Quantum spin structures and phase separation in the Hubbard model

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Quantum Spin Structures 
and Phase Separation in the 
Hubbard model

by

Zahid Bin Asghar

A Doctoral Thesis
submitted in partial fulfilment of the requirements
for the award of the degree
Doctor of Philosophy
of
Loughborough University

Supervisors: Prof. A. S. Alexandrov and Dr. J.H. Samson

July 2001

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A POEM FOR MY PARENTS

When I was speechless, you were my voice.
When I was weak, you were my strength.

You held my hand at every difficulty.
You poured oceans of love, and gave mountains of compassion
And affection unsurpassed.
You continue to be my light at every turn of my life.

May God bless you, for I can never thank you enough.

Your Son Zahid.
DEDICATION

I dedicate this thesis to my parents for supporting, guiding, encouraging and inspiring me, and to my special sisters Safina Kauser and Rabina Asghar for their unfailing support and encouragement. I hope Safina will also accomplish her task, and become a great fashion designer.
ACKNOWLEDGMENTS

I would like to thank everyone in the Physics department for making my study here in Loughborough so enjoyable. I thank my supervisors Dr. John H Samson and Prof. Sasha Alexandrov for being there whenever I needed them and my Director of research Dr Klaus Neumann, Mrs Maureen McKenzie, Debbie and Denise. I express my sincere gratitude to Prof. Feodore Kusmartsev.
ABSTRACT

In this thesis we focus on a systematic study of the ground state of the one-dimensional one-band Hubbard model in the Hartree-Fock approximation. Phases with non-uniform charge density and states with coexisting phases separated by a domain wall are included in the study. We calculate the full Hartree-Fock phase diagram for uniform and non-uniform phases, and we show that at particular electron densities the uniform phase is unstable to phase separation.

Supercell calculations are carried out, and we use the computational minimisation procedure to calculate the Hartree-Fock energies for the self-consistent spin configurations.
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Introduction

In our endless quest to seek knowledge, to improve our understanding of the creation around us. Man is ever searching for clues and explanations to give insight to some very strange phenomena. Certainly Condensed Matter Physics represents such challenges to us, even the most commonly observed effects such as magnetism can allude the consciousness of direct explanation. Science over the centuries, has crossed many difficult bridges none more so than recent development of subjects like Quantum Mechanics.

We seek to know how and why such peculiarities of nature take place, and under what conditions they are most likely to occur.

Indeed, quantum mechanics provides answers to many of the fundamental questions of condensed matter physics. However it would be true to say that there are very few exact solutions, the simple reason being that we are dealing with large number of interacting particles, whence there is hardly a single worthwhile problem with realistic interactions which can be solved precisely. One has to make do with approximate solutions, which either contain the essential features of the whole problem or, at least contain within themselves a criterion of validity.

So it should come as no surprise then, that we will be using approximate physical theory in this thesis, Hartree-Fock approximation on the one dimensional Hubbard Model, based on skilled intuition and powerful use of mathematical techniques will provide more conceptual insight than the exact numerical solutions. Hartree-Fock approximation has come a long way since Hartree’s first proposal of his famous self-consistent field method, in which every electron in an atom is given its own personal wave function and energy level. The whole construct of atomic theory, molecular physics, nuclear shell structure and of course condensed matter theory has essentially been erected on this basis.
In this thesis I will endeavour to unravel another small piece in the infinite jigsaw of the universe, it is through the eyes of science that one is humbled to the very magnificence of nature.

Chapter 1 gives an outline of an idealised theory of solids relevant to the thesis. In Chapter 2 we look into Hartree-Fock solutions for the one-dimensional Hubbard model. In Chapter 3 we give a review of other theories of interacting fermions systems with the emphasis on real systems. Research done on the bipolaronic superconductivity with Prof. Alexanrov is presented in Chapter 4.

One-dimensional systems and their relevance to current research is elucidated in Chapter 5. Differences between 1D and 3D fermionic systems are also highlighted. In Chapter 6 the computational procedure which minimises the energy of the Hubbard Hamiltonian using the Hartree-Fock approximation is introduced. The main results of this thesis are reported in Chapter 7, and we conclude with Chapter 8.
Chapter 1

Development of an idealised Theory of Solids

1.1 Periodic potential

In typical solids, atoms are a few angstroms apart [3][4][5]. Consider the simplest of materials such as monovalent atoms, where the outer electron is seen as delocalised from the inner electrons. The positive ions thus left behind give rise to a periodic potential. For real solids many physical effects will change the potential in such a way that it does not remain totally periodic. However, in an idealised theory all such effects have to be appropriately ruled out, but may be brought back later, as we will show. Assumptions about our ideal solid:

1) The ions are rigid and fixed in position such that the ions do not change their polarisation if an electron approaches close to them, and thermal vibrations are neglected.

2) No chemical impurities or physical defects are present.

3) The surface effects are neglected.

With no danger of over simplification, the essence of the physics should be contained within our model. This approach allows one to consider a simple problem of the motion of a single electron in a rigid periodic potential. Furthermore, it gives insight to N electrons in this potential.
1.2 **Periodic Boundary Conditions**

For simplicity, we assume that the crystal under investigation is in the form of parallelepiped of sides \( N_i a_i (i = 1,2,3) \), where the \( N_i \) are integers and the \( a_i \) are the primitive translations. The crystal then contains \( N = N_1 N_2 N_3 \) unit cells. The surface states of the crystal are obviously different from those of the bulk material, and cannot be readily neglected unless we make a further assumption of periodic boundary conditions. These conditions imply that our finite crystal being studied behaves exactly as if it were part of an infinite crystal. One can then assume that all the crystal properties are satisfied by the relation:

\[
f(r + N_j a_j) = f(r)
\]  

(1)

Clearly this represents the periodic boundary condition. As \( N_j \to \infty \) we obtain the infinite crystal; for large \( N_j \) the above assumption is unlikely to affect the theory of bulk properties of the crystal.

1.3 **Bloch's theorem**

Let \( R \) be a typical lattice vector in the direct lattice, and \( T(R) \) be translation operator defined by

\[
T(R) f(r_1, r_2, ...) = f(r_1 + R, r_2 + R, ...)
\]

where \( f \) is an arbitrary function. We may apply it to express the invariance of the Hamiltonian under lattice translation.

\[
T(R)H = HT(R) \quad \forall \text{ lattice vector } R.
\]  

(2)

Which implies that all \( T(R) \) and \( H \) commute, hence they have common eigenfunctions. If we let \( \psi_l(r_1, ..., r_n) \) be one of these eigenfunctions, where \( l \) stands for a set of quantum numbers, then
Chapter 1 Development of an idealised Theory of Solids

\[ T(R)\psi_i (r_1, \ldots, r_n) = \lambda_i (R) \psi_i (r_1, \ldots, r_n). \quad (3) \]

\[ \lambda_i (R) \] are eigenvalues of \( T(R) \) independent of \( r_i \) we have from above

\[ |\psi_i (r_1 + R, \ldots)|^2 = |\lambda_i (R)|^2 |\psi_i (r_1, \ldots, r_n)|^2. \quad (4) \]

This follows from (3) without further assumptions.

Integrating over \( n \) electron coordinates, and using the fact that \( n \)-particle functions are normalised, one finds that \( |\lambda_i|^2 = 1 \). That is satisfied by \( \lambda_i (R) = e^{ik \cdot R} \). We can now write down Bloch’s theorem as follows:

\[ \psi_i (r_1 + R, \ldots, r_n + R) = e^{ik \cdot R} \psi_i (r_1, \ldots, r_n). \quad (5) \]

With the above theorems and assumptions we have some of the necessary tools to investigate our problem in this thesis, but before we proceed to such a intrepid task, we must turn our attention to the Hubbard model [1]. It was originally proposed by Hubbard, Gutzwiller [2] and Kanamori [8] in the early 1960s to model the correlation between \( d \)-electrons in the narrow band shells of transition elements. They made two fundamental approximations that these shells are so much smaller than the inter-atomic spacing that one may neglect \( d \)-electronic interactions other than those between two electrons in an orbital around the same atom, and that the interactions of other orbitals can be adequately described by mean-field methods.

Another way of looking at it is to consider the electron charge density in a \( d \)-band. It is concentrated near the atomic nuclei and is sparse between them; this localisation of the wavefunction in real-space affects the nature of the correlations. Typically the electrons on the same atom may become strongly correlated with each other but will only be weakly correlated with electrons on different atoms. Indeed, it is this very precise nature of the narrow band correlations which sets them apart from the free-electron gas.
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1.4 Hubbard Model

The generic model to describe the correlated electron problem is the Hubbard model [1]. It is the simplest model to analyse many body aspects of the electronic properties of condensed matter. All complexities of atomic physics and the corresponding multiband description of condensed matter have been stripped away until all that remains is a stark competition between chemical bonding and Coulomb repulsion. These two are the direct dominant forces that dictate the behaviour of the mobile electrons.

Due to screening of the Coulomb potential, it is assumed negligible for distant sites, as mentioned earlier. The Hubbard model is thus suitable for a short-range interaction. It is directly based on the tight-binding model in the presence of Coulomb repulsion $U$ that acts only between two neighbouring electrons. Electrons are said to be neighbours only if they are sitting close to one another on the lattice, with no other electron in between the two.

On quite general grounds, starting from a Hamiltonian for $N$ particles,

$$H = \sum_i h(r_i) + \frac{1}{2} \sum_{i \neq j} v(r_i - r_j)$$  \hspace{1cm} (6)

where the sums run from 1 to $N$, and $r_i$ labels the position of the $i$-th electron, $h(r_i)$ is the ‘one particle’ part of the Hamiltonian. It contains the kinetic energy plus all the interactions with external potentials, while $v(r_i - r_j)$ represents the electron-electron two-body interaction.
One of the best ways of representing the above Hamiltonian is by the use of Wannier functions; these functions provide a set of orthonormal basis. By implementing symmetry arguments to the problem and taking advantage of the fact that the one-particle part of the Hamiltonian is represented by non-interacting electrons, one can use Bloch's theorem readily. Bloch functions appropriate to the description of the band structure of a solid are

\[ \psi_{nk} = \exp[i\mathbf{k} \cdot \mathbf{r}] \gamma_{nk}(\mathbf{r}), \quad (7) \]

where \( n \) is a band index, \( \mathbf{k} \) runs over the first Brillouin zone, and \( \gamma_{nk}(\mathbf{r}) \) has the periodicity of the lattice:

\[ \gamma_{nk}(\mathbf{r} + \mathbf{R}) = \gamma_{nk}(\mathbf{r}). \quad (8) \]

\( \mathbf{R} \) is any lattice vector. For a lattice with \( M \) sites, the Wannier functions \( \phi_{ni}(\mathbf{r}) \) are defined via the transformation:

\[ \phi_{ni} = \frac{1}{\sqrt{M}} \sum_{\mathbf{k}} \exp[-i\mathbf{k} \cdot \mathbf{R}_i] \psi_{nk}(\mathbf{r}) \quad (9) \]

Where the index \( (i) \) labels the lattice site connected to the origin by the lattice vector \( \mathbf{R}_i \).

Using equations (3,4) we can easily obtain the relation

\[ \phi_{n0}(\mathbf{r} - \mathbf{R}_i) = \phi_{ni}(\mathbf{r}). \quad (10) \]
One can define Wannier functions for each band. Wannier functions form an orthonormal basis of single-particle functions:

\[ \sum_{ni} \phi_{ni}(r) \phi^\dagger_{ni}(r') = \delta(r - r'); \]
\[ \langle \phi_{ni} | \phi_{mj} \rangle = \delta_{nm} \delta_{ij} \] (11)

Our objectives are to diagonalise the Hamiltonian, by the use of the above formalism, and represent it in the second quantised form. Second quantisation simply allows one to compare the Hamiltonian (6) with a non-interacting ideal gas Hamiltonian, properties of which are widely known.

We need only to consider one single band, for which just one Wannier function suffices. \( \phi_0(r) \) is centred at the origin, the other given by (10):

\[ \phi_j(r) = \phi_0(r - R_j) \] (12)

The Wannier function \( \phi_0(r) \) is to some extent localised on the site, and subsequently take their largest value there, unlike the Bloch functions which are generally delocalised. Applying creation and annihilation operators \( c_j^\dagger \sigma \) and \( c_j \sigma \) respectively
for electrons in state $\phi_j(r)$ and spin $\sigma$ ($\sigma = \uparrow$ or $\downarrow$), with this prescription the initial Hamiltonian may be rewritten in the second quantisation formalism thus:

$$H = -\sum_{ij} t_{ij} c_i^\dagger c_j + \frac{1}{2} \sum_{ijkl} \langle ij|v|kl \rangle c_i^\dagger c_j^\dagger c_k c_l$$

where:

$$t_{ij} = t(R_i - R_j) = -\int dr \phi_i^*(r) h(r) \phi_j(r) = t_{ij}^*$$

$$\langle ij|v|kl \rangle = \int dr dr' \phi_i^*(r) \phi_j^*(r') v(r - r') \phi_k(r') \phi_l(r)$$

Both $h$ and $v$ have been assumed to be spin-independent. Energies are set in such a way that $t_{ii} = t(0) = 0$.

Furthermore certain approximations can be made, which retain the essential physics of strongly correlated electrons, but are necessary in order to simplify the mathematics. To that end it is assumed that $t_{ij} = t(R_i - R_j)$ decays rapidly with distance, hence the only matrix elements worth retaining are the nearest neighbour sites. Indeed for isotropic systems one can approximate $t_{ij} as:

$$t_{ij} = \begin{cases} t & \text{for (i, j) nearest neighbours ('n.n')} \\ 0 & \text{otherwise} \end{cases}$$

The electron-electron Coulomb interaction is assumed to be effectively screened when electrons are far apart. The dominant contribution to the second term of the Hamiltonian is when the two electrons are on the same site ($i = j = k = l$)
Chapter 1 Development of an idealised Theory of Solids

\[ \langle ij|v|kl \rangle = \begin{cases} U & \text{if } i = j = k = l \\ 0 & \text{otherwise} \end{cases} \quad (17) \]

Atomically speaking the ionisation $E_i$ energy is defined as the energy that must be supplied in order to remove an electron from a neutral atom, and the electron affinity $E_A$ is the energy that is gained when an additional electron is added to a neutral atom. So the coulomb energy may be thought of as $U = E_A - E_i$.

