filled case, as known, the hopping term gives no contribution. The denominator contains 14 terms

$$\begin{aligned}
z &= z_1 \beta_s^{16} \beta_c^2 + z_2 \beta_s^{14} \beta_c^2 + z_3 \beta_s^{12} \beta_c^2 \\
&+ z_4 \beta_s^{12} + z_5 \beta_s^{10} \beta_c^2 + z_6 \beta_s^{10} \\
&+ z_7 \beta_s^8 \beta_c^2 + z_8 \beta_s^8 + z_9 \beta_s^6 \beta_c^2 \\
&+ z_{10} \beta_s^6 + z_{11} \beta_s^4 \beta_c^2 + z_{12} \beta_s^4 \\
&+ z_{13} \beta_s^2 + z_{14} .
\end{aligned} \tag{5.8}$$

The corresponding coefficients are

$$z_1 = 0.0003718400856 ,$$

$$z_2 = 0.0003570801752 ,$$

$$z_3 = 0.0007193949334 ,$$

$$z_4 = 0.0007576480344 ,$$

$$z_5 = 0.0006638303715 ,$$

$$z_6 = 0.0007614173043 ,$$

$$z_7 = 0.0004880385316 ,$$

$$z_8 = 0.0002434989460 ,$$

$$z_9 = 0.0004287877524 ,$$

$$z_{10} = 0.00006057236108 ,$$

$$z_{11} = 0.0001356821879 ,$$

$$z_{12} = 0.00001158317770 ,$$

$$z_{13} = 0.5774363336 \times 10^{-6} ,$$

and

$$z_{14} = 0.4840878366 \times 10^{-7} .$$

In view of the special significance of the two dimensional square lattice, we will give also explicit analytical values of  $z_i$ . This is also commendable due to the fact that, in the case of half filled Hubbard Hamiltonian the same terms are obtained,

thus these results can be used immediately for an eight site variational cluster calculation for the Hubbard Hamiltonian. The denominator will read

$$\begin{aligned}
Z = & 2 t_1^2 + 4 t_2^2 \beta_s^6 \beta_c^2 + 4 t_3^2 \beta_s^{12} \beta_c^2 + 8 t_4^2 \beta_s^8 \beta_c^2 \\
& + 8 t_5^2 \beta_s^{10} \beta_c^2 + 4 t_6^2 \beta_s^8 \beta_c^2 + 4 t_7^2 \beta_s^6 \beta_c^2 \\
& + 8 t_8^2 \beta_s^{12} \beta_c^2 + 8 t_9^2 \beta_s^6 \beta_c^2 + 4 t_{10}^2 \beta_s^4 \beta_c^2 \\
& + 4 t_{11}^2 \beta_s^{14} \beta_c^2 + 8 t_{12}^2 \beta_s^6 \beta_c^2 + 8 t_{13}^2 \beta_s^8 \\
& + 8 t_{14}^2 \beta_s^{10} + 4 t_{15}^2 \beta_s^{10} + 2 t_{16}^2 \beta_s^8 \\
& + 8 t_{17}^2 \beta_s^{10} + 8 t_{18}^2 \beta_s^6 + 8 t_{19}^2 \beta_s^8 \\
& + 2 t_{20}^2 \beta_s^4 + 4 t_{21}^2 \beta_s^{10} + 4 t_{22}^2 \beta_s^{12} \\
& + 4 t_{23}^2 \beta_s^{12} + 2 t_{24}^2 \beta_s^{12} + 8 t_{25}^2 \beta_s^8 \\
& + 8 t_{26}^2 \beta_s^4 + 8 t_{27}^2 \beta_s^6 + 4 t_{28}^2 \beta_s^2 \\
& + 8 t_{29}^2 \beta_s^6 + 8 t_{30}^2 \beta_s^{12} + 4 t_{31}^2 \beta_s^8 \\
& + 4 t_{32}^2 \beta_s^{10} + 4 t_{33}^2 \beta_s^4 + 8 t_{34}^2 \beta_s^{10} \\
& + 8 t_{35}^2 \beta_s^{10} \beta_c^2 + 2 t_{36}^2 \beta_s^{16} \beta_c^2 + 8 t_{37}^2 \beta_s^6 \beta_c^2 \\
& + 8 t_{38}^2 \beta_s^4 \beta_c^2 + 4 t_{39}^2 \beta_s^4 \beta_c^2 + 2 t_{40}^2 \beta_s^4 \beta_c^2 \\
& + 2 t_{41}^2 \beta_s^{12} \beta_c^2 + 8 t_{42}^2 \beta_s^8 \beta_c^2 + 4 t_{43}^2 \beta_s^6 \beta_c^2 \\
& + 2 t_{44}^2 \beta_s^8 \beta_c^2 + 8 t_{45}^2 \beta_s^{10} \beta_c^2 + 8 t_{46}^2 \beta_s^8 \beta_c^2 .
\end{aligned} \tag{5.9}$$

The 46 terms appearing in Eq. (5.9) are the following

$$\begin{aligned}
t_1 &= \frac{1}{256} - \frac{1}{\pi^4} \frac{49}{81} + \frac{1}{\pi^8} \frac{20480}{729} - \frac{1}{\pi^{12}} \frac{3211264}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561} , \\
t_2 &= \frac{1}{256} - \frac{1}{\pi^4} \frac{4}{81} + \frac{1}{\pi^8} \frac{2048}{729} - \frac{1}{\pi^{12}} \frac{26144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561} , \\
t_3 &= \frac{1}{256} + \frac{1}{\pi^4} \frac{97}{324} + \frac{1}{\pi^8} \frac{3712}{729} + \frac{1}{\pi^{12}} \frac{1589248}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561} ,
\end{aligned}$$

$$\begin{aligned}
t_4 &= \frac{1}{256} + \frac{1}{\pi^4} \frac{4}{81} - \frac{1}{\pi^8} \frac{512}{81} + \frac{1}{\pi^{12}} \frac{917504}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_5 &= \frac{1}{256} + \frac{1}{\pi^4} \frac{14}{81} - \frac{1}{\pi^8} \frac{256}{27} - \frac{1}{\pi^{12}} \frac{917504}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_6 &= \frac{1}{256} + \frac{1}{\pi^4} \frac{25}{324} - \frac{1}{\pi^8} \frac{1408}{729} + \frac{1}{\pi^{12}} \frac{409600}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_7 &= \frac{1}{256} - \frac{1}{\pi^4} \frac{17}{162} - \frac{1}{\pi^8} \frac{7168}{729} + \frac{1}{\pi^{12}} \frac{2392064}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_8 &= \frac{1}{256} + \frac{1}{\pi^4} \frac{53}{162} - \frac{1}{\pi^{12}} \frac{1736704}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_9 &= \frac{1}{256} - \frac{1}{\pi^4} \frac{4}{81} + \frac{1}{\pi^8} \frac{512}{729} + \frac{1}{\pi^{12}} \frac{262144}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{10} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{14}{81} + \frac{1}{\pi^8} \frac{8960}{729} - \frac{1}{\pi^{12}} \frac{917504}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{11} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{73}{162} + \frac{1}{\pi^8} \frac{7168}{729} - \frac{1}{\pi^{12}} \frac{557056}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{12} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{4}{81} + \frac{1}{\pi^8} \frac{2560}{729} + \frac{1}{\pi^{12}} \frac{917504}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{13} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{4}{81} - \frac{1}{\pi^8} \frac{6656}{729} - \frac{1}{\pi^{12}} \frac{262144}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{14} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{25}{324} - \frac{1}{\pi^8} \frac{128}{81} + \frac{1}{\pi^{12}} \frac{1064960}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{15} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{4}{81} - \frac{1}{\pi^8} \frac{2048}{729} + \frac{1}{\pi^{12}} \frac{262144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{16} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{4}{81} - \frac{1}{\pi^8} \frac{2560}{729} - \frac{1}{\pi^{12}} \frac{262144}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{17} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{4}{81} + \frac{1}{\pi^8} \frac{512}{81} - \frac{1}{\pi^{12}} \frac{262144}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{18} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{65}{324} - \frac{1}{\pi^8} \frac{128}{81} - \frac{1}{\pi^{12}} \frac{409600}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{19} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{4}{81} + \frac{1}{\pi^{12}} \frac{262144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{20} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{97}{324} - \frac{1}{\pi^8} \frac{1408}{729} + \frac{1}{\pi^{12}} \frac{770048}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{21} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{4}{81} + \frac{1}{\pi^8} \frac{2048}{729} + \frac{1}{\pi^{12}} \frac{262144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561},
\end{aligned}$$