Pauli principle demands that when two electrons are on the same site their spins must be aligned oppositely: $\sigma' = -\sigma = \overline{\sigma}$. Through such a path one eventually arrives at the simplest one-band Hubbard Hamiltonian:

\[
H = - \sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + h.c. + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (18)
\]

where $\hat{n}_{i\sigma} \equiv c_{i\sigma}^\dagger c_{i\sigma}$, the sums run over lattice sites, the symbol $\langle ij \rangle$ indicates a sum over nearest-neighbour pairs, the usual convention applies that the sums are made over ordered nearest-neighbour pairs, so that the pairs are only counted once, and h.c. is the Hermitian Conjugate. Under this convention, the summand will be symmetrical under the interchange $i \Leftrightarrow j$. The electron creation and annihilation operators $c_{i\sigma}$, $c_{i\sigma}^\dagger$ being fermionic in nature satisfy the following anticommutation rules:

\[
\left[ c_{i\sigma}, c_{j\sigma'}^\dagger \right] = \delta_{\sigma\sigma'} \delta_{ij} \quad (19)
\]

where

\[
\left[ c_{i\sigma}, c_{j\sigma'} \right] = 0, \quad \left[ c_{i\sigma}^\dagger, c_{j\sigma'}^\dagger \right] = 0
\]

These anticommutation relations ensure that no more than one particle can be in any given state, thus enforcing Pauli exclusion principle.
1.5 Simple Examples

Taking the limiting cases one obtains a soluble Hamiltonian namely:

• limits $t \rightarrow 0$ and $U \rightarrow 0$

i) $U \rightarrow 0$.

This is usual tight binding model for a single band

$$H = - \sum_{\langle ij \rangle \sigma} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + h.c.$$ 

As the Hamiltonian stands it is not diagonal. The diagonalisation procedure is to simply revert from Wannier states to Bloch waves. This is merely performing Fourier transforms of type below:

$$c_{i\sigma} = \frac{1}{\sqrt{M}} \sum_{k} \exp[i k \cdot R_i] c_{k\sigma} \quad -\frac{\pi}{a} \leq k \leq \frac{\pi}{a} \quad \text{(First Brillouin Zone)}$$

$$H = - \sum_{\langle ij \rangle \sigma} \frac{1}{M} \sum_{kk'} \exp[-i k \cdot R_i] \exp[i k' \cdot R_j] c_{k\sigma}^\dagger c_{k'\sigma} + h.c.$$ 

$$H = - \frac{t}{M} \sum_{\langle ij \rangle \sigma} \sum_{kk'} \exp[-i k \cdot R_i] \exp[i k' \cdot (R_{i+1})] c_{k\sigma}^\dagger c_{k'\sigma} + h.c.$$ 

After applying symmetry conditions we arrive at our final Hamiltonian

$$H = - \frac{t}{M} \sum_{kk' \sigma} M \delta_{kk'} \exp[i k a] c_{k\sigma}^\dagger c_{k'\sigma} + h.c.$$
more conveniently written as

$$H = \sum_{k\sigma} E(k)c_{k\sigma}^{\dagger}c_{k\sigma}$$

$$E(k) = -2t\cos(ka)$$ with lattice spacing $a$.

The effect of adding further hopping integrals between first, second and third neighbour merely produces more structure in the energy dispersion relation.

$$E(k) = -2t\cos(ka) - 2t'\cos(2ka) - 2t''\cos(3ka).$$

Figure 2. Energy dispersion $E(k)$.

Figure 3. Modification of the $E(k)$ by the hopping terms.

$E(k) = -2t\cos(ka) - 2t'\cos(2ka) - 2t''\cos(3ka)$. 

$t' = t'' = \frac{1}{2}t$
ii) $t \to 0$

The atoms that constitute the lattice are so far apart that the hopping $t$ is negligible. In this limit the Hamiltonian is trivially diagonal.

$$H = \sum_i U n_i^\uparrow n_i^\downarrow$$ (22)

Its eigenvectors are thus,

$$|n_0^\uparrow, n_0^\downarrow, \ldots, n_N^\uparrow, n_N^\downarrow\rangle$$

where $n_{i\sigma} = 0$ or $1$ with corresponding eigenvalues, given by

$$E = \sum_i \epsilon_i$$ (23)

where

$$\epsilon_i = Un_i^\uparrow n_i^\downarrow = \begin{cases} 0 & \text{Whether a site is unoccupied or singly occupied.} \\ U & \text{When a site is doubly occupied.} \end{cases}$$

Comparing this with the simple notion of atoms, one can see that $U = E_r - E_A$. Thus for $N$ electrons and $N$ atoms, the allowed energies are,

$$E = E_0, E_0 + U, E_0 + 2U \ldots$$

where $E_0 = N\epsilon_0 = 0$ is the lowest energy with all atoms singly occupied.
1.6 Variational Methods

To show that variational methods [7] at best provide an upper bound on the ground state energy we need to calculate the expectation value of the Hamiltonian for a general wavefunction $\psi$,

$$\langle H \rangle = \frac{\int \psi^* \hat{H} \psi \, d\tau}{\int \psi^* \psi \, d\tau} \quad (24)$$

where $\psi = \sum_n a_n u_n$

$$\int \psi^* \hat{H} \psi \, d\tau = \int (\sum_n a_n^* u_n^*) \hat{H} (\sum_m a_m u_m) \, d\tau$$

$$= \sum_{nm} a_n^* a_m \int u_n^* \hat{H} u_m \, d\tau$$

$$= \sum_{nm} a_n^* a_m E_m \delta_{nm}$$

hence

$$\int \psi^* \hat{H} \psi \, d\tau = \sum_n |a_n|^2 E_n \quad (25)$$

If $E_0$ is the ground state then obviously it has to be smaller than all the other $E_n$ s, which means that

$$\int \psi^* \hat{H} \psi \, d\tau \geq E_0 \sum_n |a_n|^2 \quad (26)$$

The denominator of Equation (24) is

$$\int \psi^* \psi \, d\tau = \sum_n |a_n|^2$$

thus we have proof that

$$\langle H \rangle \geq E_0 \quad (27)$$
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1.7 Hartree-Fock Variational Approach

The Hartree scheme [4] is to take the wave function of the system as a product of \( N \) one-electron functions, and then the one-electron problem is solved by supposing the electron to move in the average potential due to all the other electrons. This scheme takes into account some electron-electron interactions. Hartree-Fock (HF) method is an improvement of the Hartree scheme in that it uses antisymmetrised products of one-electron functions otherwise known as Slater determinant, in effect taking account of the Pauli principle.

1.8 The Hartree-Fock Approximation

Adding an external potential to Hamiltonian (6),

\[
H = \sum_{i=1}^{N_a} (t_i + u_i) + \frac{1}{2} \sum_{i,j=1 \atop i \neq j}^{N_a} v_{ij} \tag{28}
\]

Where \( t_i \) is the kinetic energy of the system, \( u_i \) is the external potential, \( N_a \) is the number of electrons, and \( v_{ij} \) is the particle-particle interaction term which depends on the relative positions of the particles. If one assumes the potential to be local in the \( x \)-representation then the above equation (28) becomes

\[
H = \sum_{i=1}^{N_e} \left[ -\frac{\hbar^2}{2m} \nabla_i^2 + u(x_i) \right] + \frac{1}{2} \sum_{i,j=1 \atop i \neq j}^{N_e} v(x_i - x_j) \tag{29}
\]

Our objective is to approximate the two-particle operator by an effective single-particle potential.
Chapter 1 Development of an idealised Theory of Solids

\[ H_{HF} = \sum_{i=1}^{N} h_{HF} = \sum_{i=1}^{N} (t_i + V_{HF}^{(i)}) \]

(30)

where \( V_{HF}^{(i)} \) is the effective single particle potential called the Hartree-Fock potential. One can now apply \( H_{HF} \) to the usual eigenvalue equation

\[ H_{HF} \Phi = E \Phi \]

The eigenfunctions are then simply Slater determinants

\[ \Phi(\ldots, \varphi_i, \ldots) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \varphi_1(x_1) & \cdots & \varphi_1(x_N) \\ \vdots & \ddots & \vdots \\ \varphi_N(x_1) & \cdots & \varphi_N(x_N) \end{vmatrix} = \frac{1}{\sqrt{N!}} \det[\varphi_i(x_j)] \]

(31)

The single particle orbitals \( \varphi_i \) are formally obtained from the eigenvalue equation

\[ h_{HF} \varphi_i = \tilde{E} \varphi_i. \]

(32)

The above equation is fruitless as long as we have no knowledge of the Hartree-Fock potential. One has to make the ansatz of a Slater determinant of single-particle orbitals for the exact many-body wavefunction in order to determine the single-particle orbitals. By minimising the total energy of the system with respect to the single-particle orbitals we will be able to obtain the Hartree-Fock equation for these orbitals.

Applying Ritz' variational theorem [6] to the expectation value of the exact Hamiltonian in a Slater determinant of single-particle orbitals:

\[ \frac{\delta}{\delta q_{\alpha}(x)} \left[ \langle \Phi | \hat{H} | \Phi \rangle - \sum_{i=1}^{N_i} \epsilon_i \int dy \varphi_i(y) \varphi_i^*(y) \right] = 0 \]
The Lagrangian multipliers $\epsilon_i$ above arise from the constraint that the single-particle orbitals have to be normalised.

$$\langle \Phi | H | \Phi \rangle = \sum_{i=1}^{N_v} \langle i | \hat{p} | i \rangle + \frac{1}{2} \left( \sum_{i,j=1}^{N_v} \langle ij | \hat{V} | ij \rangle - \sum_{i,j=1}^{N_v} \langle ij | \hat{V} | ji \rangle \right)$$

Performing the variation explicitly, equation (33) becomes

$$\frac{\delta}{\delta \varphi^{*}_\alpha (x)} \left\{ \sum_{i=1}^{N_v} \int dy \varphi^{*}_i (y) \left[ -\frac{\hbar^2}{2m} \nabla^2 + u(y) \right] \varphi(y) + \frac{1}{2} \sum_{i,j=1}^{N_v} \iint dy dy' \varphi^{*}_i (y) \varphi^{*}_j (y') \nu (y-y') \varphi_i (y) \varphi_j (y') - \frac{1}{2} \sum_{i,j=1}^{N_v} \iint dy dy' \varphi^{*}_i (y) \varphi^{*}_j (y') \nu (y-y') \varphi_j (y) \varphi_i (y') \right. \\
\left. - \sum_i \epsilon_i \int dy \varphi^{*}_i (y) \varphi_i (y) \right\} = 0$$

$$= \left[ -\frac{\hbar^2}{2m} \nabla^2 + u(x) \right] \varphi_\alpha (x) + \frac{1}{2} \sum_{j=1}^{N_v} \int dy' \varphi^{*}_j (y') \nu (x-y') \varphi_\alpha (x) \varphi_j (y') + \frac{1}{2} \sum_{i=1}^{N_v} \int dy \varphi^{*}_i (y) \nu (y-x) \varphi_\alpha (y) \varphi_i (x) - \frac{1}{2} \sum_{i=1}^{N_v} \int dy \varphi^{*}_i (y) \nu (y-x) \varphi_\alpha (y) \varphi_i (x) - \epsilon_\alpha \varphi_\alpha (x).$$
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We see that 2\textsuperscript{nd} and 3\textsuperscript{rd} terms are equal, and the 4\textsuperscript{th} and 5\textsuperscript{th} terms are equal. By defining the density and the density matrix we can simplify the result further.

\[ \rho(y) = \sum_{i=1}^{N} \phi_i^*(y) \phi_i(y) \quad \text{and} \quad \rho(x, y) = \sum_{i=1}^{N} \phi_i^*(y) \phi_i(x) \]

Finally we arrive at the Hartree-Fock equation

\[
\left[ -\frac{\hbar^2}{2m} \nabla^2 + u(x) + \int dy \rho(y) v(x-y) \right] \phi_\alpha(x) - \int \rho(x, y) v(x-y) \phi_\alpha(y) dy = \varepsilon_\alpha \phi_\alpha(x). \tag{35}
\]

For optimal effective single-particle potential we learn from above equation (35) that \(v_{HF}\) should act thus on the single-particle orbitals:

\[ v_{HF} \phi_i = u(x) \phi_i(x) + \int \rho(y) v(x-y) \phi_i(x) dy - \int \rho(x, y) v(x-y) \phi_i(x) dy \]

The Lagrangian parameter \(\varepsilon_\alpha\) in equation (35) must be real, and the eigenfunctions \(\phi_\alpha\) must be orthogonal.

1.9 Self-consistent procedure

Clearly one cannot solve the Hartree-Fock equation like a normal eigenvalue problem, instead we have to turn to the self-consistent procedure. The procedure starts with

1) an initial approximation \(\phi_i(x), i = 1, ..., N\)

2) the Hartree-Fock potential \(v_{HF}\) is calculated from the density matrix

\[ \rho(x, y) = \sum_{i=1}^{N} \phi_i^*(y) \phi_i(x) \]
3) once $v_{HF}$ is found, it is used to calculate the eigenvalue equation

$$(t + v_{HF})\varphi_\alpha = \varepsilon_\alpha \varphi_\alpha.$$ 

4) Select N orbitals $\varphi^{(new)}_\alpha$ with the lowest eigenvalues $\varepsilon_\alpha$.

The last step has to be performed since there are infinitely many solutions to the eigenvalue equation. Once these orbitals have been found one simply repeats the process again until this iterative scheme achieves self-consistency, that is the procedure converges so that the new orbitals obtained in the last step (4) are the same as the ones used in previous step (1).

Assuming that we eventually solve our Hartree-Fock equation for a single-particle problem, one can then obtain the Hartree-Fock approximation of the total energy of the system by inserting the Slater determinants of the occupied orbitals in equation (34).

$$E_{HF} = \langle \Phi | H | \Phi \rangle = \sum_{i=1}^{N} \langle i | H | i \rangle + \frac{1}{2} \left( \sum_{i,j=1}^{N} \langle ij | v | ij \rangle - \sum_{i,j=1}^{N} \langle ij | v | ji \rangle \right). \tag{36}$$
1.10 References


Chapter 2

Development of Hartree-Fock solutions to the 1D Hubbard model for calculation and comparison with recent results.

2 Hartree-Fock Solutions to 1D Hubbard Model

2.1 Spin Structures in the Hubbard model

Spin ordered states arise quite generally in many systems such as Heisenberg antiferromagnets [1], and in the ground state of any classical Heisenberg model, at least with unfrustrated interactions, as well as itinerant antiferromagnets [2]. Figure 1 shows some spin configurations that we will be studying in this thesis.

a) Spin Density Wave

An electron distribution with uniform charge density but with local spin polarisation.

b) Antiferromagnetic

c) Ferromagnetic
Figure 4. (b) and (c) are special case of a.