$$\begin{aligned}
t_{22} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{14}{81} + \frac{1}{\pi^8} \frac{8960}{729} + \frac{1}{\pi^{12}} \frac{917504}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{23} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{65}{324} + \frac{1}{\pi^8} \frac{3712}{729} + \frac{1}{\pi^{12}} \frac{1064960}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{24} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{47}{324} - \frac{1}{\pi^8} \frac{1408}{729} - \frac{1}{\pi^{12}} \frac{1589248}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{25} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{4}{81} - \frac{1}{\pi^8} \frac{512}{81} - \frac{1}{\pi^{12}} \frac{917504}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{26} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{53}{162} + \frac{1}{\pi^{12}} \frac{1736704}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{27} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{14}{81} - \frac{1}{\pi^8} \frac{256}{27} + \frac{1}{\pi^{12}} \frac{917504}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{28} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{73}{162} + \frac{1}{\pi^8} \frac{7168}{729} + \frac{1}{\pi^{12}} \frac{557056}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{29} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{14}{81} - \frac{1}{\pi^8} \frac{2560}{729} + \frac{1}{\pi^{12}} \frac{262144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{30} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{14}{81} + \frac{1}{\pi^8} \frac{512}{81} + \frac{1}{\pi^{12}} \frac{262144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{31} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{25}{324} - \frac{1}{\pi^8} \frac{1408}{729} - \frac{1}{\pi^{12}} \frac{409600}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{32} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{17}{162} - \frac{1}{\pi^8} \frac{7168}{729} - \frac{1}{\pi^{12}} \frac{2392064}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{33} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{97}{324} + \frac{1}{\pi^8} \frac{3712}{729} - \frac{1}{\pi^{12}} \frac{1589248}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{34} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{4}{81} + \frac{1}{\pi^8} \frac{2560}{729} - \frac{1}{\pi^{12}} \frac{917504}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{35} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{14}{81} - \frac{1}{\pi^8} \frac{2560}{729} - \frac{1}{\pi^{12}} \frac{262144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{36} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{49}{81} + \frac{1}{\pi^8} \frac{20480}{729} + \frac{1}{\pi^{12}} \frac{3211264}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{37} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{25}{324} - \frac{1}{\pi^8} \frac{128}{81} - \frac{1}{\pi^{12}} \frac{1064960}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{38} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{14}{81} + \frac{1}{\pi^8} \frac{512}{81} - \frac{1}{\pi^{12}} \frac{262144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{39} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{65}{324} + \frac{1}{\pi^8} \frac{3712}{729} - \frac{1}{\pi^{12}} \frac{1064960}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561},
\end{aligned}$$

$$\begin{aligned}
t_{40} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{47}{324} - \frac{1}{\pi^8} \frac{1408}{729} + \frac{1}{\pi^{12}} \frac{1589248}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{41} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{97}{324} - \frac{1}{\pi^8} \frac{1408}{729} - \frac{1}{\pi^{12}} \frac{770048}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{42} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{4}{81} - \frac{1}{\pi^8} \frac{6656}{729} + \frac{1}{\pi^{12}} \frac{262144}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{43} &= \frac{1}{256} - \frac{1}{\pi^4} \frac{4}{81} - \frac{1}{\pi^8} \frac{2048}{729} - \frac{1}{\pi^{12}} \frac{262144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{44} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{4}{81} - \frac{1}{\pi^8} \frac{2560}{729} + \frac{1}{\pi^{12}} \frac{262144}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561}, \\
t_{45} &= \frac{1}{256} + \frac{1}{\pi^4} \frac{65}{324} - \frac{1}{\pi^8} \frac{128}{81} + \frac{1}{\pi^{12}} \frac{409600}{6561} + \frac{1}{\pi^{16}} \frac{16777216}{6561},
\end{aligned}$$

and

$$t_{46} = \frac{1}{256} + \frac{1}{\pi^4} \frac{4}{81} - \frac{1}{\pi^{12}} \frac{262144}{6561} - \frac{1}{\pi^{16}} \frac{16777216}{6561}.$$

The corresponding expectation values for the central pair are

$$\begin{aligned}
\langle S_4^z S_5^z \rangle &= s_1 \beta_s^{16} \beta_c^2 + s_2 \beta_s^{14} \beta_c^2 + s_3 \beta_s^{12} \beta_c^2 \\
&+ s_4 \beta_s^{12} + s_5 \beta_s^{10} \beta_c^2 + s_6 \beta_s^{10} \\
&+ s_7 \beta_s^8 \beta_c^2 + s_8 \beta_s^8 + s_9 \beta_s^6 \beta_c^2 \\
&+ s_{10} \beta_s^6 + s_{11} \beta_s^4 \beta_c^2 + s_{12} \beta_s^4 \\
&+ s_{13} \beta_s^2 + \dots
\end{aligned} \tag{5.10}$$

The corresponding coefficients are

$$s_1 = -0.00005101479050,$$

$$s_2 = -0.00004488543295,$$

$$s_3 = -0.001043929306,$$

$$s_4 = -0.0001580605796,$$



$$\begin{aligned}
s_5 &= -0.00008843412780 , \\
s_6 &= -0.0001579100956 , \\
s_7 &= -0.00007477181265 , \\
s_8 &= -0.00004738797292 , \\
s_9 &= -0.00007611151555 , \\
s_{10} &= -0.00001304543154 , \\
s_{11} &= -0.00002501476658 , \\
s_{12} &= -0.3990166730 \times 10^{-5} ,
\end{aligned}$$

and

$$s_{13} = -0.1506255736 \times 10^{-6} .$$

While for the spin  $z$  component we obtain

$$\begin{aligned}
\langle S_4^z S_5^z \rangle &= s_{14} \beta_s^{16} \beta_c^2 + s_{15} \beta_s^{14} \beta_c^2 + s_{16} \beta_s^{12} \beta_c^2 \\
&+ s_{17} \beta_s^{12} + s_{18} \beta_s^{10} \beta_c^2 + s_{19} \beta_s^{10} \\
&+ s_{20} \beta_s^8 \beta_c^2 + s_{21} \beta_s^8 + s_{22} \beta_s^6 \beta_c^2 \\
&+ s_{23} \beta_s^6 + s_{24} \beta_s^4 \beta_c^2 + s_{25} \beta_s^4 \\
&+ s_{26} \beta_s^2 + s_{27} .
\end{aligned} \tag{5.11}$$

Where

$$\begin{aligned}
s_{14} &= -0.0008366401926 , \\
s_{15} &= -0.0006248903067 , \\
s_{16} &= -0.0008992436667 ,
\end{aligned}$$

$$\begin{aligned}
s_{17} &= -0.0005682360259 , \\
s_{18} &= -0.0004978727787 , \\
s_{19} &= -0.0001903543261 , \\
s_{20} &= -0.0001220096329 , \\
s_{21} &= 0.00006087473649 , \\
s_{22} &= 0.0001071969381 , \\
s_{23} &= 0.00004542927081 , \\
s_{24} &= 0.0001017616410 , \\
s_{25} &= 0.00001447897212 , \\
s_{26} &= 0.1010513584 \times 10^{-5} ,
\end{aligned}$$

and

$$s_{27} = 0.1089197632 \times 10^{-6} .$$

As in one dimensional half filled case in order to check the program, we computed

$$\begin{aligned}
\sum_{\langle i,j \rangle} \langle n_i n_j \rangle &= s_{28} \beta_s^{16} \beta_c^2 + s_{29} \beta_s^{14} \beta_c^2 + s_{30} \beta_s^{12} \beta_c^2 \\
&+ s_{31} \beta_s^{12} + s_{32} \beta_s^{10} \beta_c^2 + s_{33} \beta_s^{10} \\
&+ s_{34} \beta_s^8 \beta_c^2 + s_{35} \beta_s^8 + s_{36} \beta_s^6 \beta_c^2 \\
&+ s_{37} \beta_s^6 + s_{38} \beta_s^4 \beta_c^2 + s_{39} \beta_s^4 \\
&+ s_{40} \beta_s^2 + s_{41} .
\end{aligned} \tag{5.12}$$

With

$$s_{28} = 0.0033464 ,$$

$$\begin{aligned}
s_{29} &= 0.0032136 , \\
s_{30} &= 0.0064744 , \\
s_{31} &= 0.0068188 , \\
s_{32} &= 0.0059744 , \\
s_{33} &= 0.0068524 , \\
s_{34} &= 0.0043920 , \\
s_{35} &= 0.0021912 , \\
s_{36} &= 0.0038588 , \\
s_{37} &= 0.00054448 , \\
s_{38} &= 0.0012208 , \\
s_{39} &= 0.0001042 , \\
s_{40} &= 0.519692 \times 10^{-5} ,
\end{aligned}$$

and

$$s_{41} = 0.435676 \times 10^{-6} .$$

The Bethe-Peierls condition (5.7) takes the form

$$\beta_c^2 = \frac{6z_4\beta_s^{12} + 5z_6\beta_s^{10} + 4z_8\beta_s^8 + 3z_{10}\beta_s^6 + 2z_{12}\beta_s^4 + z_{13}\beta_s^2}{z_2\beta_s^{14} + 2z_3\beta_s^{12} + 3z_5\beta_s^{10} + 4z_7\beta_s^8 + 5z_9\beta_s^6 + 6z_{11}\beta_s^4} . \quad (5.13)$$

As it is known, for the half filled case the Hamiltonian (3.1) reduces to the Heisenberg one. Thus we minimize the expectation value of  $\langle \vec{S}_4 \cdot \vec{S}_5 \rangle$ . We reach the minimum energy for the following variational parameters

$$\beta_s = 0.8825 , \text{ and } \beta_c = 1.2078 . \quad (5.14)$$

The energy minimum, i.e. the ground state expectation value per site and  $J$ , it is obtained to be -0.6495. Which is three per cent less than -0.6692, obtained by Trivedi and Ceperley (1989) using Green function Monte Carlo method. Our result stands at the level of energies obtained by other variational methods. However, our method firstly has the power that using just eight sites we can reach a compatible result with other methods implying a larger number of sites. The energy by terms is the following

$$\langle S_4^x S_5^x \rangle = -0.217085, \quad (5.15)$$

$$\langle S_4^z S_5^z \rangle = -0.215330. \quad (5.16)$$

The value of  $\sum_{\langle i,j \rangle} \langle n_i n_j \rangle$ , was obtained to be equal with nine, i.e. the number of bonds which are counted. This, as mentioned previously, guarantees the accuracy of the used program.