2.2 Hartree-Fock Hamiltonian

Take the Hubbard Hamiltonian in one dimension,

\[ H = H_0 + U \sum_{i=1}^{N} n_{i\uparrow} n_{i\downarrow}, \]

where \( n_i \) is the number operator, and

\[ H_0 = -\sum_{ij} t_{ij} c_{i\uparrow}^\dagger c_{j\uparrow} = -t \sum_{i=1}^{N} \sum_{s=\uparrow}^{\downarrow} (c_{i\uparrow}^\dagger c_{(i+1)s} + c_{is}^\dagger c_{(i-1)s}). \]

Figure 5. A linear chain
Chapter 2 Hartree-Fock Solutions to 1D Hubbard Model

Here $i$ and $j$ are site indices, $s = \uparrow, \downarrow$ is spin index and $U$ is the on-site Coulomb repulsion. We shall be considering the one-dimensional model with nearest-neighbour hopping, $t_{ij} = t$ for $|i - j| = 1$ and $t = 0$ otherwise, and arbitrary band filling ($0 < n < 2$).

$N_a$ is the number of sites, which is best taken as infinite. $c_a^\dagger$ creates an electron of spin $s \in \{\uparrow, \downarrow\}$ on site $i$. The true ground state for $U \neq 0$ will be correlated. The Hartree-Fock (HF) seeks the best (lowest-energy) uncorrelated many-electron ground state. An uncorrelated state with fixed electron number is the Slater determinant:

$$|\psi\rangle = \prod_{k=1}^{nN} c_i^\dagger |0\rangle.$$  \hspace{1cm} (3)

Where the $|0\rangle$ is the vacuum (no electrons) and $c_k^\dagger$ creates an electron in the $k$-th energy level on the non-interacting Hamiltonian:

$$H_{HF} = \sum_{k=1}^{2N} \varepsilon_k c_k^\dagger c_k$$

$$= \sum_{i=1}^{N} \sum_{j=1}^{N} \sum_{s=\uparrow, \downarrow}^{1} \sum_{t=\uparrow, \downarrow}^{1} h_{ij} c_i^\dagger c_j.$$  \hspace{1cm} (4)

$$[c_k^\dagger, c_{k'}]_s = \delta_{kk'}$$

$$[c_k^\dagger, c_{k'}^\dagger]_s = [c_k, c_{k'}]_s = 0$$  \hspace{1cm} (5)

HF solutions are correct in the limit of large orbital degeneracy. When two or more quantum states have the same value of the energy, they are then said to be degenerate; often degeneracy [2] is closely associated with the symmetry of the system. The HF wavefunction obey certain equivalence restrictions such as the orbital function for $4S\uparrow$ is the same as the orbital function $4S\downarrow$; these equivalence restrictions are direct consequences of conservation laws. Symmetry requirements are also fulfilled by the HF wavefunctions. However the unrestricted HF wavefunctions break both symmetry
Chapter 2 Hartree-Fock Solutions to 1D Hubbard Model

and equivalence requirements. The effect of broken symmetry is to take into account the electronic correlations partially [3].

The unrestricted HF approximation minimises $\langle \Phi | H | \Phi \rangle$, the expectation value of the Hubbard Hamiltonian (1) in the space of Slater determinants $|\Phi\rangle$. $|\Phi\rangle$ is the ground state of the non-interacting (HF) Hamiltonian with parameters $\Phi = \{(\phi, \theta, \Delta, w)\}$. The complete $\{(\phi, \theta, \Delta, w)\}$ set forms the Slater space. The scalar potential $w$ interacts with the electron density, and the vector magnetic field $\Delta$ interacts with the spin density, hence only $4N_a$ parameters are required. Consider a $4N_a$-parameter family of non-interacting Hamiltonians:

$$ H_{HF}(\Phi) = H_0 + \sum_i (w_i n_i - \Delta \cdot S_i) $$

(6)

The $nN_a$-electron ground state in this Hamiltonian is the Slater determinant $|\Phi\rangle$.

Where the total wavefunction of the electron system can be written in the form of an antisymmetric product of one-electron wavefunctions expressed in terms of a single determinant. The elements of the determinant are assumed orthogonal to each other.

These states are true ground states of the non-interacting many electron system in a spin- and site- dependent Hamiltonian, but are variational approximations to the ground states of the interacting Hamiltonian (1).
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with

\[ S_i = \frac{1}{2} \sum_{\mu} c_i^\dagger \sigma_{\mu} c_i \] 

where \( \sigma_{\mu} \) represents Pauli spin matrices, and

\[ n_i = \sum_{\mu} c_i^\dagger c_i . \]

In the case of the Hubbard model, the HF Hamiltonian above corresponds to non-interacting electrons moving in an on-site charge and spin dependent potential on each site. The Green function for the above tight-binding case is defined as

\[
\left[ G_{ij} \right]_{st} (E) = \langle is | (E - H_{HF})^{-1} |jt \rangle
\]  

(7)

where \( |is\rangle \) is a one-electron Wannier orbital.

\[
G_{ij} (E) = [(E - H)^{-1}]_{ij} = E^{-1} \delta_{ij} + E^{-2} H_{ij} + E^{-3} H_{ik} H_{kj} + E^{-4} H_{ik} H_{kj} H_{ij} + ... 
\]  

(8)

For spin density waves, as in fig.(1a), the tight-binding Green functions take the form

\[
G_{ij} (E) = g_{ij} (E) - \frac{1}{2} \Delta \sum_j g_{ij} (E) e_j \cdot \sigma g_{ji} (E) \\
+ w \sum_j g_{ij} (E) e_j g_{ji} (E) + ... 
\]  

(9)

where \( g_{ij} (E) \) is the tight-binding Green Function of the band Hamiltonian \( H_o \) (2).

\[
G = (E - H)^{-1} = \sum_n (E - E_n)^{-1} |n\rangle \langle n| 
\]  

(10)

\[
(E - E_n)^{-1} = P(E - E_n)^{-1} - i\pi \delta(E - E_n) 
\]  

(11)

The local density of states \( n_i (E) \) on site \( i \) can easily be evaluated in terms of the imaginary Greens function.
\[
\frac{1}{\pi} \text{Im} G_{ij} = n_i(E)
\] (12)

Figure 7. Green Functions (a) \( g_{ii} \), and (b) \( G_{ii} \)

Since the HF states are torque free, that is \( \Delta_j + \Delta_{-i} \) must be parallel to \( \Delta_0 \) (or vanish) for each \( i \). This condition strongly imposes that the local Green function be parallel to the onsite exchange field.

The above condition guarantees that

\[
(e_{i-k} + e_{i+k}) \parallel e_i \quad \forall i, k
\] (13)

where the unit vector \( e_i \) are the directions of \( \Delta_i \), this is true for the spin density wave.

Samson [9] imposed a stronger restriction on the local Greens function to be parallel to the on-site exchange field. Instead of the more general tight binding Green's function given by equation (9) employed here, he considered the Green's function of the type given below,
\[ G_{ij}(E) = a_{ij}(E) + b_{ij}(E) \cdot \sigma \quad (14) \]

where \( a_{ij} \) and \( b_{ij} \) are some two by two matrices,

\[ b_u(E) \parallel \Delta_i \text{ at site } i \forall E. \]

As a direct consequence of these assumptions the configurations necessarily had to be coplanar. In our more general case these assumptions cannot be justifiably be applied, however we will consider the Green functions of the type in equation (9).

This condition is valid for the uniform one-cell case and is considered generally applicable to the non-uniform case. It ensures that the expected configurations are coplanar, implying vanishing torque on the local moments [4]. This will be tested numerically. It can be seen more clearly if one considers the following scenario.

\[ \text{Figure 8. Vectorial representation for three different spin orientations} \]

The magnetisation on site B is given by

\[ m_B = \alpha \Delta_B + \beta (\Delta_a + \Delta_c) + T \quad (15) \]

where \( T \) represents further sites, \( \alpha \) and \( \beta \) depend further on the exchange splitting \( \Delta \). However self consistency condition demands that the magnetisation on site \( i \) is,

\[ m_i = \frac{\Delta_i}{U} \quad (16) \]

which simply leads to,

\[ m_B = \frac{\beta U (m_A + m_C)}{1 - \alpha U} \quad (17) \]
Hence, it is reasonably safe to assume coplanarity, although a twist on the next nearest neighbours can not be ruled out, for spin spirals the condition
\[ \Delta_{i-1} + \Delta_{i+1} = 2\Delta_i \cos \theta \]
en ensures that there is no torque between sites.

We rewrite the interaction term for Hartree-Fock Hamiltonian (6), imposing it with the constraints implied by the tight-binding Green function (coplanar) as

\[
\sum_i (w_i I - \frac{1}{2} \Delta_i \cdot \sigma) = \sum_i \begin{pmatrix} w_i - \frac{1}{2} \Delta_{ix} & -\frac{1}{2} \Delta_{iz} + \frac{i}{2} \Delta_{iy} \\ \frac{1}{2} \Delta_{ix} - \frac{1}{2} i \Delta_{iy} & w_i + \frac{1}{2} \Delta_{iz} \end{pmatrix}
\]

We assume the spin quantisation axis to be \( z \) axis. For coplanar configurations \( \Delta_y = 0 \).

Again we take the Hubbard Hamiltonian,

\[ H = H_0 + U \sum_{i=1}^{N_\text{c}} n_{i\uparrow} n_{i\downarrow}, \]

the most general self-consistent field approximations are obtained by calculating the energy as the expectation value of \( H \), replacing the expectation value of any four-creation destruction operators by the product of two two-creation destruction operators, and minimising with respect to the state vector [5]. The way in which the factorisation is made makes the difference between Hartree and Hartree-Fock approximation.

\[ \langle n_{i\uparrow} n_{i\downarrow} \rangle \rightarrow \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle \text{ Hartree approximation.} \]

\[ \langle n_{i\uparrow} n_{i\downarrow} \rangle \rightarrow \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle - \langle c_{i\uparrow}^\dagger c_{i\downarrow} \rangle \langle c_{i\downarrow}^\dagger c_{i\uparrow} \rangle \text{ Hartree-Fock approximation.} \]

The interaction potential can be transformed into two feasible forms:
(19) and

\[
\langle n_{i\uparrow} n_{i\downarrow} \rangle = \left\langle \frac{1}{4} (n_{i\uparrow} + n_{i\downarrow})^2 - \frac{1}{4} (n_{i\uparrow} - n_{i\downarrow})^2 \right\rangle 
\]

\[
= \frac{\langle n_i \rangle \langle n_i \rangle}{4} - \langle S_z \rangle \langle S_z \rangle 
\]

and

\[
\langle n_{i\uparrow} n_{i\downarrow} \rangle = \left\langle \frac{1}{2} (n_{i\uparrow} + n_{i\downarrow}) - \frac{1}{2} (n_{i\uparrow} - n_{i\downarrow}) \right\rangle 
\]

\[
= \left\langle \frac{1}{2} (n_{i\uparrow} + n_{i\downarrow}) + S_z (n_{i\uparrow} - n_{i\downarrow}) \right\rangle, 
\]

\[
= \frac{1}{2} \langle n_i \rangle + 2 \langle S_z \rangle \langle S_z \rangle 
\]

where \( \langle n_i \rangle = \langle n_{i\uparrow} \rangle + \langle n_{i\downarrow} \rangle \) and \( \langle S_z \rangle = \frac{1}{2} (\langle n_{i\uparrow} \rangle - \langle n_{i\downarrow} \rangle) \) are the mean fields for the charge and spin respectively. Decomposition (19) contains both spin-spin and charge-charge correlations, it is also hoped that such a decomposition will give lower ground state energy. Apply the HF type factorisation to the Hubbard Hamiltonian above,

\[
H = H_0 + U \sum_i (n_{i\uparrow} - \langle n_{i\uparrow} \rangle)(n_{i\downarrow} - \langle n_{i\downarrow} \rangle) + U \sum_i \langle n_{i\uparrow} \rangle n_{i\downarrow} + \langle n_{i\downarrow} \rangle n_{i\uparrow} - U \sum_i \langle n_{i\uparrow} \rangle \langle n_{i\downarrow} \rangle. 
\]  

(21)

\[
H_{HF} = H_0 + \sum_i (w_i n_i - \Delta_i \cdot S_i) = H_0 + \sum_i ((w_i - \frac{1}{2} \Delta_i) n_{i\uparrow} + (w_i + \frac{1}{2} \Delta_i) n_{i\downarrow}) 
\]  

(22)

\[
H_{HF} = H_0 + \sum_i ((w_i - \frac{1}{2} \Delta_i) n_{i\uparrow} + (w_i + \frac{1}{2} \Delta_i) n_{i\downarrow}) 
\]

Let \( \beta_{i\uparrow} = w_i - \frac{1}{2} \Delta_i \) and \( \beta_{i\downarrow} = w_i + \frac{1}{2} \Delta_i \)

\[
H_{HF} = H_0 + \sum_i (\beta_{i\uparrow} n_{i\uparrow} + \beta_{i\downarrow} n_{i\downarrow}) 
\]  

(23)
\[ H_{HF} | \Phi \rangle = E(\Phi) | \Phi \rangle \] (24)

\[ E_{HF} = \min_{\{w, \Delta\}} \langle \Phi | H | \Phi \rangle \] (25)

We take the number of sites \( N_a \to \infty \) and work in the canonical ensemble in \( 4 N_a \) dimensional space, with a fixed number \( n \) of electrons per site. The general problem is a minimisation of a function with a large number of local minima and saddle points, dependent on boundary condition and differing little in energy. We wish to find \( | \Phi \rangle \) that minimises [9],

\[ E_{HF}(\Phi) = \min_{\Phi} \langle \Phi | H | \Phi \rangle = \min_{\Phi} \langle \Phi | H_{HF} | \Phi \rangle + \langle \Phi | \left( U \sum_{i=1}^{N_a} n_{i+} n_{i-} \right) + \Delta_i \cdot S_i - w_i n_i | \Phi \rangle \]

(26)

where \( \Phi \) parameterises the space of Slater determinants, using (25) and applying (21) to (23),

\[ E_{min} = \min_{\Phi} E_{HF}(\Phi) = \min_{\Phi} \left( \langle \Phi | H - H_{HF} | \Phi \rangle + E(\Phi) \right) \] (27)

\[ E_{min} = \min_{\Phi} \left( E(\Phi) + \sum_i U \langle \Phi | (n_{i+} - \langle n_{i+} \rangle)(n_{i-} - \langle n_{i-} \rangle) | \Phi \rangle \right) \]

\[ -\langle \Phi | (\beta_{i+} - U \langle n_{i+} \rangle) n_{i+} + (\beta_{i-} - U \langle n_{i-} \rangle) n_{i-} | \Phi \rangle + U \left( \sum_i \langle n_{i+} | n_{i-} \rangle \right) \] (28)

Taking the second term as,

\[ \sum_i (U \langle \Phi | (n_{i+} - \langle n_{i+} \rangle)(n_{i-} - \langle n_{i-} \rangle) | \Phi \rangle) \]
This is valid only for an uncorrelated state such as the Slater determinant.

\[
E_{\text{min}} = \min_{\Phi} (E(\Phi) + \frac{1}{U} \sum_i (\beta_{i\uparrow} - U\langle n_{i\uparrow} \rangle)(\beta_{i\downarrow} - U\langle n_{i\downarrow} \rangle) - \frac{1}{U} (\sum_i \beta_{i\uparrow}\beta_{i\downarrow}))
\]

(30)

where \( \langle n_{i\sigma} \rangle = \frac{1}{2} \langle n_i \rangle - \langle S_{i\sigma} \rangle \) and \( \langle n_{i\uparrow} \rangle = \frac{1}{2} \langle n_i \rangle + \langle S_{i\uparrow} \rangle \)

(31)

Finally we obtain the \( E_{\text{min}} \), which needs to be minimised for a complete range of parameters, incidentally the expression of \( E_{\text{min}} \) obtained here is similar to one calculated by Ichimura et al [6] for two dimensional Hubbard model.

\[
E_{\text{min}} = \min_{\Phi} \left( E(\Phi) + \sum_i w_i \langle n_i \rangle - \Delta_i \langle S_{i\sigma} \rangle - U \frac{\langle n_i \rangle \langle n_i \rangle}{4} - \langle S_{i\sigma} \rangle \langle S_{i\sigma} \rangle \right)
\]

(32)

The HF condition is achieved by setting:

\[
\beta_{i\uparrow} = U\langle n_{i\uparrow} \rangle
\]

\[
\beta_{i\downarrow} = U\langle n_{i\downarrow} \rangle
\]

(33a,b)

We can prove this by partially differentiating \( E(\Phi) \):

Let the susceptibilities be defined as \( \chi_{\sigma \sigma'} = \frac{\partial}{\partial \beta_{i\sigma}} \langle n_i \rangle \) and \( \chi_{\uparrow \uparrow} = \frac{\partial}{\partial \beta_{i\uparrow}} \langle n_i \rangle \)

Restating equation (30) as

\[
E_{\text{min}} = \min_{\Phi} (\langle \Phi | H_{HF} | \Phi \rangle + \frac{1}{U} \sum_i (\beta_{i\uparrow} - U\langle n_{i\uparrow} \rangle)(\beta_{i\downarrow} - U\langle n_{i\downarrow} \rangle) - \frac{1}{U} (\sum_i \beta_{i\uparrow}\beta_{i\downarrow}))
\]

(34)
\[
\frac{\partial}{\partial \beta_{iT}} E_{HF} = \min_{\Phi} (\Phi| \frac{\partial}{\partial \beta_{iT}} H_{HF} | \Phi) \\
+ \frac{1}{U} \sum_i \left[ \frac{\partial}{\partial \beta_{iT}} (\beta_{iT} - U \langle n_{i\uparrow} \rangle) \right] (\beta_{iT} - U \langle n_{i\uparrow} \rangle) + \frac{1}{U} \sum_i (\beta_{iT} - U \langle n_{i\uparrow} \rangle) \left[ \frac{\partial}{\partial \beta_{iT}} (\beta_{iT} - U \langle n_{i\uparrow} \rangle) \right] \\
- \frac{1}{U} (\sum_i \beta_{iT}) \tag{35}
\]

For minimum energy \( \frac{\partial E_{HF}}{\partial \beta_{iT}} = 0 \) and \( \frac{\partial E_{HF}}{\partial \beta_{iT}} = 0 \). \( E_{\text{min}} = E_{HF} \)

Equation (35) can be written in terms of the susceptibilities at the self-consistent state, and from equation (23),

\[
\frac{\partial}{\partial \beta_{iT}} E_{HF} = n_{iT} + \frac{1}{U} \sum_i [(1 - U \chi_{\uparrow \uparrow})](0) + \frac{1}{U} \sum_i (0)[0 - U \chi_{\uparrow \uparrow}] - \frac{1}{U} (\sum_i \beta_{iT}).
\]

\( \Rightarrow \frac{\partial E_{HF}}{\partial \beta_{iT}} = n_{iT} - \frac{1}{U} (\beta_{iT}). \tag{36} \)

similarly for the down-spin,

\[
\frac{\partial E(\Phi)}{\partial \beta_{iT}} = n_{iT} - \frac{1}{U} (\beta_{iT}). \tag{37} \]

At the self-consistent condition these derivatives must vanish, thus leading to equations (33a,b). From these relations we can directly write down the self-consistent fields below,

\[
w_i = \frac{1}{2} U \langle n_i \rangle \tag{38} \]

\[
\Delta_i = 2U \langle S_i \rangle \tag{39} \]

We have shown above that at the self-consistent state, we don’t need to worry about the susceptibilities since they are multiplied by zero. The Slater determinant \( \Phi \) is just a stationary function at the saddle point so its form does not matter.
2.3 Calculating the bandstructures

Bandstructures for the Spin Spirals

Bandstructures of the HF Hamiltonian are calculated in a standard manner. For the Spin Spiral case one takes the restricted Hamiltonian that is not translationally invariant, however under a translation by \( r \) combined with a spin rotation of \( Q \cdot r \) about the y axis it is invariant. This invariance implies that Bloch’s theorem is valid; hence the wavefunctions comply to it, such that for spin up we have,

\[
\Psi_{k\uparrow}(r) = e^{i k \cdot r} e^{-\frac{1}{2} i Q \cdot \sigma_y} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = e^{i k \cdot r} \begin{pmatrix} \cos\left(\frac{1}{2} Q \cdot r\right) - i \sigma_y \sin\left(\frac{1}{2} Q \cdot r\right) \\ 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix},
\]

(40)

\[
\Psi_{k\downarrow}(r) = e^{i k \cdot r} \begin{pmatrix} \cos\left(\frac{1}{2} Q \cdot r\right) & -\sin\left(\frac{1}{2} Q \cdot r\right) \\ \sin\left(\frac{1}{2} Q \cdot r\right) & \cos\left(\frac{1}{2} Q \cdot r\right) \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = e^{i k \cdot r} \begin{pmatrix} \cos\left(\frac{1}{2} Q \cdot r\right) \\ \sin\left(\frac{1}{2} Q \cdot r\right) \end{pmatrix}
\]

(41)

and similarly for spin down,

\[
\Psi_{k\downarrow}(r) = e^{i k \cdot r} e^{-\frac{1}{2} i Q \cdot \sigma_y} \begin{pmatrix} 0 \\ 1 \end{pmatrix} = e^{i k \cdot r} \begin{pmatrix} -\sin\left(\frac{1}{2} Q \cdot r\right) \\ \cos\left(\frac{1}{2} Q \cdot r\right) \end{pmatrix}
\]

(42)
These wavefunctions are the eigenfunctions of the HF Hamiltonian in (6). The hopping matrix couples $\Psi_{k\uparrow}$ and $\Psi_{k\downarrow}$. Taking the cell size as 1, we can employ these wavefunctions in Hamiltonian (43) to calculate the energies.

$$H_{HF} \begin{pmatrix} \Psi_{k\uparrow}(r) \\ \Psi_{k\downarrow}(r) \end{pmatrix} = E \begin{pmatrix} \Psi_{k\uparrow}(r) \\ \Psi_{k\downarrow}(r) \end{pmatrix} \tag{43}$$

For the Spin Spirals there is no charge density modulation so we can set $\omega_i = 0$, and the vector magnetic field as (see Figure 1a),

$$\Delta_i = \Delta e_i,$$

where $$e_i = (\sin Q_i, 0, \cos Q_i). \tag{44}$$

Taking $t_{ij} = 1$ for the nearest neighbour and 0 otherwise.

$$H_{HF} \Psi_{k\uparrow}(r) = -e^{i(k(r+1) - e^{i(k(r-1)} \left( \begin{array}{c} \cos \frac{Q}{2}(r+1) \\ \sin \frac{Q}{2}(r+1) \end{array} \right) - \frac{1}{2} \Delta e^{ikr} \left[ \begin{array}{cc} \cos Qr & \sin Qr \\ -\cos Qr & \sin Qr \end{array} \right] \left( \begin{array}{c} \cos \frac{Q}{2}r \\ \sin \frac{Q}{2}r \end{array} \right) \right. \tag{45}$$

$$H_{HF} \Psi_{k\downarrow}(r) = (-2 \cos k \cos \frac{Q}{2} - \frac{1}{2} \Delta) \Psi_{k\uparrow}(r) - (2i \sin k \sin \frac{Q}{2}) \Psi_{k\downarrow}(r) \tag{46}$$

Similarly for the spin down,

$$H_{HF} \Psi_{k\downarrow}(r) = e^{i(k(r+1) - \cos \frac{Q}{2}(r+1)} \left( \begin{array}{c} -\sin \frac{Q}{2}(r+1) \\ \cos \frac{Q}{2}(r+1) \end{array} \right) - e^{-i(k(r-1)} \left( \begin{array}{c} -\sin \frac{Q}{2}(r-1) \\ \cos \frac{Q}{2}(r-1) \end{array} \right) - \frac{1}{2} \Delta e^{ikr} \left[ \begin{array}{cc} \cos Qr & \sin Qr \\ -\cos Qr & \sin Qr \end{array} \right] \left( \begin{array}{c} -\sin \frac{Q}{2}r \\ \cos \frac{Q}{2}r \end{array} \right) \right. \tag{47}$$

$$H_{HF} \Psi_{k\uparrow}(r) = (-2 \cos k \cos \frac{Q}{2} + \frac{1}{2} \Delta) \Psi_{k\downarrow}(r) + (2i \sin k \sin \frac{Q}{2}) \Psi_{k\uparrow}(r).$$

It is clear that the hopping couples $\Psi_{k\uparrow}(r)$ and $\Psi_{k\downarrow}(r)$, the matrix representation of the HF Hamiltonian becomes:
$$H_{HF} = \begin{pmatrix} -2\cos k \cos \frac{1}{2}Q - \frac{1}{2}\Delta & -(2i \sin k \sin \frac{1}{2}Q) \\ (2i \sin k \sin \frac{1}{2}Q) & -2\cos k \cos \frac{1}{2}Q + \frac{1}{2}\Delta \end{pmatrix}$$

The secular equation for the energies can be easily calculated from the determinant of the matrix $E - H_{HF}$ being equated to 0.

$$(-2\cos k \cos \frac{1}{2}Q + \frac{1}{2}\Delta - E)(-2\cos k \cos \frac{1}{2}Q - \frac{1}{2}\Delta - E) - 4(\sin^2 k \sin^2 \frac{1}{2}Q) = 0$$

The band energies are obtained by solving the quadratic equation:

$$E(k) = -2\cos k \cos \frac{1}{2}Q \pm \sqrt{\frac{1}{4}\Delta^2 + 4(\sin^2 k \sin^2 \frac{1}{2}Q)}$$


Figures (9-14) show the energy dispersion for different values for Q and $\Delta$.

For $Q = 0, \Delta = 0$ we revert back to our delocalised Bloch electrons, Figure 9:
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Figure 10. Ferromagnetic for $\Delta = 1, Q = 0$.

Figure 11. $Q = \frac{\pi}{2}, \Delta = 0$.

Figure 12. $Q = \frac{\pi}{2}, \Delta = 1$.
The total moment can be evaluated in terms of the elliptic integral of the first kind [10],

\[ F(\Phi, p) = \int_0^\Phi \frac{dk}{\sqrt{1 - p^2 \sin^2 k}} \]  

\[(51)\]
The eigenfunctions are linear combinations of $\psi_{k\uparrow}$ and $\psi_{k\downarrow}$. In the limit as $\Delta \to \infty$ they should be purely $\psi_{k\uparrow}$ and $\psi_{k\downarrow}$. Furthermore, the HF Hamiltonian for the SS can be diagonalised thus,

$$H_{HF} = \begin{pmatrix} (-2\cos k \cos \frac{1}{2}Q - \frac{1}{4}\Delta)a & -(2i\sin k \sin \frac{1}{2}Q)b \\ (2i\sin k \sin \frac{1}{2}Q)a & (-2\cos k \cos \frac{1}{2}Q + \frac{1}{4}\Delta)b \end{pmatrix}$$

$$= -2\cos k \cos \frac{1}{2}Q \pm \sqrt{\frac{1}{4}\Delta^2 + 4(\sin^2 k \sin^2 \frac{1}{2}Q)} \begin{pmatrix} a \\ b \end{pmatrix}$$

$$\Rightarrow a = \frac{2i\sin k \sin \frac{1}{2}Qb}{-\frac{1}{4}\Delta \mp \sqrt{\frac{1}{4}\Delta^2 + 4(\sin^2 k \sin^2 \frac{1}{2}Q)}}$$

The moment of the states is the probability of finding it in $\psi_{k\uparrow}$ minus that of finding it in $\psi_{k\downarrow}$.

$$m = \frac{|a|^2 - |b|^2}{|a|^2 + |b|^2}$$

$$= \frac{4(\sin^2 k \sin^2 \frac{1}{2}Q) - \frac{1}{4}\Delta^2 - \left[\frac{1}{4}\Delta^2 + 4(\sin^2 k \sin^2 \frac{1}{2}Q)\right] \mp \Delta \sqrt{\frac{1}{4}\Delta^2 + 4(\sin^2 k \sin^2 \frac{1}{2}Q)}}{4(\sin^2 k \sin^2 \frac{1}{2}Q) + \frac{1}{4}\Delta^2 + \left[\frac{1}{4}\Delta^2 + 4(\sin^2 k \sin^2 \frac{1}{2}Q)\right] \pm \Delta \sqrt{\frac{1}{4}\Delta^2 + 4(\sin^2 k \sin^2 \frac{1}{2}Q)}}$$

which simplifies to,

$$m = \mp \frac{1}{\sqrt{1 + \frac{16(\sin^2 k \sin^2 \frac{1}{2}Q)}{\Delta^2}}}$$

Figures 15 and 16 show the moments for the SS configuration.
The magnetisation is just the integration of the moments bound by the Fermi Energy.

\[ M = \frac{1}{2\pi} \left( \int_{k: E_t(k) < E_F} dk - \int_{k: E_t(k) > E_F} dk \right) \frac{1}{\sqrt{1 + \frac{16\sin^2 k \sin^2 \frac{1}{2} Q}{\Delta^2}}} \]
which can be written

$$M(k_F) = \frac{1}{\pi} \int_{k_F-}^{k_F+} \frac{1}{\sqrt{1 + \frac{16(\sin^2 k \sin^2 \frac{1}{2} Q)}{\Delta^2}}} dk$$

$$= \frac{1}{\pi} F(\tan^{-1}\left(\sqrt{1 + \frac{16(\sin^2 k \sin^2 \frac{1}{2} Q)}{\Delta^2}}\right) \tan k_F, \left(\Delta^2 / 16(\sin^2 k \sin^2 \frac{1}{2} Q) + 1\right))$$

The energy of the configurations, following equation (20), is

$$V_{HF} = \frac{1}{2\pi} \sum_{\text{Bands } k : E(k) > E_F} \int E(k) dk + wn + \frac{\Delta^2}{4U} + \frac{1}{4} Un^2$$

For the SS energies this can be evaluated in terms of the elliptic integral of the second kind, $E(\Phi, k)$ [10].