The following case analysed, as for the one dimensional case, is the  $n = 5/6$  filling. The obtained results are given in the Appendix, as it follows. Appendix 1, contains the expression of the denominator. The corresponding Hamiltonian terms are in Appendix 2  $\langle S_4^z S_5^z \rangle$ ; in Appendix 3  $\langle S_4^x S_5^x \rangle$ ; in Appendix 4  $\langle n_4 n_5 \rangle$ ; and in Appendix 5 the hopping term. Being  $n$  the same value as in the one dimensional case, we can use the same equation in order to determine it, i.e. Eq. (4.21). By making the minimization, we obtain for the variational parameters  $\alpha_s \sim 0.87$ ,  $\alpha_c \sim 0.94$ ,  $\beta_s \sim 0.98$ , and  $\beta_c \sim 1.15$ . While  $\mu$  it is obtained to be equal with 0.7. For the kinetic energy -0.4374 it is obtained, which is situated between the Gutzwiller approximation value of  $\sim -0.5$  and  $\sim -0.4$  of Yokoyama and Shiba (1987). The last value was obtained with use of variational Gutzwiller Monte Carlo method. Our result is not changing appreciable with the  $J/t$  value. The same is true for the  $\langle S_4^z S_5^z \rangle$  expectation value, which also stays at the constant value of -0.14034 with varying  $J/t$ . However, the  $\langle S_4^x S_5^x \rangle$  expectation value is changing

with  $J/t$ , from  $-0.152$  for  $J/t \sim 0.1$  up to  $-0.128$  for  $J/t \sim 1$ . One interesting fact is that this variation is compensated by the  $\langle n_4 n_5 \rangle$  term, in such a way that for different values of  $J/t$  the energy minimum it is obtained roughly at the same values of the variational parameters. For these expectation values we do not have any source for comparison. However, Yokoyama and Shiba (1987) obtained in the  $n \sim 0.8$  range for the interaction part of the Hamiltonian  $\sim -0.5 - \sim -0.625$   $J/t$ . While Bonca, Prelovsek, and Sega (1989) are not giving any concrete values for the ground state energy, or correlations. Our results for the interaction term is  $-0.51786$  per site and  $J/t$  which is in agreement with the result of Yokoyama and Shiba. We give the final result as compared also with the half filled case.

Expectation Values	Band Filling	Results
$E_{kin}/N$	$n = 1$	0
$S_4^x S_5^x$	$n = 1$	-0.21708
$S_4^z S_5^z$	$n = 1$	-0.21533
$S_4 \cdot S_5$	$n = 1$	-0.64949
$n_4 n_5$	$n = 1$	1
$E_{pot}/N$ (J/t)	$n = 1$	-0.89949
$E_{kin}/N$	$n = 5/6$	-0.43740
$S_4^x S_5^x$	$n = 5/6$	-0.15278
$S_4^z S_5^z$	$n = 5/6$	-0.14034
$S_4 \cdot S_5$	$n = 5/6$	-0.44590
$n_4 n_5$	$n = 5/6$	0.28785
$E_{pot}/N$ (J/t)	$n = 5/6$	-0.51786

As for the one dimensional case, the potential energy is increasing with doping. However, this increase is more then in one dimensional case, that is  $\sim 0.38$ . While in one dimension  $\sim 0.24$  it is obtained. This can be understood starting from the kinetic energy which is lower in two dimension than in the case of the linear chain. Concerning the hole-hole correlations, as it was mentioned in the previous chapters, the value of the variational parameter  $\alpha$  can elucidate if some attraction between holes is favored within the systems. This analysis is interesting due to

the fact that Bonca, Prelovsek, and Sega (1989) obtains that the effective binding energy for two holes is negative for all range of  $J/t$  and the hole density correlation shows attraction for  $J/t > 0.1$ . Their result shows that attraction occurs for next-nearest neighboring holes for  $J/t < 0.5$  and for nearest neighboring holes for  $J/t > 0.5$ . However, as mentioned by themselves, substantial binding energy of the two holes may be attributed to the very specific boundary condition which they used. In our calculations, due to the Bethe-Peierls condition, we can approximately determine the nearest neighbour correlation of the bulk. The obtained results shows hole-hole repulsion, at least for the  $J/t < 0.5$  domain. For higher values of the  $J/t$  parameter, because of the importance of this issue, numerical subrutines will be also used parallel with the Maple program. Needless to say, our study is not complete, more work must be considered, and it is already under progress, in order to elucidate the behaviour of the t-J model on square lattice.

# Conclusions

In the present work we have given a variational description of the ground state properties of the  $t$ - $J$  model. The treatment is on the line of the Gutzwiller method, however, we improved both the Ansatz and the evaluation of the expectation values. We were interested in the properties of the normal ground state, that is why we were not considering any projected long range ordered states, as in the previous treatments. In such a way we avoid predicting spurious ordering instabilities. In the limit of half filling our Ansatz corresponds to a quantum paramagnetic ( $RVB$ ) ground state of the Heisenberg model. Away from half filling the Ansatz corresponds to a normal conductor. In the present work we brought essential improvements in the treatment of short range order effects. As variational parameters we introduced new type of parameters in order to control nearest neighbour hole-hole, and spin-spin correlations.

The other essential aspect of our treatment is the introduction of a cluster approximation. As it is known, the exchange hole effect inherited from the Fermi sea can account for a good part of antiparallel spin configurations in the large  $U$  limit, in low dimensions. In order to keep this feature, we took multielectron configuration amplitudes from the Fermi sea ground state, and modify these with variational parameters. We took clusters which are sufficiently large so that there is a central pair of site completely surrounded by cluster sites. The method being applicable in any dimension, we analysed the one dimensional chain and two

dimensional square lattice. The Bethe-Peierls condition is a guarantee that the correlation functions obtained for the central pair are a good approximation for the bulk.

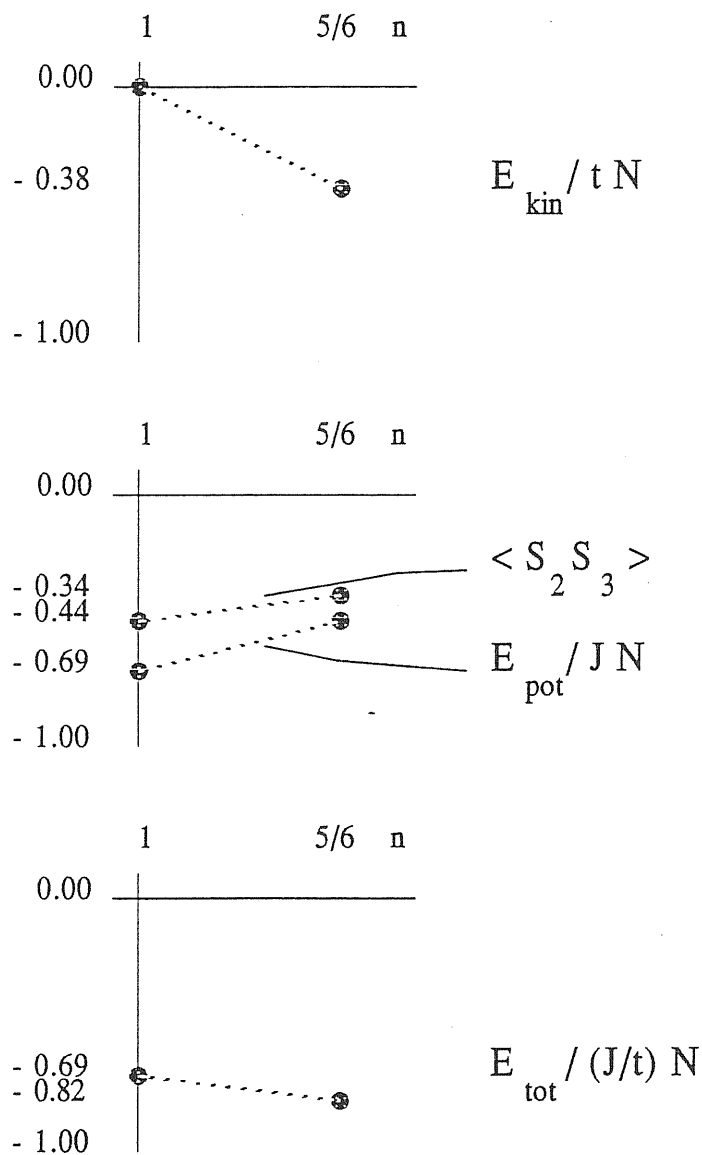
For the linear chain, to accomplish the desired property of the cluster, four sites are taken to construct it. For half filled case, the t-J model reduces to the Heisenberg Hamiltonian, the obtained energy is 98.7 per cent of the exact value, which considering the simplicity of the calculation technique is a remarkable result. For the  $n = 5/6$  less than half filled case the kinetic energy will give slightly more than fifty per cent of the obtained ground state energy. No reliable results exists for the less than half filling case in the one dimensional t-J model to make a comparison. The spin-spin and charge-charge correlations are also computed.

In the case of square lattice, by considering all the nearest neighbours of a central pair we were led to work with an eight site cluster. The calculations were more lengthy than in the previous case, because of the total 6561 configurations which must be taken into account. The first case analysed was the half filled system, i.e. the Heisenberg model. After making the minimization we obtained for the energy -0.6495, which is two per cent higher than the energy values obtained by Monte Carlo methods. The  $n = 5/6$  less than half filling case was also analysed for the two dimensional square lattice. After making the energy minimization, -0.4374 it is obtained for the kinetic energy term. This value is situated between the results obtained by the Gutzwiller approximation -0.5, and by the Gutzwiller

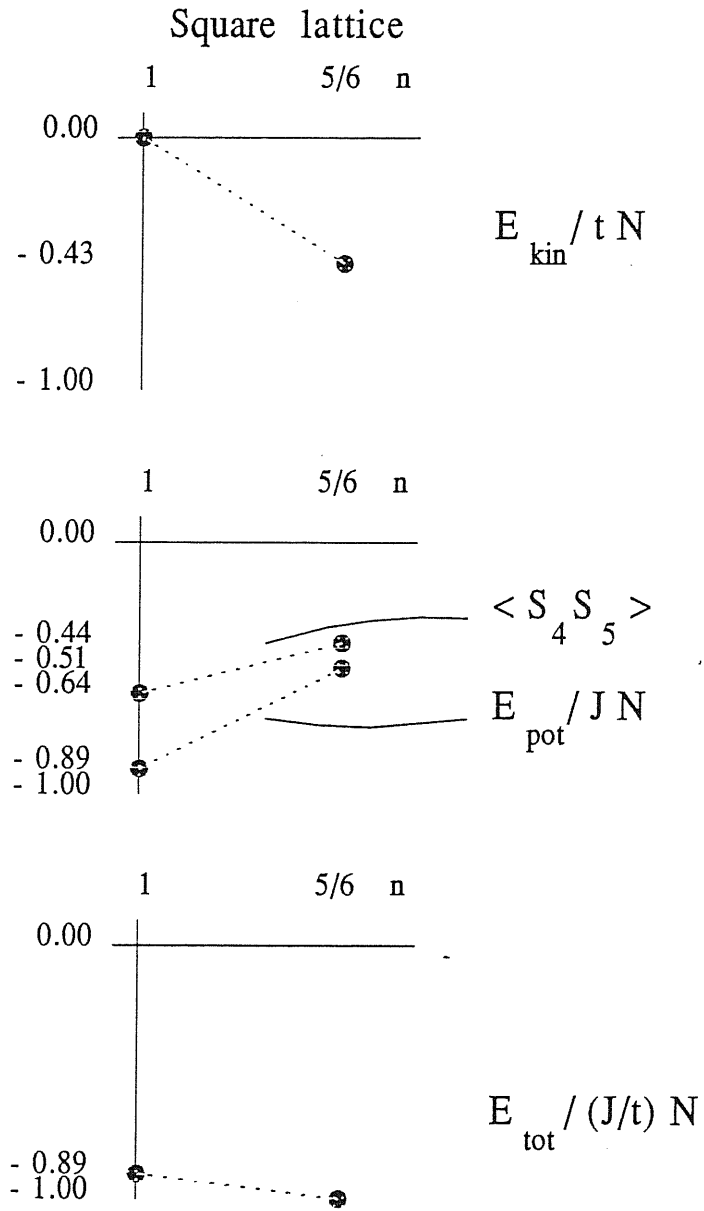


variational Monte Carlo method of Yokoyama and Shiba (1987) of -0.4. For the interaction term of the Hamiltonian we obtained -0.51786 per site and  $J/t$ , which is also in agreement with the range of energies obtained by Yokoyama and Shiba (1987) of  $\sim -0.5 - -0.625$  per site and  $J/t$ . In order to compare the one and two dimensional cases, we give the following simple graphics. For the linear chain.

### Linear chain



In the case of square lattice.



The same filling factor was analysed in both the one and two dimensional case. The kinetic energy it is obtained at a lower value in two dimension, i.e. -0.437 compared with -0.381 in one dimension. This can be understood because of the extra degree of freedom in the square lattice, i.e., a larger coordination. Concerning the first neighbour spin-spin correlation, and thus the potential energy it turns to be less damaged by doping in two dimension than in one . Although our trial state is paramagnetic, this finding is in line, of course, with the well-known fact that antiferromagnetism tendencies are more robust in two dimension than in one. Quantum fluctuations in two dimension are not so strong than in one dimension. Due to this, the effect of doping is lower in one dimension, the energy variation is 0.24, than in the case of the square lattice, case in which it is obtained 0.38.

Furthermore, some very interesting conclusions can be drawn from the slope of the total energy variation versus the band filling. Relating our calculation to the Hubbard Hamiltonian, we could argue that for  $U \rightarrow \infty$ , the ground state energy is given by the spinless Fermion wave function. This is due to the fact that for one hole, the Nagaoka state is the ground state. By increasing the doping, being at large  $U$  limit the potential energy gives no contribution, while the kinetic one should be the lowest for the spinless Fermionic case. In order to check such a state, we compute for the spinless Fermions the variation of the chemical potential, for  $n = 5/6$  doping, and compare the results with the slope of the total energy variation. The results obtained are in agreement with the calculated ones, i.e.,

for one dimension the sloap is  $\sim 0.78$ , expected  $\sim 0.92$ , while in two dimension the sloap is  $\sim 0.66$ , and expected  $\sim 0.79$ . We used the values given in the figure, because these are for the  $J/t \sim 0.1$  range. This result suggests that for large  $U$  limit, the ground state of the Hubbard Hamiltonian is degenerate, with one of the states being the spinless Fermionic one.

The results obtained show no attractive force between two nearest neighboring holes in the both studied cases. All the states which would have led to real space bonding between the holes were situated at high energetic levels. We find this behaviour for all  $J/t$  values. This is surprising, since small size Lanczos calculations made by Bonca, Prelovsek and Sega (1989) have indicated a switch from hole-hole repulsion for  $J/t < 0.5$ , to attraction for  $J/t > 0.5$ . On the other hand, similar calculations of Parola *et al.* (1989) for the Hubbard model seem to indicate just repulsion. More work is in progress, to elucidate the reasons of these discrepancies.

Mostly, all the results are presented with numerical values, however every calculation was made in algebraic form by use of the Maple algebraic manipulation program. This is necessary in order to perform the Bethe-Peierls conditions and to control the number of electrons per site, i.e. in order to evaluate the chemical potential. In view of the special significance of the two dimensional square lattice, the results so obtained allow to obtain in some limiting cases approximate but analytical results for the Hubbard Hamiltonian.

# Appendix 1

The denominator of the two dimensional square lattice for  $n=5/6$  is the following.

$$\begin{aligned}
Z = & 0.001572058370 \alpha_c \alpha_s^2 \beta_s^4 \beta_c^2 \mu^{10} + 0.0001767671380 \alpha_c \alpha_s^2 \beta_s^8 \beta_c^2 \mu^{12} \\
& + 0.0005640640131 \alpha_s^2 \beta_s^4 \beta_c^2 \mu^{12} + 0.000166763109 \alpha_s^2 \beta_s^6 \beta_c^2 \mu^8 \\
& + 0.003240192543 \alpha_c^2 \alpha_s^2 \beta_s^2 \mu^{10} + 0.003317027022 \alpha_c^2 \alpha_s^4 \beta_s^2 \mu^8 \\
& + 0.00100758436 \alpha_c^2 \alpha_s^8 \beta_s^2 \mu^6 + 0.0001784567677 \alpha_c^2 \alpha_s^4 \beta_s^4 \mu^8 \\
& + 0.0004417247350 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^6 + 0.0005202822471 \alpha_s^2 \beta_s^6 \beta_c^2 \mu^{10} \\
& + 0.0009570614248 \alpha_c^2 \alpha_s^6 \beta_s^2 \mu^6 + 0.0003207957321 \alpha_c^2 \alpha_s^{10} \beta_s^2 \mu^4 \\
& + 0.0006778913172 \alpha_s^2 \beta_s^4 \beta_c^2 \mu^8 + 0.002749515178 \mu^{10} + 0.001369067401 \mu^{12} \\
& + 0.000329598968 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^{12} + 0.00195730212 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^8 \\
& + 0.0005663643994 \beta_c^2 \mu^{10} + 0.0005433904152 \alpha_c^2 \alpha_s^2 \beta_s^4 \mu^{10} \\
& + 0.0002289447656 \alpha_s^4 \beta_s^2 \beta_c^2 \mu^6 + 0.0002508315528 \alpha_s^2 \beta_s^8 \beta_c^2 \mu^{10} \\
& + 0.001649273354 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^{10} + 0.006655826733 \alpha_s^2 \beta_s^4 \mu^{10} \\
& + 0.00240964779 \beta_s^2 \beta_c^2 \mu^{20} + 0.0007767803430 \beta_s^{10} \beta_c^2 \mu^{14} \\
& + 0.001130478264 \alpha_s^2 \beta_s^8 \mu^{12} + 0.0007397524436 \beta_s^6 \beta_c^2 \mu^{10} \\
& + 0.00009371686186 \alpha_s^2 \beta_s^{10} \mu^{12} + 0.002916197766 \alpha_c^2 \alpha_s^{10} \mu^4 \\
& + 0.00194686951 \alpha_s^2 \beta_s^4 \mu^8 + 0.0002607896987 \alpha_s^4 \beta_s^8 \mu^{10} \\
& + 0.000268409634 \beta_s^{10} \beta_c^2 \mu^{16} + 0.00002339518742 \beta_s^{16} \beta_c^2 \mu^{16}
\end{aligned}$$