In general the procedure would be to fix $U$ and $n$, and then calculate the self-consistent $w_i$ and $\Delta_i$ for each $\theta_i$. This is exactly equivalent to minimising the energy with respect to all the parameters. Instead of having spin directions on sites it would be advantageous to have them on the bonds. Following the method by Korenman et al [7], a unitary transformation is required for each site. We start by defining a set of local and global operators with respect to the axes.

Let $c_{\beta\sigma} = \begin{pmatrix} c_{\sigma} \\ c_{\alpha} \end{pmatrix}$ be the annihilation operator with respect to the global spin axes, and $d_i$ be the operator with respect to the local axes. Then
\[ c_{i\beta} = U(i)_{\beta\gamma} d_{\gamma} \]  
(60)

\[ c_{i\alpha}^\dagger = U^\dagger(i)_{\gamma\alpha} d_{\gamma}^\dagger \]  
(61)

where the unitary matrix \( U(i) \) is defined as,

\[
U(i) = \begin{pmatrix}
    e^{-\frac{1}{2}(\phi_i + b_i)} \cos_2 \theta_i & -e^{-\frac{1}{2}(\phi_i + b_i)} \sin_2 \theta_i \\
    e^{\frac{1}{2}(\phi_i + b_i)} \sin_2 \theta_i & e^{\frac{1}{2}(\phi_i + b_i)} \cos_2 \theta_i
\end{pmatrix}
\]  
(62)

Here \((\theta_i, \phi_i)\) is the local spin quantisation axis and \( b_i \) is an additional gauge freedom related to the rotation about the local axis. The spin quantisation axis has been transformed from the \( z \)-axis to the local axis \( e_i = (\sin \theta_i, 0, \cos \theta_i) \). We can now immediately transform the HF Hamiltonian into these new operators.

\[
H_{HF} = -\sum_j t_j U^\dagger(i)_{\gamma\alpha} U(i)_{\alpha\beta} d_{\gamma}^\dagger d_{\beta} - \sum_i \frac{1}{2} \Delta \sigma_{\alpha\beta}^z d_{i\alpha}^\dagger d_{i\beta} + \omega_i n_i
\]  
(63)

Clearly, the hopping term is replaced by the matrix,

\[
\bar{t}_{ij} = t_{ij} U^\dagger(i) U(j)
\]  
(64)

we only need to work in the \( \phi = 0 \) plane, and we can also set the gauge freedom term \( b = 0 \). This reduces to,

\[
\bar{t}_{ij} = t_{ij} \begin{pmatrix}
    \cos \frac{1}{2} (\theta_i - \theta_j) & \sin \frac{1}{2} (\theta_i - \theta_j) \\
    -\sin \frac{1}{2} (\theta_i - \theta_j) & \cos \frac{1}{2} (\theta_i - \theta_j)
\end{pmatrix}
\]  
(66)
Now returning to the example of SS, all the nearest-neighbour bonds are equal, and the hopping angle matrix becomes,

\[
\tilde{t}_{r,\text{rest}} = t_q \begin{pmatrix} \cos \frac{1}{2}(Q) & \mp \sin \frac{1}{2}(Q) \\ \pm \sin \frac{1}{2}(Q) & \cos \frac{1}{2}(Q) \end{pmatrix}
\]  

(67)

The bandstructure is found from the eigenequation straight away much more easily than before, with \( w_i = 0 \),

\[
\begin{pmatrix} \cos \frac{1}{2}(Q) & -\sin \frac{1}{2}(Q) \\ \sin \frac{1}{2}(Q) & \cos \frac{1}{2}(Q) \end{pmatrix} e^{ik(a-b)} \begin{pmatrix} \cos \frac{1}{2}(Q) & \sin \frac{1}{2}(Q) \\ -\sin \frac{1}{2}(Q) & \cos \frac{1}{2}(Q) \end{pmatrix} e^{-ik(a-b)} - \frac{1}{2}\Delta \begin{pmatrix} a \\ b \end{pmatrix} = E \begin{pmatrix} a \\ b \end{pmatrix}
\]

(68)

The determinant turns out exactly as before,

\[
\begin{vmatrix} E + 2 \cos k \cos \frac{1}{2}Q + \frac{1}{2}\Delta & -(2i \sin k \sin \frac{1}{2}Q) \\ (2i \sin k \sin \frac{1}{2}Q) & E + 2 \cos k \cos \frac{1}{2}Q - \frac{1}{2}\Delta \end{vmatrix} = 0
\]

(69)

\[
\Rightarrow E(k) = -2 \cos k \cos \frac{1}{2}Q \pm \sqrt{\left[\Delta^2 + 4(\sin^2 k \sin^2 \frac{1}{2}Q)\right]}
\]

(70)

(With the Brillouin zone \(-\pi < k \leq \pi\))
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2.4 Reference:


Chapter 3

In this chapter, several theoretical models appropriate for strongly correlated systems will be expounded; a mention will be made about their applicability to real systems. Theoretical studies have taken two lines of approach: namely the pertubative renormalisation-group calculations and lattice specific models. We will focus on the latter approach.

3 Theories of interacting fermions

From any theoretical model, one wants to work out the ground state properties of some material. This can be done in a variety of ways depending on the material in question, since two different materials will not have the same ground state. Strictly speaking ground state properties of any system (material) manifest themselves around zero temperature. For temperatures above absolute zero, we cannot be certain about the ground state properties due to the emergence of excitations.

In monovalent elements, such as sodium metal the ground state of the electrons is a simple Fermi sea filled up to the level of one electron per atom. In metals such as mercury and niobium the electrons make up Cooper pairs and superconduct in the ground state; for iron the ground state for the electrons is ferromagnetic. Just a handful of metals has shown that finding the ground state is no trivial matter.

![Ground state configuration for the antiferromagnetic insulating state of a CuO2 plane.](image)
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Theories of Interacting Fermions

Figure 2. A Bipartite Lattice

3.1 Cuprate Superconductors

For the specific case of cuprate superconductors; it is widely believed that the basic superconducting unit is that formed by a two-dimensional CuO$_2$ layer, as shown in Figure 1. The one-band Hubbard model and the t-J model both try to capture the physics of the CuO$_2$ plane with a relative degree of success, even though the effects of approximations and projection operators tend to overemphasise the effects of correlation relative to what is actually happening in the physical system. Figure 2 shows a bipartite layer. It consists of a union of two interpenetrating sublattices, A and B, in such a manner that site A always has site B as a neighbour and vice versa. Evidently a non-bipartite will not share this property; this is the case for triangular or hexagonal lattice. A non-bipartite lattice can be responsible for frustration effect as discussed below.

A bipartite lattice has the special property that there is a reciprocal space point, $Q$, for which $E(k+Q) = -E(k)$. This point $Q$ is at the corner of the Brillouin zone and is associated with natural antiferromagnetism for the lattice. This property shows that the Fermi surface is mapped onto itself by a translation through $Q$, and secondly holes are mapped onto particles and vice versa, this is known as nesting of the Fermi surface. The geometry of the lattice is an extremely important parameter in all these models. The fermionic characteristics are strongly modified by the local connectivity of the atoms.
3.2 Heisenberg Model

Ever since the development of quantum mechanics, local magnetic moments of atoms have played a pivotal role in many of the theories discussed here. Heisenberg [1] developed his theory based on this idea. He utilised the fact that the coupling between the neighbouring local moments is no other than the quantum mechanical exchange interaction. Heisenberg model and its variants such as Ising model have enjoyed a particular level of success in giving remarkable insight to areas of phase transition and magnetism. For the first time one was able to understand the formation of various magnetic structures such as Antiferromagnetism, Ferromagnetism, and Spin Density waves just to mention a few.

For the sake of completeness the formalism behind Heisenberg and other spin lattice models will be given, as they are widely used in the literature. Clearly, the motivation for studying such models is due to discoveries of new materials such as heavy-fermion compounds or the high temperature superconductors amongst the plethora of new organic and inorganic compounds.

3.3 The Spin Operator Formalism

The spin operator has a SU(2) symmetry. It is commonly written within the second quantisation formalism thus,

\[ S_i = \frac{1}{2} \psi_i^s \sigma \psi_i^s, \quad \psi_i^s = \begin{pmatrix} c_i^s \\ c_i^{-s} \end{pmatrix}, \]  

(1)

where \( \sigma \) is the vector of Pauli matrices:

\[
\sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_y = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \text{and} \quad \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}. \]  

(2)

The action of an SU(2) matrix on the two-spinor may be shown to induce a rotation of the spin basis,
\[ \psi' \rightarrow \psi'' = U \psi', \quad U \in \text{SU}(2), \]  

(3)

\[ S \rightarrow S' = \frac{1}{2} \psi_i^{*+} \sigma \psi_i', \]  

(4)

\[ S' = \frac{1}{2} \psi_i^{*+} (U^{-1} \sigma U) \psi_i' = MS, \]  

(5)

where the rotation matrix is \( M^{ab} = U^{-1} \sigma_a U \sigma_b \) [26].

### 3.4 One-dimensional Heisenberg Hamiltonian

The Heisenberg Model is the standard model for magnetism, and holds a similar position for magnets as band theory does for metals.

\[ H = -J \sum_i S_i \cdot S_{i+1} \]  

(6)

(Spin \( S = \frac{1}{2} \) for electrons). Site \( i \) is at position \( R_i = ai \), where \( a \) is the lattice spacing. Ferromagnetism (\( J > 0 \)) can be described by the above Hamiltonian [3]. It is customary to introduce a new set of spin reversal operators in terms of \( S (S^x, S^y, S^z) \),

\[ S_i^+ = S_i^x + iS_i^y = c_i^\dagger c_i = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix} \]  

(7)

\[ S_i^- = (S_i^+)^\dagger = S_i^x - iS_i^y = c_i^\dagger c_i = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}. \]  

(8)

The spin operators form an SU(2) Lie algebra, with the usual commutation relations:

\[ [S^x, S^y] = iS^z, \]
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The new operators also obey the SU(2) algebra:

\[ [S^+, S^-] = 2S^z, \quad [S^z, S^\pm] = \pm S^\mp. \]  

Express the product \( S_i \cdot S_j \) as

\[ S_i \cdot S_j = S_i^+ S_j^- + S_i^- S_j^+ = \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z. \]

In the ground state \( |0\rangle \), all the spins point up-wards. The operator \( S_i^+ \) increases the \( z \) component of the spin at site \( i \), whereas \( S_i^- \) operator decreases the \( z \) component of the spin at site \( i \). Clearly for fermions \( S = \frac{1}{2} \), the \( S_i^- \) corresponds to a spin flip (i.e. the \( z \) component changes from \( \frac{1}{2} \) to \( -\frac{1}{2} \)). The corresponding new state is denoted by \( |i\rangle; |\bar{i}\rangle = S_i^- |0\rangle \). This implies the following:

\[ S_i^z |i\rangle = \begin{cases} S |i\rangle & i \neq j; \\ (S - 1) |i\rangle & i = j; \end{cases} \]

\[ S_j^- S_{j+1}^- |i\rangle = \begin{cases} 0 & i = j + 1; \\ |i-1\rangle & i = j; \\ 0 & 0 \text{ otherwise.} \end{cases} \]

\[ S_j^+ S_{j+1}^+ |i\rangle = \begin{cases} |i+1\rangle & i = j; \\ 0 & i = j + 1; \\ 0 & 0 \text{ otherwise.} \end{cases} \]

The isotropic Heisenberg Hamiltonian is given below [27][28].
The Ising model can be seen as a special case of Heisenberg model, where only the $z$ component of spins is used.

3.5 Ising model at a glance

When the $x$-, $y$- components of the interaction are negligible the Heisenberg Hamiltonian reduces to the Ising Hamiltonian. The Ising interactions are used for classical spins to model problems of magnetic ordering [3] [4].

\[ H = -J \sum_{<ij>} \frac{1}{2} (S_i^+ S_j^- + S_i^- S_j^+) + S_i^z S_j^z \]  

(15)

All spins are quantised with respect to the $z$ axis, each having an eigenvalue $\pm \frac{1}{2}$ of its component $S_i^z$. Both Heisenberg and Ising models fail for the narrow d-band transition elements, where the competing itinerant electrons overpower the localised electrons; the d-electrons are not localised.
3.6 $J_1 - J_2$ Type models

The $J_1 - J_2$ type models are used to study frustration in Heisenberg antiferromagnets,

$$H = -J \sum_i S_i S_{i+1} - J' \sum_i S_i S_{i+2}.$$ (17)

Frustration occurs in systems that have a high degree of degeneracy, in other words frustration occurs when it becomes impossible to simultaneously satisfy all the interactions having the same energy.

![Figure 3. $J_1 - J_2$ model of a linear chain with nearest neighbour ($J_1$) and next nearest neighbour $J_2$.](image)

Usual convention is to take $J_1 = -J$ and $J_2 = -J'$. A good review is given by Schulz et al [5]. Majumdar et al [6] have studied the above Hamiltonian (17) for the case $J_1, J_2 > 0$, finding a spiral ground state in the limit $J_1 \ll J_2$ for the classical case, where the even and odd sites decouple and the ground state becomes degenerate. We will also see the multiplicity of ground states in this work. Haldane [7] found local singlet formation for $\frac{J_2}{J_1} = 1$, of the order unity or larger. In certain situations the classical Heisenberg model possess a line of degenerate ground states, as seen in the
two dimensional antiferromagnetic square lattice with nearest- and next-nearest-neighbour exchange interactions, with \( \frac{J_1}{2} < J_2 \) \([29][30]\).

3.7 The Hubbard Model revisited

\[
H = -\sum_{<ij>\sigma} t_{ij} \sigma_i \sigma_j + U \sum_i n_i^\dagger n_i
\]

(18)

The Hubbard Hamiltonian (18) is considered in the limit of large ratios of \( \frac{U}{t} \), with the band filling of less than one half. In the large U-limit double occupancy is projected out. Following Fulde \([8]\), if we let \( P \) be a projection operator which projects the states it acts on onto the reduced Hilbert space and satisfies the Gutzwiller projection relation \([11]\), \( P^2 = P \). Then the operator \( Q = 1 - P \) projects onto the space of configurations with double occupancy. The reduced Hamiltonian will have a form determined by these projection operators:

\[
\tilde{H} = PHP - \frac{1}{U} PHQHP
\]

(19)

From the definition of \( P \) and \( Q \), it follows that,

\[
QHP = \sum_{<ij>\sigma} t_{ij} n_{i-\sigma}^\dagger \sigma_i \sigma_j (1-n_{j-\sigma})
\]

(20)

\[
PHQ = \sum_{<ij>\sigma} t_{ij} (1-n_{i-\sigma}) \sigma_i^\dagger \sigma_j n_{j-\sigma}
\]

(21)
Limiting the calculations to nearest-neighbour hopping \((t_{ij} = -t)\) [9], we obtain the following reduced Hamiltonian,

\[
\tilde{H} = \sum_{\langle ij \rangle} t_{ij} c_{i\sigma}^\dagger c_{j\sigma} + J \sum_{\langle ij \rangle} \left( S_i S_j - \frac{n_{i\sigma} n_{j\sigma}}{4} \right) - J \sum_{\langle ijk \rangle} (c_{i\sigma}^\dagger n_{j-\sigma} c_{i\sigma} - c_{i\sigma}^\dagger c_{j\sigma}^\dagger c_{j\sigma} c_{i-\sigma})
\]  

(22)

The brackets \(\langle ij \rangle\) and \(\langle ijk \rangle\) denote pairs of nearest neighbours, and a three-site term respectively, where \(i\) and \(k\) are neighbours of \(j\). The \(c_{i\sigma}^\dagger, c_{i\sigma}\) are the electron creation and annihilation operators which act in the reduced Hilbert space, with \(J = \frac{4t^2}{U}\).

\[
c_{i\sigma}^\dagger = c_{j\sigma}^\dagger (1 - n_{j-\sigma}),
\]

(23)

\[
c_{j\sigma} = c_{j\sigma} (1 - n_{j-\sigma}),
\]

(24)

where the spin operators \(S_i = \frac{1}{2} \sum_{\alpha\beta} c_{i\alpha}^\dagger \sigma_{\alpha\beta} c_{i\beta}\) with \(\sigma_{\alpha\beta}\) as the Pauli matrices and \(n_{di}\) as the charge operators

\[
n_{di} = n_{i\sigma} + n_{i,-\sigma}.
\]

(25)

### 3.8 The t-J model

The three-site terms in \(\tilde{H}\) contribute only when the system deviates from half filling: these terms are responsible for describing indirect hopping processes between next-nearest neighbour sites \(i\) and \(k\). The order of the three-site terms is \(\frac{t}{U}\) as compared to the first term. We are then justified in dropping these terms if we are close to half filling. If this applies the Hubbard Hamiltonian (18) transforms over to the \(t - J\) model Hamiltonian:
Effectively the Hamiltonian (18) has been replaced by a reduced Hamiltonian $\tilde{H}$, which has the Hubbard $U = \infty$, as a direct consequence of the action of the projection operators that forbid double occupancy. What remains is a Heisenberg type antiferromagnetic coupling [10]. At half filling, the lower Hubbard band will be full, and hence may be expected to have an antiferromagnetic ground state.

The projection operators ensure that the $t - J$ model will always have strong correlations even if $J$ is set to zero since double occupancy is forbidden. This implies that the creation operators (23) can only give a non-zero result if the site $i$ is unoccupied, pointing out the fact that the usual fermion commutation rules cannot be applied for these composite particles.

### 3.9 Falicov-Kimball Model

Falicov and Kimball introduced their model to study metal-insulator transitions in mixed valence compounds of rare earth and transition metal oxides as an effect of the interactions between localised f-electrons and itinerant d-electrons [12][13].

$$H = -\sum_{ij} t_{ij} c_i^{\dagger} c_j + U \sum_i w_i c_i^{\dagger} c_i$$

The above Hamiltonian defines the spinless Falicov-Kimball model. As usual the operators $c_i, c_i^{\dagger}$ are fermionic creation and annihilation operators for the spinless
electron at site \( i \), \( w_i \) is the occupation number of the ions, which takes a value of 1 or 0 at each site depending on whether the site \( i \) is occupied or unoccupied, respectively, by an ion. The first term needs no introduction, the second term represents an on-site interaction between electrons and ions that can be repulsive or attractive depending on the sign of \( U \).

The total number \( N_i \) of ions and the total number \( N_e \) of electrons is conserved.

\[
N_e = \sum_i c_i^\dagger c_i, \quad N_i = \sum_i w_i
\]  

(28)

The moving particles play the role of the d-band electrons and the ions play the role of f electrons. It can be seen as a model, in which only up-spin are allowed to hop and the down-spins are anchored to the sites.

3.10 Metal Insulator transitions

![Figure 4. The zero-temperature electrical conductivities of phosphorus-doped silicon.](image)
Metal-insulator transitions are accompanied by huge resistivity changes [15] as shown above in Figure 4. It shows the electrical conductivity of P-doped Si at very low temperatures as a function of the P donor concentration. Strong electron-electron correlations lead to insulating phases categorised by Mott insulator. Fascinating behaviour occurs near the critical region of the transition point, the metallic state shows fluctuations and ordering in the spin, charge, and orbital degrees of freedom [16]. In the early years of quantum mechanics the theoretical description for metals and insulators was based on the weak or noninteracting electron systems. The theory makes a general distinction between metals and insulators at zero temperature based on the filling of the electronic bands. Fermi level lies in a band gap in insulators and for metals it lies inside a band. In the non-interacting theory, the formation of band structure is totally due to the periodic structure of the atoms in the crystal.

This basic distinction between insulators and metals was proposed in the days when quantum mechanics was in its infancy (1930’s), then came semiconductors which were insulators with small energy gap between the highest filled band and the lowest empty band. The band picture was quite successful in many respects, however in the case of transition-metal oxides with partially filled d-electron band were in many cases insulators or extremely poor metals at best. Typical example is that of NiO, the explanation for this was given by Mott [17]. Mott explained this effect by considering a lattice model with a single electronic orbital on each site. Without electron-electron interaction, a single band would be formed from the overlap of the atomic orbitals in this system, where the band becomes full when two electrons with opposite spins occupy each site.

However two electrons sitting on the same site (with opposite spins) will feel a large Coulomb repulsion, which Mott argued would split the band into two. With one electron per site the system would be an insulator. If one considers the electron-electron interaction for the partially filled, but with low density of atoms, then according to Mott a sharp transition of the type in Figure 4 will occur from metallic to insulating state as the distance of the atoms exceeds some critical length.
\[ a_{\text{crit}} = \frac{Ah^2\pi^2}{me^2}, \]

where \( A \) is some dimensionless constant. Thus concluding that metallic states do not survive at low conduction electron densities for partially filled narrow bands. This is similar to Anderson localisation, where the metallic ground state is also destroyed. It happens if the potential due to impurities is of the same order as the bandwidth.

### 3.11 Kondo Lattice Model

Heavy quasi-particles called *heavy fermions* are found within the Fermi-liquid states of intermetallic compounds containing actinides or rare-earth elements. Heavy fermion compounds contain two different types of electrons. One set forms the conduction electrons in the \( s, p, d \) – atomic orbitals and move through a lattice forming broad bands. The other set is the electrons in the inner \( f \) orbital. These \( f \) orbitals are essentially ionic in nature and keep to themselves, hybridising only weakly with the rest of conduction electrons. Hund’s coupling makes the electron-electron interaction between the \( f \) electrons larger [22]. The Anderson model and the Kondo lattice model are the two standard models used in literature for modelling heavy-fermions. In the Kondo model charge fluctuations are of \( f \) electrons is completely omitted and the lowest \( f \)-ion multiplet is taken into account as a localised spin.

\[
H_{\text{KLM}} = \sum_{k\sigma} E(k)c_{k\sigma}^\dagger c_{k\sigma} + J \sum_s S_{ei} \cdot S_i \quad (29)
\]

where the spin-density operators for the impurity and conduction electron are,

\[
S_{ei} = \frac{1}{2} \sum_{\alpha\beta} \sigma_{\alpha\beta} c_{i\alpha}^\dagger c_{i\beta}, \quad S_i = \frac{1}{2} \sum_{\alpha\beta} \sigma_{\alpha\beta} d_{i\alpha}^\dagger d_{i\beta}. \quad (30)
\]

The Kondo lattice model reduces to the Kondo model (31) for a single impurity.
Kondo considered the problem of a magnetic impurity embedded in a sea of conduction electrons [21]. The properties of normal pure metal are drastically affected by the addition of an impurity atom. If one dissolves a transition metal ion or a rare earth impurity, a number of anomalous transport properties are observed. A characteristic property of the system is that the resistance as a function of temperature shows a minimum rather than a monotonic decrease.

Here $S_c$ is the spin of the magnetic impurity placed at the origin and $S(0)$ is spin of the conduction electrons given by,

$$S(0) = \frac{1}{2} \sum_{\alpha \beta} c_{\alpha \sigma}^\dagger \sigma_{\alpha \beta} c_{\beta \kappa}$$

(32)

with $\sigma_{\alpha \beta}$ as the Pauli matrices and $E(k)$ as the energy dispersion. The Hamiltonian (27) describes the interactions of conduction electrons with impurities that have an internal degree of freedom.
3.12 Anderson Model

Anderson suggested his model for the description of a magnetic impurity embedded in a metal [18].

![Figure 5. Two orbitals D and C with orbital energies $E_d$ and $E_e$, respectively, coupling factor $\Delta$.](image)

The above Figure 5 depicts the simplest type of a strongly correlated system consisting of electrons distributed over D orbital and partially filled band conduction electrons. The C electrons are dispersive, with a dispersion $E_e(k)$ and non-interacting with $U_e = 0$. We assume that the corresponding energies are $E_d$ and $E_e$ respectively with $E_d < E_e$. The Hamiltonian for the above scenario is given by,

$$H = \sum_{k\alpha} E_e(k)n_{k\alpha} + E_d \sum_\sigma n_{d\sigma} - \Delta \sum_{k\alpha} (c_{k\alpha}^\dagger d_\sigma + d_\sigma^\dagger c_{k\alpha}) + U_{\text{e}} n_{e\uparrow} n_{d\downarrow}$$  \hspace{1cm} (33)
The $c^\dagger_{\kappa \sigma}$, $d^\dagger_{\sigma}$ create electrons with spin $\sigma$ in the C and D orbitals respectively, where as the $c_{\kappa \sigma}$ and $d_{\sigma}$ annihilate electrons with spin $\sigma$ in the C and D orbitals respectively. The number operators for the orbital C and D are $n_{d\sigma} = d^\dagger_{\sigma} d_{\sigma}$ and $n_{c\sigma} = c^\dagger_{k\sigma} c_{k\sigma}$ respectively.

When $\Delta = 0$, the ground state of the system is fourfold degenerate, and has the energy $E_0 = E_c + E_d$. One electron is in the D orbital while the other is in the C orbital. A state with a double occupied D orbital has a high energy because of the large coulomb repulsion $U$. The C orbital is assumed to be extended and the coulomb repulsion is assumed negligible, as are the interactions between electrons in the C and D orbital.

The four eigenstates of the total spin $S$ are:

\begin{align*}
|\phi_{1,5,:,:0} &= \frac{1}{\sqrt{2}}(c^\dagger_i d^\dagger_i - c^\dagger_i d^\dagger_i)|0\rangle, \\
|\phi_{2,5,:,:1} &= c^\dagger_i d^\dagger_i|0\rangle, \\
|\phi_{3,5,:,:1} &= \frac{1}{\sqrt{2}}(c^\dagger_i d^\dagger_i + c^\dagger_i d^\dagger_i)|0\rangle, \\
|\phi_{4,5,:,:1} &= c^\dagger_i d^\dagger_i|0\rangle.
\end{align*}

The system has one excited state of the form

\begin{align*}
|\phi_{\alpha} &= c^\dagger_i c^\dagger_i|0\rangle.
\end{align*}

The excitation energy is $E_{ex} = 2E_c$. As in the t-J model, if we assume $U \rightarrow \infty$, then we can ignore the state $|\phi_{\alpha} = d^\dagger_i d^\dagger_i|0\rangle$ since it has energy in the order of $U$. In many of these lattice site models discussed here, a large class of wavefunctions belonging to higher energies is routinely neglected, which makes the single-electron states extremely simple. This may seems like that we are disregarding many essential features of physics compared with say the infinite energy levels of the hydrogen atom. However this simplification as mentioned in Chapter 1 is justified because the atomic
energy spacings are much larger than the thermal energies and necessary for the problem to be solvable [18].

The Hamiltonian (33) simply describes two independent systems, the band electrons and the \( d \) electrons. The \( d \) electron system splits into \( N_d \) independent sites. The physical properties are determined trivially from the Fermi level \( E_F, E_d \), and \( E_d + U \). For \( E_d < E_F \) and \( E_d + U < E_F \) the \( d \) site are fully occupied, equivalently they are empty for \( E_d > E_F \) and \( E_d + U > E_F \). There are no unpaired magnetic moments, and the system is diamagnetic. For \( E_d < E_F \) and \( E_d + U > E_F \) the minimum energy configuration will have as many unpaired electrons on the \( d \) sites as possible, which means that the system will have magnetic moments on most sites. If there is exactly one electron per site then the system will be paramagnetic with magnetic moments \( \mu = \mu_B \), where \( \mu_B \) is the Bohr magneton.