$$\begin{aligned}
& + 0.000417954148 \alpha_c^2 \alpha_s^{14} \mu^2 + 0.003181960486 \alpha_s^{10} \beta_s^2 \mu^4 \\
& + 0.004129416803 \alpha_s^4 \beta_s^4 \mu^{10} + 0.00646907934 \alpha_s^4 \beta_s^2 \mu^8 \\
& + 0.0001235045859 \alpha_s^2 \beta_s^8 \mu^{10} + 0.001979280951 \beta_s^6 \beta_c^2 \mu^{14} \\
& + 0.001909911915 \beta_s^4 \beta_c^2 \mu^{14} + 0.006081706872 \alpha_c^2 \alpha_s^4 \mu^8 \\
& + 0.0001467723801 \alpha_s^4 \beta_c^2 \mu^4 + 0.002701764773 \alpha_c^2 \alpha_s^2 \mu^{10} \\
& + 0.0008061489834 \alpha_s^{12} \alpha_c^2 \mu^2 + 0.001219911263 \beta_c^2 \beta_s^8 \mu^{14} \\
& + 0.0007717003007 \alpha_c^2 \beta_s^2 \mu^{12} + 0.003665347159 \alpha_s^4 \beta_s^2 \mu^{10} \\
& + 0.00229767765 \beta_s^4 \beta_c^2 \mu^{10} + 0.003913430476 \beta_s^4 \beta_c^2 \mu^{12} \\
& + 0.0000892806017 \alpha_s^4 \beta_s^4 \beta_c^2 \mu^8 + 0.00001484145187 \mu^{16} + 0.0002543192626 \mu^{14} \\
& + 0.001701605654 \mu^8 + 0.0007499046013 \alpha_s^6 \alpha_c^2 \beta_s^2 \mu^8 \\
& + 0.0000946518426 \alpha_s^2 \beta_s^{10} \beta_c^2 \mu^{12} + 0.00124285733 \alpha_s^8 \alpha_c^2 \mu^4 \\
& + 0.000751559016 \alpha_s^6 \alpha_c^2 \mu^8 + 0.00116254747 \alpha_s^4 \beta_s^2 \mu^6 \\
& + 0.0006901640148 \alpha_s^6 \beta_s^4 \mu^6 + 0.00004189986010 \beta_s^{14} \beta_c^2 \mu^{16} \\
& + 0.003807024124 \alpha_s^2 \beta_s^4 \mu^{12} + 0.0001697285391 \beta_s^{12} \beta_c^2 \mu^{16} \\
& + 0.007146917365 \alpha_s^2 \beta_s^2 \mu^{10} + 0.0007513090983 \alpha_s^2 \beta_c^2 \mu^8 \\
& + 0.003009013608 \alpha_s^8 \alpha_c^2 \mu^6 + 0.003453062045 \beta_s^4 \mu^{10} \\
& + 0.0002227849772 \beta_c^2 \mu^{12} + 0.0004853757703 \alpha_s^2 \mu^{12} \\
& + 0.0003570651255 \beta_s^8 \mu^{16} + 0.0003093569257 \beta_s^6 \mu^{16} \\
& + 0.00004297879312 \beta_s^2 \mu^{16} + 0.004704932683 \beta_s^6 \mu^{12} \\
& + 0.003236016528 \beta_s^6 \mu^{14} + 0.0004723335682 \beta_s^{10} \mu^{16}
\end{aligned}$$

$$\begin{aligned}
& + 0.001124603225 \beta_s^2 \mu^{14} + 0.004670916135 \beta_s^2 \mu^{12} \\
& + 0.0001447254006 \beta_s^4 \mu^{16} + 0.0002010858267 \beta_s^{12} \mu^{16} \\
& + 0.006468986435 \beta_s^4 \mu^{12} + 0.003627940484 \alpha_s^2 \mu^8 \\
& + 0.002621383959 \beta_s^4 \mu^{14} + 0.003627866739 \alpha_s^4 \mu^8 \\
& + 0.0007021508245 \beta_s^2 \mu^8 + 0.0003482061912 \beta_s^4 \mu^8 \\
& + 0.0003855743992 \alpha_s^{10} \mu^2 + 0.0009741331960 \alpha_s^8 \mu^6 \\
& + 0.0003181220568 \alpha_s^{10} \mu^4 + 0.001193946284 \alpha_s^6 \mu^4 \\
& + 0.002599524682 \beta_s^8 \mu^{14} + 0.002611294629 \alpha_s^6 \mu^6 \\
& + 0.005005829667 \beta_s^2 \mu^{10} + 0.003026173694 \alpha_s^4 \mu^6 \\
& + 0.001967610194 \beta_s^8 \mu^{12} + 0.001148953762 \beta_s^{10} \mu^{14} \\
& + 0.001232501660 \alpha_s^8 \mu^4 + 0.001231632361 \alpha_s^6 \mu^8 \\
& + 0.0001266140955 \alpha_s^{16} \alpha_c^2 + 0.002593258646 \alpha_s^2 \mu^{10} \\
& + 0.0003861659616 \alpha_c^2 \mu^{12} + 0.0003596523719 \beta_c^2 \mu^8 \\
& + 0.001313539417 \beta_s^6 \mu^{10} + 0.0009816634273 \alpha_s^4 \mu^{10} \\
& + 0.001339787696 \alpha_s^2 \mu^6 + 0.0001466499744 \alpha_s^4 \mu^4 \\
& + 0.0002421920728 \beta_s^6 \beta_c^2 \mu^{12} + 0.0003861415518 \beta_s^{10} \beta_c^2 \mu^{12} \\
& + 0.002035521349 \beta_s^2 \beta_c^2 \mu^{12} + 0.0004668584778 \alpha_s^2 \beta_s^2 \mu^6 \\
& + 0.0003837820611 \beta_s^8 \beta_c^2 \mu^{16} + 0.002282075107 \alpha_s^2 \beta_s^2 \mu^{12} \\
& + 0.002395853852 \alpha_s^6 \beta_s^4 \mu^8 + 0.00009991150928 \beta_s^4 \beta_c^2 \mu^8 \\
& + 0.0003436812023 \alpha_s^4 \beta_s^6 \mu^8 + 0.0002485788382 \beta_s^4 \beta_c^2 \mu^{16}
\end{aligned}$$

$$\begin{aligned}
& + 0.0004671326246 \alpha_s^2 \beta_c^2 \mu^6 + 0.001846252811 \alpha_s^4 \beta_s^6 \mu^{10} \\
& + 0.002645769698 \alpha_s^2 \beta_s^6 \mu^{10} + 0.005000431546 \alpha_s^2 \beta_s^2 \mu^8 \\
& + 0.003386708074 \alpha_s^6 \beta_s^2 \mu^6 + 0.004880192894 \alpha_s^6 \alpha_c^2 \mu^6 \\
& + 0.0005351389569 \alpha_s^6 \beta_s^6 \mu^8 + 0.001505890530 \alpha_s^8 \beta_s^2 \mu^6 \\
+ & 0.00004291940762 \beta_s^{12} \beta_c^2 \mu^{12} + 0.00006337531334 \beta_s^{14} \beta_c^2 \mu^{14} \\
& + 0.0006137357944 \alpha_s^8 \beta_s^2 \mu^4 + 0.0004138455440 \beta_s^2 \beta_c^2 \mu^{16} \\
& + 0.0006809760580 \beta_s^2 \beta_c^2 \mu^8 + 0.0003333567181 \beta_s^6 \beta_c^2 \mu^4 \\
& + 0.003124437355 \alpha_s^2 \beta_s^6 \mu^{12} + 0.003266785263 \alpha_s^6 \beta_s^2 \mu^8 \\
+ & 0.0002388671400 \beta_s^8 \beta_c^2 \mu^{10} + 0.0003018866920 \alpha_s^2 \beta_c^2 \mu^{10} \\
& + 0.0003249136236 \beta_s^4 \beta_c^2 \mu^8 + 0.0004809068858 \alpha_s^8 \beta_s^4 \mu^6 \\
+ & 0.0004754442069 \beta_s^2 \beta_c^2 \mu^{14} + 0.0001979785391 \beta_s^{12} \beta_c^2 \mu^{14} \\
& + 0.001192346754 \beta_s^8 \beta_c^2 \mu^{12} + 0.002919494380 \alpha_s^4 \beta_s^4 \mu^8
\end{aligned}$$



## Appendix 2

The  $z$  component of the spin-spin correlation for  $n = 5/6$  less than half filled square lattice is the following.