When \( \Delta \neq 0 \), the hybridization couples the singlets \( |\phi_{ss'}\rangle \) and \( |\phi_{ee'}\rangle \) but the exact solutions are unknown. However, a mean field treatment may bring about some of the necessary physics we are interested in.

Let \( E_0 = E_d + U \langle n_{d\uparrow} \rangle \), and \( |\psi_k\rangle = (\alpha_k c_k^\dagger + \beta_k d_k^\dagger) \).

Here the \( \langle n_{d\downarrow} \rangle = \frac{1}{2} \sum_{k,d} \langle \psi_{kd} | d_k^\dagger d_k | \psi_{kd} \rangle \), with the normalisation condition

\[
|\alpha_k|^2 + |\beta_k|^2 = 1. \tag{39}
\]

The Schrödinger equation becomes, for each \( k \),

\[
H_\uparrow = \sum_k E_c(k) n_{k\uparrow} + E_d \sum_d n_{d\uparrow} - \Delta \sum_{kd} (c_{k\dagger}^\uparrow d_k^\dagger + d_k^\dagger c_{k\dagger}^\uparrow) + U n_{d\uparrow} \langle n_{d\uparrow} \rangle \tag{40}
\]

\[
H_\downarrow = \sum_k E_c(k) n_{k\downarrow} + E_d \sum_d n_{d\downarrow} - \Delta \sum_{kd} (c_{k\dagger}^\downarrow d_k^\dagger + d_k^\dagger c_{k\dagger}^\downarrow) + U \langle n_{d\downarrow} \rangle n_{d\downarrow} \tag{41}
\]
\[ \begin{pmatrix} E_c(k) - E(k) & \Delta \\ \Delta & E_0 - E(k) \end{pmatrix} \begin{pmatrix} \alpha(k) \\ \beta(k) \end{pmatrix} = 0 \] \hspace{1cm} (42)

The energies are,

\[ E = \frac{(E_c + E_0)}{2} \pm \sqrt{\frac{(E_c + E_0)^2}{4} + \Delta^2}. \] \hspace{1cm} (43)

Figure 3. Energy dispersion of the two hybridised bands. The dotted lines represent \( E_c \) and \( E_0 \).

From the eigenvectors \( \alpha \) and \( \beta \) we can work out the moments as defined in Chapter 2.

\[ \beta^2 = \frac{\Delta^2}{(E - E_0)^2 + \Delta^2}, \] \hspace{1cm} and the localised moment \( \mu = \mu_B \left( \langle n_{d\uparrow} \rangle - \langle n_{d\downarrow} \rangle \right) \).

The Anderson Hamiltonian can be solved exactly for a single impurity by the Bethe Ansatz method [20]. As with any exact solution it provides a stringent test for any approximations, however the above treatment and the treatment in the rest of this thesis gives the physics which is much more easier to grasp.
3.13 Slave boson method

This method has the advantage over the variational approach that a systematic improvement of the result is possible at least in principle, using a pertubative expansion. The slave boson method was developed originally for $U \to \infty$ periodic Anderson model \cite{23}\cite{24}, and was later extended to general case by Kotliar et al \cite{24}. The slave boson method is no more than an attempt to replace the hardly tractable operator inequality $\sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} \leq 1$ by an equality allowing easier handling of the local constraint.

The localised $d_{i\sigma}^\dagger$ ($d_{i\sigma}$) electron operators are written as a composition of a boson $b$ and fermion $f$ operator,

$$d_{i\sigma}^\dagger = f_{i\sigma}^\dagger b_i, \text{ and } d_{i\sigma} = b_i^\dagger f_{i\sigma}. \quad (44)$$

The boson may be seen as a vacant site, so that every site is always occupied by either an $f$ fermion or $b$ boson. This can be written more succinctly by the operator equality,

$$\sum_{\sigma} f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i = 1 \quad (45)$$

The Anderson Hamiltonian (33) can now be written in terms of these new operators as,

$$H = \sum_{k\sigma} E_k n_{k\sigma} + \sum_{i\sigma} E_d f_{i\sigma}^\dagger f_{i\sigma} - \Delta \sum_{i\sigma} (c_{i\sigma}^\dagger b_i f_{i\sigma} + f_{i\sigma}^\dagger b_i c_{i\sigma})$$

$$+ \sum_i \lambda_i \sum_{\sigma} (f_{i\sigma}^\dagger f_{i\sigma} + b_i^\dagger b_i - 1) \quad (46)$$

where the Lagrange multiplier $\lambda_i$ is used to impose the local constraints on site $i$. 
Mean field approximation is applied, assuming that there is Bose condensation for the bosons, \( \langle b_i \rangle = b_0 \). The Lagrange multiplier is chosen to be uniform, \( \lambda_i = \lambda_0 \) for all the sites. The resulting Hamiltonian (46) is equivalent to (33). The mean field approach is exact in the limit of infinite degeneracy \( N \) of the localised \( f \) orbitals, where the fluctuations of the boson field vanish. Then \( \gamma_N \) correction provides a small parameter for a systematic improvement for finite \( N \) by treating the fluctuation around the mean field [25].
3.14 Reference:


Chapter 3  Theories of Interacting Fermions


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[27] Harald Ibach and Hans Luth *Solid-State Physics* (Springer-Verlag, 1993)


Chapter 4

In this Chapter, research done on bipolaronic superconductivity with Professor A. S. Alexandrov will be presented. Here we look at negative $U$ Hubbard model with short range interaction. The on-site bipolaron Hamiltonian is mapped onto the negative $U$ Hubbard Hamiltonian.

4 Bipolaronic Superconductivity

The electron-phonon interaction leads to the formation of a polaron [1], which comprises an electron and its accompanying lattice polarisation. In case of strong electron-lattice coupling, the polaron may be described in terms of localised states [2]. Each state has an electron bound to a site and is surrounded by the lattice polarisation. Such Polarons are usually termed small polarons. The attractive potential between two like-charged polarons suggests the possible formation of bipolarons [3]. The introduction of small mobile bipolarons and small polarons into the theory of superconductivity dates from the work of Alexandrov et al [5].

A marked feature of high temperature ($T_c$) cuprate superconductors is that they show behaviour very different to that predicted by the Bardeen-Cooper-Schrieffer (BCS) Fermi liquid theory [8]. In case of bipolarons, real space pairing gives rise to superconductivity in contrast to the BCS. BCS superconductivity originates from an exchange coupling between pairs of electrons $c_{k\uparrow}^\dagger c_{-k\downarrow}^\dagger$ with equal and opposite momenta, acting in a thin layer around the Fermi surface. Real space pairing involves all the electrons of the Fermi sea in the pairing mechanism.

The discrepancies found in the BCS theory can readily be remedied if one considers bipolaronic superconductivity. Strong electron-lattice coupling and weak electron-phonon coupling, leads to the formation of small polarons, because of electron–lattice
coupling the polaron binding energy is reduced further, thus making the existence of the bipolarons favourable. Phonons in our picture are defined as the vibrational modes with respect to the deformed lattice. The stability of small polarons is the consequence of weak electron-phonon coupling.

Tables 1 and 2 show the comparison between BCS Fermi liquid and the experimental results for the high $T_c$ copper oxides [4].

<table>
<thead>
<tr>
<th>Physical Property for $T\leq T_c$</th>
<th>BCS/Fermi Liquid</th>
<th>Experimental Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>NMR $1/T_1$</td>
<td>Coherent peak</td>
<td>absent</td>
</tr>
<tr>
<td>Thermal conductivity</td>
<td>Decreases</td>
<td>enhancement</td>
</tr>
<tr>
<td>Gap</td>
<td>$3.5T_c$</td>
<td>$7-8T_c$ (for $T_c=90K$)</td>
</tr>
</tbody>
</table>

Table 1. Comparison between BCS and Experiment $T\leq T_c$.

<table>
<thead>
<tr>
<th>Physical Property for $T\geq T_c$</th>
<th>BCS/Fermi Liquid</th>
<th>Experimental Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>Hall ratio</td>
<td>Constant</td>
<td>$1/T$</td>
</tr>
<tr>
<td>Themopower</td>
<td>$T$</td>
<td>Nonlinear, large</td>
</tr>
<tr>
<td>Infrared conductivity</td>
<td>Drude-law</td>
<td>Mid-Infrared maxima</td>
</tr>
</tbody>
</table>

Table 2. Comparison between BCS and Experiment $T\geq T_c$.

Without too much digression from the topic of this thesis, we will only convey the relevant physics that we are interested in, namely spin waves in the context of the Hubbard model. The pairing of real space electron changes the nature of the of the carriers from fermionic to that of bosons, what we actually end up with is looking at the problem of charged hardcore Bose gas on a lattice. Following Alexandrov [5][6] a bipolaronic Hamiltonian for a perfect lattice may be written in the form below,

$$H = -\mu \sum_i n_i + \sum_{i\neq j}(U_{ij}n_i n_j - t_{ij} b_i^\dagger b_j),$$

(1)
where the energy of the localised bipolaron is included in the definition of the bipolaron chemical potential $\mu$. $U_{ij}$ is the coulomb potential and the hopping is represented by $t_{ij}$. The singlet bipolaron creation and annihilation operators are $b_i^\dagger = c_i^r c_i^l$, $b_i = c_i^l c_i^r$ respectively. The bipolaronic occupation number is given by $n_i = b_i^\dagger b_i$.

The bipolaronic operators obey the mixed commutation rules in a subspace of empty or double occupied sites.

\begin{align}
    b_i b_i^\dagger + b_i^\dagger b_i &= 1 \\
    b_i b_j^\dagger - b_j^\dagger b_i &= 0 \text{ for } i \neq j
\end{align}

We can now employ the pseudo-spin analogy and rewrite the polaronic operators,

\begin{equation}
    b_i^\dagger = S_i^+ - iS_i^x,
\end{equation}

and

\begin{equation}
    b_i^\dagger b_i = \frac{1}{2} - S_i^z,
\end{equation}

with the pseudo spin $\frac{1}{2}$ operators $S_{i,x,y,z}^\pm = \frac{1}{2} \sigma_{x,y,z}$. $S_i^z = \frac{1}{2}$ corresponds to an empty site and $S_i^z = -\frac{1}{2}$ corresponds to a occupied bipolaronic site. These new spin operators preserve the bosonic character of the bipolarons on different sites, and their fermionic internal structure is safe guarded by the Pauli's exclusion principle incorporated in the Pauli spins $\sigma_{x,y,z}$.

### 4.1 Anisotropic Heisenberg Hamiltonian

The spin operators now allow us to rewrite the bipolaronic Hamiltonian (1) into the familiar anisotropic Heisenberg Hamiltonian,

\begin{equation}
    H = \mu \sum_i S_i^z - \sum_{i \neq j} (t_{ij} (S_i^+ S_j^- + S_i^- S_j^+) + \frac{1}{2} U_{ij} S_i^z S_j^z)
\end{equation}
with the bipolaron chemical potential playing the role of an external magnetic field. The above Hamiltonian has been thoroughly investigated in the literature in the context of quantum solids and magnetic materials. It is the usual practice to take the magnetic field or pressure as one of the independent thermodynamic variables or the molar volume is determined so as to minimise the free energy. In contrast the number density of bipolarons is determined in our case by having the magnetic field fixed by the total magnetisation. The bipolaron density is conserved,

$$\sum_i \langle S_i^z \rangle = \frac{N-n}{2}$$

where $N$ and $n$ are the numbers of cells and electrons respectively. We assume $N \leq n$. If $N < n \leq 2N$ electron hole symmetry applies so holes may be used instead of electrons.

### 4.2 Bipolaronic ground state

To calculate the ground state we can apply a mean field approach. Let an average magnetic field $H_i$ act on a spin at site $i$.

In the nearest neighbour approximation the magnetic field may be written as a local pseudofield,

$$H_i = -\langle \mu + 2J \langle S_j^z \rangle e + 2t \langle S_j^z \rangle \rangle$$

where $J = \frac{\xi}{2}U_{ij}^j, t = zt_{ij}, z$ is the co-ordination number, $\langle S_j^z \rangle = \langle S_{i,a}^z \rangle$ (averaged over the neighbours of $S_j^z$), $a$ is the lattice spacing, $e$ is the unit vector in the $z$-direction, and $S_j^z$ is a spin component perpendicular to the $z$-axis. We assume that $J, t > 0$. Multiple bipolaron occupation is prohibited due to strong repulsive
interactions. The chemical potential is determined by the condition that $\langle S_i \rangle$ is parallel to $\mathbf{H}_i$,

$$\mu = -(J + t) \cos \theta \quad (9)$$

In the absence of a macroscopic current $\langle S_i^z \rangle = 0$, and at $T=0$,

$$\langle S_i^z \rangle = \frac{1}{2} \cos \theta . \quad (10)$$

$$\langle S_i^z \rangle = \frac{1}{2} \sin \theta . \quad (11)$$

The mean field ground state has $\langle S_i \rangle$ parallel to $\mathbf{H}_i$ we find for the angle $\theta = \theta_i$ between the new direction of the spin and the $z$-axes, and $\theta'$ is the angle of the nearest neighbours of $S_i^z$. We arrive at two set of equations for $\theta$ and $\mu$,

$$\sin \theta = \frac{t \sin \theta'}{\sqrt{(\mu + J \cos \theta')^2 + t^2 \sin^2 \theta'}} . \quad (12)$$

$$\cos \theta = \frac{\mu + t \cos \theta'}{\sqrt{(\mu + J \cos \theta')^2 + t^2 \sin^2 \theta'}} . \quad (13)$$

$$\cos \theta + \cos \theta' = 2(1 - \frac{n}{N}) . \quad (14)$$

Two solutions are possible to the above equations. First solution is obtained when,

$$\cos \theta = \cos \theta' = (1 - \frac{n}{N}) \quad (15)$$

and the chemical potential,

$$\mu = -(J + t)(1 - \frac{n}{N}) \quad (16)$$

This is the pseudospin ferromagnetic solution with all the pseudospins in one direction, and the bipolaron are evenly distributed over the lattice. The energy for the ferromagnetic case can be determined from equation (3) as,
Chapter 4 Bipolaronic Superconductivity

\[ E_{\text{ferro}} = -\frac{tN}{4} \left[ 1 + (1 + \frac{J}{t})(1 - \frac{n}{N})^2 \right] \]  \hspace{1cm} (17)

The second solution is that of a bipartite lattice with two different sublattices (\( \theta \) and \( \theta' \)), it is an antiferromagnetic pseudospin solution with lower energy than the ferromagnetic state. The energy for the antiferromagnetic case is

\[ E_{\text{antiferro}} = -\frac{JN}{4} < E_{\text{ferro}}. \]  \hspace{1cm} (18)

The antiferromagnetic solution only exists if \( J > t \) and the electron density is sufficiently high,

\[ n > \frac{1}{2} \left( 1 - \sqrt{\frac{J-t}{J+t}} \right) \]  \hspace{1cm} (19)

In Chapter 7, we will see that for the one-dimensional Hubbard model at high electron densities we do indeed get antiferromagnetic order, although the nature of the spins is somewhat different from here.