$$\begin{aligned}
 \langle S_4^z S_5^z \rangle = & - 0.00006270788820 \alpha_s^2 \beta_s^8 \beta_c^2 \mu^{10} + 0.00001074469828 \beta_s^2 \mu^{16} \\
 & + 0.00003666249360 \alpha_s^4 \mu^4 - 0.0001104311837 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^6 \\
 & + 0.00001830826529 \alpha_s^2 \mu^{12} + 0.0001180833921 \beta_s^{10} \mu^{16} \\
 & - 0.00002497787732 \alpha_s^4 \beta_c^2 \mu^8 + 0.3710362968 \times 10^{-5} \mu^{16} \\
 & - 0.00002366329606 \alpha_s^2 \beta_s^{10} \beta_c^2 \mu^{12} - 0.0001415910999 \beta_c^2 \mu^{10} \\
 & + 0.0006059316489 \beta_s^4 \mu^{10} + 0.0001755377064 \beta_s^2 \mu^8 \\
 & + 0.00007733923142 \beta_s^6 \mu^{16} - 0.0009783576169 \beta_s^4 \beta_c^2 \mu^{12} \\
 & - 0.00001047496503 \beta_s^{14} \beta_c^2 \mu^{16} - 0.0001694728293 \alpha_s^2 \beta_s^4 \beta_c^2 \mu^8 \\
 & - 0.00004396477848 \alpha_s^4 \beta_s^2 \beta_c^2 \mu^8 - 0.00006214470953 \beta_s^4 \beta_c^2 \mu^{16} \\
 & + 0.0003173393538 \alpha_s^2 \beta_s^4 \mu^8 - 0.00004419178452 \alpha_s^2 \beta_s^8 \beta_c^2 \mu^{12} \\
 & - 0.00005569624428 \beta_c^2 \mu^{12} - 0.0001167831562 \alpha_s^2 \beta_c^2 \mu^6 \\
 & + 0.00004719129502 \alpha_s^4 \beta_s^2 \mu^8 + 0.0007643369186 \beta_s^4 \mu^{12} \\
 & - 0.0001410160035 \alpha_s^2 \beta_s^4 \beta_c^2 \mu^{12} - 0.0003930145926 \alpha_s^2 \beta_s^4 \beta_c^2 \mu^{10} \\
 & - 0.0001188610517 \beta_s^2 \beta_c^2 \mu^{14} + 0.00007061475506 \alpha_s^2 \beta_s^8 \mu^{12} \\
 & + 0.00002329488150 \alpha_s^4 \beta_s^4 \mu^8 + 0.00002069544552 \alpha_s^4 \mu^8 \\
 & + 0.00009630066628 \alpha_s^2 \beta_s^4 \mu^{12} - 0.00006054801820 \alpha_s^4 \beta_c^2 \mu^6
 \end{aligned}$$

$$\begin{aligned}
& + 0.0001145309903 \alpha_s^2 \mu^{10} - 0.0001878272746 \alpha_s^2 \beta_c^2 \mu^8 \\
& - 0.0004894575533 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^8 + 0.0001102801013 \alpha_s^2 \mu^6 \\
& - 0.00004154407772 \alpha_s^2 \beta_s^6 \beta_c^2 \mu^8 - 0.00003669309506 \alpha_s^4 \beta_c^2 \mu^4 \\
& - 0.00004949463478 \beta_s^{12} \beta_c^2 \mu^{14} + 0.00005027145668 \beta_s^{12} \mu^{16} \\
& + 0.00008705154776 \beta_s^4 \mu^8 + 0.0002544148181 \beta_s^{10} \mu^{14} \\
& + 0.0003021084723 \beta_s^4 \mu^{14} + 0.00007845583696 \mu^8 + 0.0003640626699 \alpha_s^2 \beta_s^2 \mu^8 \\
& + 0.00003646469944 \mu^{14} - 0.0001941950855 \beta_s^{10} \beta_c^2 \mu^{14} + 0.0001242985008 \mu^{12} \\
& - 0.00004243213480 \beta_s^{12} \beta_c^2 \mu^{16} - 0.0001003586857 \alpha_s^2 \beta_s^6 \beta_c^2 \mu^{12} \\
& + 0.0002701304447 \alpha_s^2 \beta_s^2 \mu^{10} - 0.00001584382834 \beta_s^{14} \beta_c^2 \mu^{14} \\
& + 0.0004576361202 \beta_s^2 \mu^{10} + 0.0003283848538 \beta_s^6 \mu^{10} \\
& - 0.00005723619140 \alpha_s^4 \beta_s^2 \beta_c^2 \mu^6 + 0.0004678604054 \beta_s^6 \mu^{14} \\
& - 0.0005743919406 \beta_s^4 \beta_c^2 \mu^{10} + 0.0002716816892 \alpha_s^2 \beta_s^6 \mu^{10} \\
& - 0.00008915842270 \beta_s^{10} \beta_c^2 \mu^{12} + 0.0002061540141 \alpha_s^2 \mu^8 \\
& + 0.00003618135016 \beta_s^4 \mu^{16} + 0.0007977150501 \beta_s^6 \mu^{12} \\
& - 0.0001300705618 \alpha_s^2 \beta_s^6 \beta_c^2 \mu^{10} - 0.00008991309298 \beta_c^2 \mu^8 \\
& + 0.0004841928446 \beta_s^8 \mu^{14} + 0.0001096848001 \beta_s^2 \mu^{14} \\
& - 0.00002232015042 \alpha_s^4 \beta_s^4 \beta_c^2 \mu^8 + 0.00008926628134 \beta_s^8 \mu^{16} \\
& + 0.0004455145199 \beta_s^8 \mu^{12} - 0.00005971678502 \beta_s^8 \beta_c^2 \mu^{10} \\
& - 0.00007547167300 \alpha_s^2 \beta_c^2 \mu^{10} - 0.0004123183379 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^{10} \\
& - 0.5848796856 \times 10^{-5} \beta_s^{16} \beta_c^2 \mu^{16} + 0.0004163643770 \alpha_s^2 \beta_s^4 \mu^{10}
\end{aligned}$$

$$\begin{aligned}
& + 0.00005718410176 \alpha_s^4 \mu^6 - 0.0002980866886 \beta_s^8 \beta_c^2 \mu^{12} \\
& + 0.00004898551745 \alpha_s^2 \beta_s^2 \mu^{12} - 0.0005088803368 \beta_s^2 \beta_c^2 \mu^{12} \\
& + 0.0001698263803 \mu^{10} - 0.00006546024085 \beta_s^{10} \beta_c^2 \mu^{16} \\
& - 0.0001034613860 \beta_s^6 \beta_c^2 \mu^{16} + 0.0001571113123 \alpha_s^2 \beta_s^6 \mu^{12} \\
& - 0.00001072985191 \beta_s^{12} \beta_c^2 \mu^{12} + 0.00006051159318 \alpha_s^4 \beta_s^2 \mu^6 \\
& - 0.0003049778161 \beta_s^8 \beta_c^2 \mu^{14} + 0.0003685106952 \beta_s^2 \mu^{12} \\
& - 0.0001849381109 \beta_s^6 \beta_c^2 \mu^{10} - 0.00008122840592 \beta_s^4 \beta_c^2 \mu^8 \\
& - 0.0004774779793 \beta_s^4 \beta_c^2 \mu^{14} - 0.0001702440146 \beta_s^2 \beta_c^2 \mu^8 \\
& - 0.00009594551524 \beta_s^8 \beta_c^2 \mu^{16} + 0.0001167146195 \alpha_s^2 \beta_s^2 \mu^6 \\
& - 0.0004948202385 \beta_s^6 \beta_c^2 \mu^{14} - 0.0005611867864 \beta_s^6 \beta_c^2 \mu^{12} \\
& - 0.0006024101960 \beta_s^2 \beta_c^2 \mu^{10} - 0.00008239974204 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^{12}
\end{aligned}$$

## Appendix 3

The  $\langle S_4^x S_5^x \rangle = \langle S_4^y S_5^y \rangle$  spin correlation for  $n = 5/6$  less than half filled square lattice is the following.

$$\begin{aligned}
\langle S_4^x S_5^x \rangle = & - .2495716808 \times 10^{-6} \beta_s^8 \beta_c^2 \mu^{12} - .3106466582 \times 10^{-7} \beta_s^{12} \beta_c^2 \mu^{12} \\
& - .4250307366 \times 10^{-7} \beta_s^{14} \beta_c^2 \mu^{14} - .2918814312 \times 10^{-7} \beta_s^{12} \beta_c^2 \mu^{16} \\
& - .3246766171 \times 10^{-7} \beta_s^8 \beta_c^2 \mu^{16} - .5357330914 \times 10^{-7} \beta_s^4 \beta_c^2 \mu^{16} \\
& - .6052374529 \times 10^{-6} \beta_s^4 \beta_c^2 \mu^{14} - .1564631407 \times 10^{-6} \beta_s^8 \beta_c^2 \mu^{10} \\
& - .1373222324 \times 10^{-6} \alpha_s^2 \beta_s^8 \beta_c^2 \mu^2 - .8850786432 \times 10^{-7} \alpha_s^4 \beta_c^2 \mu^6 \\
& - .1453831244 \times 10^{-7} \beta_s^{16} \beta_c^2 \mu^{16} - .6640437086 \times 10^{-7} \beta_s^{10} \beta_c^2 \mu^{16} \\
& - .8977738825 \times 10^{-7} \beta_s^{12} \beta_c^2 \mu^{14} - .2196029476 \times 10^{-6} \alpha_s^2 \beta_s^2 \beta_c^2 \mu^6 \\
& - .2196029476 \times 10^{-6} \alpha_s^2 \beta_c^2 \mu^6 - .1276566738 \times 10^{-6} \beta_s^6 \beta_c^2 \mu^{16} \\
& - .4068443268 \times 10^{-6} \beta_s^8 \beta_c^2 \mu^{12} - .1812137635 \times 10^{-7} \beta_s^{14} \beta_c^2 \mu^{16} \\
& - .1212760477 \times 10^{-5} \beta_s^4 \beta_c^2 \mu^{12} - .2532895252 \times 10^{-6} \beta_s^{10} \beta_c^2 \mu^{14} \\
& - .4968157904 \times 10^{-6} \beta_s^6 \beta_c^2 \mu^{14} - .3118745480 \times 10^{-6} \alpha_s^2 \beta_s^4 \beta_c^2 \mu^8 \\
& - .4785797350 \times 10^{-7} \alpha_s^2 \beta_s^{10} \beta_c^2 \mu^{12} - .9082312783 \times 10^{-6} \beta_s^2 \beta_c^2 \mu^{10} \\
& - .9850707286 \times 10^{-7} \alpha_s^2 \beta_s^6 \beta_c^2 \mu^8 - .320025661 \times 10^{-7} \alpha_s^4 \beta_s^4 \beta_c^2 \mu^8 \\
& - .2160949243 \times 10^{-6} \beta_s^{10} \beta_c^2 \mu^{12} - .1899960523 \times 10^{-6} \alpha_s^2 \beta_s^6 \beta_c^2 \mu^{10} \\
& - .6855339043 \times 10^{-6} \alpha_s^2 \beta_s^2 \beta_c^2 \mu^{10} - .3118745480 \times 10^{-6} \alpha_s^2 \beta_c^2 \mu^8 \\
& - .8850786432 \times 10^{-7} \alpha_s^4 \beta_s^2 \beta_c^2 \mu^6 - .7097162039 \times 10^{-6} \beta_s^6 \beta_c^2 \mu^{12}
\end{aligned}$$

$$\begin{aligned}
& - .7690670514 \times 10^{-6} \alpha_s^2 \beta_s^2 \beta_c^2 \mu^8 - .3608625325 \times 10^{-6} \beta_s^6 \beta_c^2 \mu^{10} \\
& - .6275161540 \times 10^{-6} \alpha_s^2 \beta_s^4 \beta_c^2 \mu^{10} - .6119542120 \times 10^{-7} \alpha_s^4 \beta_c^2 \mu^4 \\
& - .1519781324 \times 10^{-6} \beta_s^2 \beta_c^2 \mu^{14} - .9099789954 \times 10^{-7} \beta_c^2 \mu^{12} \\
& - .2849871124 \times 10^{-6} \alpha_s^2 \beta_s^4 \beta_c^2 \mu^{12} - .8525932339 \times 10^{-6} \beta_s^4 \beta_c^2 \mu^{10} \\
& - .8919621680 \times 10^{-7} \alpha_s^2 \beta_s^6 \beta_c^2 \mu^{12} - .1857083414 \times 10^{-6} \beta_c^2 \mu^8 \\
& - .1051316050 \times 10^{-6} \alpha_s^2 \beta_s^2 \beta_c^2 \mu^{12} - .3093994178 \times 10^{-6} \beta_s^2 \beta_c^2 \mu^8 \\
& - .1857083414 \times 10^{-6} \beta_s^4 \beta_c^2 \mu^8 - .320025661 \times 10^{-7} \alpha_s^4 \beta_c^2 \mu^8 \\
& - .7729909604 \times 10^{-6} \beta_s^2 \beta_c^2 \mu^{12} - .2600374363 \times 10^{-6} \beta_c^2 \mu^{10} \\
& - .9081013616 \times 10^{-7} \alpha_s^2 \beta_s^8 \beta_c^2 \mu^{12} - .1106915700 \times 10^{-6} \alpha_s^2 \beta_c^2 \mu^{10} \\
& - .9835753948 \times 10^{-7} \alpha_s^4 \beta_s^2 \beta_c^2 \mu^8
\end{aligned}$$

## Appendix 4

The value of the charge-charge correlation for  $n = 5/6$  less than half filled square lattice is the following.

$$\begin{aligned}
 - (1/4) \langle n_4 n_5 \rangle = & - .00006270788820 \alpha_s^2 \beta_s^8 \beta_c^2 \mu^{20} - .00001074469828 \beta_s^2 \mu^{16} \\
 & - .00003666249360 \alpha_s^4 \mu^4 - .0001104311837 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^6 \\
 & - .00001830826529 \alpha_s^2 \mu^{12} - .0001180833921 \beta_s^{10} \mu^{16} \\
 & - .00002497787732 \alpha_s^4 \beta_c^2 \mu^8 - .3710362968 \times 10^{-5} \mu^{16} \\
 & - .00002366329606 \alpha_s^2 \beta_s^{10} \beta_c^2 \mu^{12} - .0001415910999 \beta_c^2 \mu^{10} \\
 & - .0006059316489 \beta_s^4 \mu^{10} - .0001755377064 \beta_s^8 \mu^8 \\
 & - .00007733923142 \beta_s^6 \mu^{16} - .0009783576169 \beta_s^4 \beta_c^2 \mu^{12} \\
 & - .00001047496503 \beta_s^{14} \beta_c^2 \mu^{16} - .0001694728293 \alpha_s^2 \beta_s^4 \beta_c^2 \mu^8 \\
 & - .00004396477848 \alpha_s^4 \beta_s^2 \beta_c^2 \mu^8 - .00006214470953 \beta_s^4 \beta_c^2 \mu^{16} \\
 & - .0003173393538 \alpha_s^2 \beta_s^4 \mu^8 - .00004419178452 \alpha_s^2 \beta_s^8 \beta_c^2 \mu^{12} \\
 & - .00005569624428 \beta_c^2 \mu^{12} - .0001167831562 \alpha_s^2 \beta_c^2 \mu^6 \\
 & - .00004719129502 \alpha_s^4 \beta_s^2 \mu^8 - .0007643369186 \beta_s^4 \mu^{12} \\
 & - .0001410160035 \alpha_s^2 \beta_s^4 \beta_c^2 \mu^{12} - .0003930145926 \alpha_s^2 \beta_s^4 \beta_c^2 \mu^{10} \\
 & - .0001188610517 \beta_s^2 \beta_c^2 \mu^{14} - .00007061475506 \alpha_s^2 \beta_s^8 \mu^{12} \\
 & - .00002329488150 \alpha_s^4 \beta_s^4 \mu^8 - .00002069544552 \alpha_s^4 \mu^8 \\
 & - .00009630066628 \alpha_s^2 \beta_s^4 \mu^{12} - .00006054801820 \alpha_s^4 \beta_c^2 \mu^6
 \end{aligned}$$

$$\begin{aligned}
& - .0001145309903 \alpha_s^2 \mu^{10} - .0001878272746 \alpha_s^2 \beta_c^2 \mu^8 \\
& - .0004894575533 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^8 - .0001102801013 \alpha_s^2 \mu^6 \\
& - .00004154407772 \alpha_s^2 \beta_s^6 \beta_c^2 \mu^8 - .00003669309506 \alpha_s^4 \beta_c^2 \mu^4 \\
& - .00004949463478 \beta_s^{12} \beta_c^2 \mu^{14} - .00005027145668 \beta_s^{12} \mu^{16} \\
& - .00008705154776 \beta_s^4 \mu^8 - .0002544148181 \beta_s^{10} \mu^{14} \\
& - .0003021084723 \beta_s^4 \mu^{14} - .00007845583696 \mu^8 - .0003640626699 \alpha_s^2 \beta_s^2 \mu^8 \\
& - .00003646469944 \mu^{14} - .0001941950855 \beta_s^{10} \beta_c^2 \mu^{14} - .0001242985008 \mu^{12} \\
& - .00004243213480 \beta_s^{12} \beta_c^2 \mu^{16} - .0001003586857 \alpha_s^2 \beta_s^6 \beta_c^2 \mu^{12} \\
& - .0002701304447 \alpha_s^2 \beta_s^2 \mu^{10} - .00001584382834 \beta_s^{14} \beta_c^2 \mu^{14} \\
& - .0004576361202 \beta_s^2 \mu^{10} - .0003283848538 \beta_s^6 \mu^{10} \\
& - .00005723619140 \alpha_s^4 \beta_s^2 \beta_c^2 \mu^6 - .0004678604054 \beta_s^6 \mu^{14} \\
& - .0005743919406 \beta_s^4 \beta_c^2 \mu^{10} - .0002716816892 \alpha_s^2 \beta_s^6 \mu^{10} \\
& - .00008915842270 \beta_s^{10} \beta_c^2 \mu^{12} - .0002061540141 \alpha_s^2 \mu^8 \\
& - .00003618135016 \beta_s^4 \mu^{16} - .0007977150501 \beta_s^6 \mu^{12} \\
& - .0001300705618 \alpha_s^2 \beta_s^6 \beta_c^2 \mu^{10} - .00008991309298 \beta_c^2 \mu^8 \\
& - .0004841928446 \beta_s^8 \mu^{14} - .0001096848001 \beta_s^2 \mu^{14} \\
& - .00002232015042 \alpha_s^4 \beta_s^4 \beta_c^2 \mu^8 - .00008926628134 \beta_s^8 \mu^{16} \\
& - .0004455145199 \beta_s^8 \mu^{12} - .00005971678502 \beta_s^8 \beta_c^2 \mu^{10} \\
& - .00007547167300 \alpha_s^2 \beta_c^2 \mu^{10} - .0004123183379 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^{10} \\
& - .5848796856 \times 10^{-5} \beta_s^{16} \beta_c^2 \mu^{16} - .0004163643770 \alpha_s^2 \beta_s^4 \mu^{10}
\end{aligned}$$

$$\begin{aligned}
& - .00005718410176 \alpha_s^4 \mu^6 - .0002980866886 \beta_s^8 \beta_c^2 \mu^{12} \\
& - .00004898551745 \alpha_s^2 \beta_s^2 \mu^{12} - .0005088803368 \beta_s^2 \beta_c^2 \mu^{12} \\
& - .0001698263803 \mu^{10} - .00006546024085 \beta_s^{10} \beta_c^2 \mu^{16} \\
& - .0001034613860 \beta_s^6 \beta_c^2 \mu^{16} - .0001571113123 \alpha_s^2 \beta_s^6 \mu^{12} \\
& - .00001072985191 \beta_s^{12} \beta_c^2 \mu^{12} - .00006051159318 \alpha_s^4 \beta_s^2 \mu^6 \\
& - .0003049778161 \beta_s^8 \beta_c^2 \mu^{14} - .0003685106952 \beta_s^2 \mu^{12} \\
& - .0001849381109 \beta_s^6 \beta_c^2 \mu^{10} - .00008122840592 \beta_s^4 \beta_c^2 \mu^8 \\
& - .0004774779793 \beta_s^4 \beta_c^2 \mu^{14} - .0001702440146 \beta_s^2 \beta_c^2 \mu^8 \\
& - .00009594551524 \beta_s^8 \beta_c^2 \mu^{16} - .0001167146195 \alpha_s^2 \beta_s^2 \mu^6 \\
& - .0004948202385 \beta_s^6 \beta_c^2 \mu^{14} - .0005611867864 \beta_s^6 \beta_c^2 \mu^{12} \\
& - .0006024101960 \beta_s^2 \beta_c^2 \mu^{10} - .00008239974204 \alpha_s^2 \beta_s^2 \beta_c^2 \mu^{12}
\end{aligned}$$



## Appendix 5

The kinetic energy of the  $n = 5/6$  less than half filled square lattice is the following.

$$\begin{aligned}
 \langle c_{4,\sigma}^\dagger c_{5,\sigma}^\dagger \rangle = & + .9598080485 \times 10^{-5} \alpha_s^4 \beta_s^5 \mu^{10} + .00001459014814 \alpha_s^4 \beta_s^2 \mu^{10} \\
 & + .3500212278 \times 10^{-5} \alpha_s^6 \beta_s^4 \mu^6 + .00009821893131 \alpha_s^2 \beta_s^4 \mu^{10} \\
 & + .00008035708779 \alpha_s^5 \beta_s \mu^8 + .00004064295705 \beta_s^3 \alpha_s \mu^{10} \\
 & + .00002708191415 \alpha_s^2 \beta_s^3 \mu^8 + .00007041379845 \alpha_s^6 \beta_s \mu^6 \\
 & + .1372170905 \times 10^{-5} \mu^{12} + .8739781111 \times 10^{-6} \mu^{14} \\
 & + .6672610146 \times 10^{-5} \alpha_s \beta_s^6 \mu^{10} + .00002081435569 \alpha_s^2 \beta_s^6 \mu^{10} \\
 & + .00001234964626 \alpha_s^7 \beta_s \mu^4 + .00001270562972 \alpha_s^4 \beta_s^2 \mu^6 \\
 & + .00002209960864 \alpha_s \beta_s^7 \mu^{12} + .00001646619505 \alpha_s^6 \beta_s \mu^4 \\
 & + .6563439628 \times 10^{-5} \alpha_s^5 \beta_s^2 \mu^6 + .0001037970164 \alpha_s^2 \beta_s^3 \mu^{10} \\
 & + .00002771324792 \alpha_s^3 \beta_s^4 \mu^8 + .00001828019583 \alpha_s^4 \beta_s^3 \mu^8 \\
 & + .00002075443577 \alpha_s^4 \beta_s \mu^6 + .8925094273 \times 10^{-5} \alpha_s^4 \beta_s^2 \mu^8 \\
 & + .00002777900811 \alpha_s \beta_s \mu^{12} + .00001303814526 \alpha_s^4 \beta_s \mu^{10} \\
 & + .00006810414422 \alpha_s \beta_s^3 \mu^{12} + .00001364020560 \alpha_s \beta_s \mu^{10} \\
 & + .00003422641480 \alpha_s^5 \beta_s^4 \mu^8 + .00005569117351 \alpha_s^2 \beta_s^5 \mu^{10} \\
 & + .00002680238454 \alpha_s^2 \beta_s^2 \mu^8 + .00003734877592 \alpha_s \beta_s^6 \mu^{12} \\
 & + .00004574987479 \alpha_s^5 \beta_s^3 \mu^8 + .4902733482 \times 10^{-5} \alpha_s^9 \mu^2
 \end{aligned}$$

$$\begin{aligned}
& + .8759259317 \times 10^{-5} \alpha_s^4 \mu^8 + .5322102329 \times 10^{-5} \beta_s^8 \mu^{14} \\
& + .9938668161 \times 10^{-5} \alpha_s^8 \mu^6 + .7572527460 \times 10^{-5} \beta_s^3 \mu^{12} \\
& + .00001130200349 \alpha_s^3 \mu^6 + .4902733482 \times 10^{-5} \alpha_s^{10} \mu^2 \\
& + .00001118855849 \alpha_s^9 \mu^4 + .00002275057254 \alpha_s^2 \mu^8 \\
& + .4682454674 \times 10^{-5} \beta_s^2 \mu^{14} + .00001271527305 \beta_s^5 \mu^{14} \\
& + .1389479885 \times 10^{-5} \beta_s^9 \mu^{14} + .00002577393099 \alpha_s^2 \mu^{10} \\
& + .00003819943924 \alpha_s^6 \mu^6 + .00001130200349 \alpha_s^4 \mu^6 \\
& + .8296495031 \times 10^{-5} \beta_s^5 \mu^{12} + .00002992672236 \alpha_s^5 \mu^6 \\
& + .00001655021929 \alpha_s^7 \mu^4 + .00001655021929 \alpha_s^6 \mu^4 \\
& + .7495397174 \times 10^{-5} \alpha_s^8 \mu^4 + .7571312361 \times 10^{-5} \alpha_s^4 \mu^{10} \\
& + .1624485551 \times 10^{-5} \beta_s^4 \mu^{12} + .8760151029 \times 10^{-5} \alpha_s \mu^{12} \\
& + .00002665223463 \alpha_s^3 \mu^8 + .00001086772197 \alpha_s \mu^{10} \\
& + .5162600645 \times 10^{-5} \beta_s^2 \mu^{12} + .00001082625312 \beta_s^3 \mu^{14} \\
& + .7820167203 \times 10^{-5} \beta_s^6 \mu^{12} + .00001271196483 \beta_s^7 \mu^{14} \\
& + .00001607673749 \beta_s^6 \mu^{14} + .00003535102436 \alpha_s^5 \mu^8 \\
& + .1909556000 \times 10^{-5} \beta_s \mu^{14} + .00001256690516 \beta_s^4 \mu^{14} \\
& + .00001918736648 \alpha_s^6 \beta_s^3 \mu^6 + .3375067483 \times 10^{-5} \alpha_s^2 \beta_s^7 \mu^{10} \\
& + .5787484529 \times 10^{-5} \alpha_s^4 \beta_s^3 \mu^6 + .00001211014501 \alpha_s^8 \beta_s \mu^6 \\
& + .00008215483522 \alpha_s^3 \beta_s^2 \mu^8 + .00002347854186 \alpha_s^5 \beta_s \mu^6 \\
& + .9838405846 \times 10^{-5} \alpha_s^3 \beta_s^5 \mu^8 + .00003738506270 \alpha_s^6 \beta_s^2 \mu^6
\end{aligned}$$

$$\begin{aligned}
& + .6895105909 \times 10^{-5} \alpha_s \beta_s^5 \mu^{10} + .00003954751948 \alpha_s \beta_s^2 \mu^{12} \\
& + .4784568368 \times 10^{-5} \alpha_s^5 \beta_s^5 \mu^8 + .00005776743117 \alpha_s \beta_s^5 \mu^{12} \\
& + .00008669893029 \alpha_s \beta_s^4 \mu^{12} + .00004742603276 \alpha_s^2 \beta_s \mu^8 \\
& + .3471680221 \times 10^{-5} \alpha_s^8 \beta_s^2 \mu^6 + .00001954612379 \alpha_s^2 \beta_s^4 \mu^8 \\
& + .4116548789 \times 10^{-5} \alpha_s^7 \beta_s^2 \mu^4 + .4164084149 \times 10^{-5} \alpha_s \beta_s^8 \mu^{12} \\
& + .00001819798250 \beta_s^2 \alpha_s \mu^{10} + .00002777655251 \alpha_s^4 \beta_s^4 \mu^{10} \\
& + .0001110634110 \alpha_s^2 \beta_s^2 \mu^{10} + .00001383629053 \alpha_s^5 \beta_s^3 \mu^6 \\
& + .00009151806080 \alpha_s^2 \beta_s \mu^{10} + .00002585288648 \beta_s^4 \alpha_s \mu^{10} \\
& + .00001157496896 \alpha_s^3 \beta_s^2 \mu^6 + .00002869404322 \alpha_s^4 \beta_s^3 \mu^{10} \\
& + .00001148890434 \alpha_s^9 \beta_s \mu^4 + .1794824598 \times 10^{-5} \alpha_s^4 \beta_s^6 \mu^{10} \\
& + .00005420510969 \alpha_s^3 \beta_s^3 \mu^8 + .00005384417188 \alpha_s^5 \beta_s^2 \mu^8 \\
& + .00007930173044 \alpha_s^3 \beta_s \mu^8 + .00002767258106 \alpha_s^3 \beta_s \mu^6
\end{aligned}$$

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