We may conclude that at \( T=0 \) the bipolarons exist either as a homogeneous ferromagnetic quantum fluid or at higher density as a mixture of an inhomogeneous antiferromagnetic Bose-Einstein condensate and a charge density wave. We must stress that the real spins of the system are always zero, it is only the pseudospins which are being referred to here. Figure 2 below shows real spin singlet in a occupied site and an empty site.

\[ \begin{align*}
&\uparrow \downarrow \quad \bigcirc \quad \uparrow \downarrow \quad \bigcirc \quad \uparrow \downarrow \quad \bigcirc \\
\text{Figure 2. Occupied and empty sites.}
\end{align*} \]
4.3 T-n phase diagram

Robaszkiewicz et al [9] have applied a mean field analysis on the Hamiltonian (6). They solved the effective pseudospin Hamiltonian by means of Bogoliubov variational principle [8]. At finite temperatures thermal fluctuations become extremely important as well as quantum fluctuations. Under the condition $J \gg t$ the Bose-Einstein condensate disappears first with increasing temperature at $T = t$, followed by the disappearance of charge ordered state at $T = J$.

![Image](image.png)

The above Figure 3 shows the bipolaronic liquid consisting of four phases. Two of them are low-temperature phases namely a bipolaronic superfluid (BS) and a mixed phase described above. The other two phases occur at high temperatures; one is the unusual metal (N) of nondegenerate bipolarons with an elementary charge of 2e. The other phase is a charge ordered state (CO). In the BS phase, the low-lying excitations are collective modes of phase fluctuations, which are coupled to the electron density fluctuations in the superconducting phase.
4.4 Reference:


Chapter 5

The discovery of High Temperature Superconductors [3] in 1986, with a variety of heavy-fermion and related non-Fermi Liquid systems, has opened the floodgates of renewed research in the arena of one dimensionality. Precise understanding of the one-dimensional models may provide deeper insights into the properties of three-dimensional systems. Literature is inundated with numerous papers. The importance of current research will be discussed in this chapter.

5 One-dimensional materials

Fundamental differences between 1D and 3D fermionic systems must be highlighted. In 1D we have the absence of fermionic particles characterised by spin-charge separation, and non-universal power law correlations. Whereas the 3D system is usually characterised by a Fermi Liquid theory, describing the vicinity of the 3D Fermi surface, which is based on the existence of quasi-particles evolving out of electron or hole excitations of the Fermi gas. These quasi-particles obey the usual Fermi-Dirac statistics, possess the same quantum number as the bare counterparts, also the spin, and charge excitations are collective.

5.1 Phase Transitions

One of the most fundamental problems in condensed matter is to understand the phenomenon of phase transitions, in particular why all elements and many compounds crystallise in periodic structure. We will endeavour to gain some insight into this ancient conundrum in Chapter 6. A phase transition occurs at those values of the external parameters for which one or more of the observables become singular. The transition can be classed by the nature of the singularity -whether it is discontinuous or divergent. A phase transition separates the different phases of the system. An order parameter is necessary to distinguish different phases. For instance in our supercell

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calculations, we expect the parameters \( \{\theta, \Delta, \nu\} \) to change drastically near the phase transition point.

One-dimensional solids are particularly interesting in the context of fundamental studies on phase transitions. In fact, much of the motivation in this field arises from the hope of finding the key to High Temperature Superconductors. A famous theorem by Landau states that phase transitions are impossible in 1D systems. The long-range order is unstable with respect to the creation of domain walls, because the entropy terms in the free enthalpy will always overcompensate the energy needed to form new walls. However, one may insist that although phase transitions are highly unlikely, the 1D system might be very close to a phase transition even at high temperatures.

Expectation values of spin are another good order parameter, it allows the calculation of spontaneous magnetisation. The anomalous average \( \langle c^\dagger_{k_1} c^\dagger_{-k_2} \rangle \) for superconductors is zero for normal state but finite for the superconducting state.

We will not digress too much from the focus of our research. Related topics are mentioned only for the sake of completeness. Our attention is primarily in one-dimension. Furthermore, a large number of compounds have been found whose behaviour is substantially determined by 1D or 2D effects. The dimensionality plays a crucial role in determining the phenomenology at work. In low dimensions, the fluctuations become increasingly pronounced so that highly anharmonic configurations can result. A wide variety of materials with one-dimensional structural and electronic properties have been discovered, ranging from heavy-doped conjugate polymers [1] to organic superconductors [2].

Little [4] in 1964 suggested that one could form a one dimensional superconductor using the \textit{backbone} of polyacetylene. He proposed that some of the hydrogen atoms could be replaced by some specifically designed substituents\$ \$; see Figure 1.
This was one of the first proposed designs for a one-dimensional superconductor. The endeavour to find room temperature superconductivity has led to renewed efforts both experimentally and theoretically in the avenue of one-dimensionality. Organic superconductors have long way to go before they can even catch up with their counterparts in the high temperature society, such as cuprates. These cuprates have a very impressive superconducting temperature \( T_c \): HgBa\(_2\)Ca\(_2\)Cu\(_3\)O\(_4\) has \( T_c \) around 140K [5]. Organic conducting polymers are considered as novel materials with a large potential for new applications. Doped polyacetylene broke the conduction barrier not long after Little’s proposal and even dominates polymer research platform today.

An intriguing concept with all these materials is their dependence on doping. This shouldn’t come as too much of a surprise, since increase in the amount of dopants either creates more charge or holes which can directly affect the electronic structure. In the case of cuprates for example strontium doped lanthanum cuprate \( \text{La}_{2-x}\text{Sr}_x\text{CuO}_4 \), the parent \( \text{La}_2\text{CuO}_4 \) is an insulating antiferromagnet, where \( x \) is the percentage of dopant. Upon addition of strontium the stoichiometry of the parent is changed in such a way that superconductivity is produced. It is for this reason that we have tried to calculate a general supercell with varying electron concentration \( n \).
It is believed that the onset of superconductivity in these \((\text{La}_{2-x}\text{Sr}_x\text{CuO}_4)\) ceramics is just the interplay between strong antiferromagnetic correlations and Mott transition in the proximity of half-filled bands [6].

5.2 Spin Peierls and Peierls distortions

In one-dimensional crystals, which are essentially linear chains, periodic distortions of the chains can introduce energy band gaps. These distortions are usually called Peierls distortions [8]. Peierls showed that a monoatomic metallic chain is unstable and will undergo a metal-insulator transition at low temperatures. This effect occurs as a consequence of electron-lattice coupling. Spin Peierls transition occurs when spins arranged in equidistant points on a lattice are changed into pairs. The lattice adjusts to paired arrangement of electrons, the elementary cell is doubled, and the Brillouin zone is halved. In comparison with previous models discussed here, Peierls and spin Peierls distortion are of great relevance to the research presented in this thesis.

Take a normal infinite chain with spacing \(a\) and hopping matrix \(t\). From Chapter 1, we recall that for a tight binding system of the type below in Figure 2 the energy dispersion is given by,

\[
E(k) = -2t \cos(ka) .
\]

![Figure 2](image)

If one now alters the chain in such a manner that it needs two hopping integrals instead of one, then the period of the chain doubles and as mentioned earlier the Brillouin zone folds in half, extending from \(-\frac{\pi}{2a}\) to \(\frac{\pi}{2a}\); see Figure 3.
Chapter 5

We can illustrate this by considering the above Figure 3, and determining its secular equation by the usual method, spin indices along with other interactions will be ignored just the hopping terms will be taken into account. Furthermore we assume that the distortion is only slight such that the lattice spacing can be taken as \( a \), Figure 3 above shows an exaggerated effect of distortion.

Site \( i \) \[ e^{ik(r+1)a}t_2\alpha + e^{ik(r-1)a}t_1\beta = E\alpha e^{ika} \]

Site \( i + 1 \) \[ e^{ik(r+1)a}t_1\alpha + e^{ik(r-1)a}t_3\alpha = E\beta e^{ika} \]

The determinant can be written thus,

\[
\begin{vmatrix}
-E & e^{ika}t_1 + e^{-ika}t_2 \\
 e^{ika}t_2 + e^{-ika}t_1 & -E
\end{vmatrix} = 0
\]

The new dispersion relation for the energy is shown in Figure 4. At the boundaries of the Brillouin zone, a gap has opened up of the magnitude \( 2|t_1 - t_2| \). If we take the electron filling \( n = 1 \), for the half-filled case, we find for the original undistorted chain Figure 2 the Fermi wave vector is \( k_F = \pm \frac{\pi}{2a} \). The distortion of the chain has split the band into lower and upper bands, with a well-defined band gap, the lower band is now completely full while the upper is empty. This is rather surprising since we started with a metallic state and have now ended up with an insulating state albeit with lower ground state energy (the sum of the energies of the occupied electronic states).
The lowering of the energy of the distorted chain is not limited to the half filled case: it could happen for any Fermi wave vector, $k_F$, in the undistorted chain (Chapter 6 will bring more light on this). The total energy of the system will be lowered by a periodic distortion of the lattice of wavelength $\frac{\pi}{k_F}$. The distortion is commensurate if the wavelength is a rational multiple of the lattice spacing; otherwise it is said to be incommensurate if the wavelength is an irrational multiple of the atomic spacing [10]. We are inevitably led to draw the conclusion that one-dimensional metals are not energetically stable, and the preferred ground state is that of an insulator.

### 5.3 Soliton lattice and charge density waves

A phase transition is marked by the fact that a particular change of the system has occurred; the most interesting part of the transition is the place (in one-dimension it’s a point) where this transition takes place, the phase separation. In one-dimensional systems, this phase separation can form a soliton lattice line. The soliton lattice states are characterised by a domain wall which separates say a degenerate ferromagnetic ground state into antiferromagnetic domain wall, see Figures 5 and 6 below, in
another words a wall between two symmetry related states. A soliton lattice is a lattice of domain walls.

![Figure 5. Domain Wall phase separation](image)

One can apply the sine-Gordon equation to the above scenarios and obtain a model solitonic solution [12] by considering the phase transition as a kink in space [14]. A soliton may then be viewed as the quasi-particle corresponding to solitary waves; it is free to move along the one-dimensional chain because the total energy of the system does not depend on the position of the soliton. However, a confined soliton may have to overcome an energy barrier before it can move from site to site. In polyacetylene, the solitons are free to move since it has a degenerate ground state [13]. A charge density wave (CDW) is a spatial modulation of the electron density given in Chapter 2.
as a sum of the local electron density per site. An essential feature of the CDW is its coupling with the mass density (the background ions) in real systems.

5.4 One-dimensional substances

Before the advent of conducting polymers, investigations of one-dimensional conductivity were mainly based on organic charge transfer salts. These salts were successfully grown into single crystals, which made them easy to work with [7]. Single crystals of TTF-TCNQ undergo metal-insulator transition and have very high conductivity in comparison with conventional organic conductors. These salts helped in understanding Peierls transition and CDW, although any attempts to find high temperature superconductivity were deemed futile.

Another example of charge transfer salt is that of Bechgaard salt, which comprises of an organic donor and an inorganic acceptor, and goes by the name of TMTSF. These salts tend to be metallic under normal conditions, and at low temperatures superconduct. Other Bechgaard salts undergo metal-insulator transition via the Peierls mechanism. Krogmann salts [9] are a good example for solids with only one set of chains, commonly known as KCP. Krogmann salts have a metallic chain which can undergo Peierls distortion.
5.5 Reference:


Chapter 6

In this chapter, we will introduce the computational procedure that minimises the energy of the Hubbard Hamiltonian using the Hartree-Fock approximation.

6 Computational method

Our task is to minimise the energy of the system with respect to N variables as efficiently as possible. Chart 1 highlights the overall picture of the computational code developed for the minimisation of the HF energies. In the unrestricted Hartree-Fock approximation we minimise with respect to all the parameters. This is a very difficult task for a large system as the energy differences between local minima may be tiny. In chapter 2, where most of the underlying mathematics was developed for the computational method, a mention was made about the self-consistent procedure. This is a very powerful method as it can solve a complex problem by iteration procedure.

Yang et al [1], Poilblanc et al [2], Kato et al [5] and many other authors in the literature utilise the self-consistent iteration procedure. It is a rather straightforward task to implement such a procedure. Given an initial distribution of the spin-up and spin-down densities, the relevant mean-field band Hamiltonian is numerically diagonalised. The expectation values of the density operator are then calculated; these in turn are used to calculate a new distribution of spin-up and spin-down densities. The procedure is repeated using these updated values of spin-up and spin-down densities until a convergence is reached. An important point to note is that the initial guess for the parameter must be good enough to render convergence, otherwise the procedure would never converge.

This procedure was applied to our problem. Admittedly it is quite fast if one happens to be near the convergence limit, otherwise it is slower than the minimisation approach. Another disadvantage is that different initial conditions can sometimes lead
to a different convergent solution. Then one has no choice but to try many different initial conditions, and pick the lowest-energy solution as the ground state.

After weighing the advantages and disadvantages of the self-consistent procedure, we return to the minimisation procedure. This has a clear advantage that a convergence is guaranteed for almost any initial condition, we say almost because there are times when no convergence will take place, and then one needs to change the initial conditions. A discussion is in order for Chart 1. It gives an overview of the minimisation procedure without mentioning the detailed structure of the C++ code, however Charts 2 and 3 are more involved in terms of the C++ functions [3] employed in the actual program.

**Powell's method** is utilised thoroughly, since it is a direction-set method that uses a search matrix. The search matrix is initialised at the beginning of the algorithm. If we start at point \( P \) and proceed in some direction \( n \), then our minimisation routine proceeds to some minimum point and change the search direction and carries on along the second direction to its minimum, cycling through the whole set of directions as many times as necessary, until the function stops decreasing.
Chapter 6: Computational Method

Minimisation

1. Initialise all the Parameters

   - For the particular Cell Size calculate the Bandstructure and the moments, $E(k)$

2. Calculate the Fermi level $E_F$

3. Integrate up to the Fermi Level

4. Calculate $H_{HF}$

5. Make a New Guess for the Parameters.

   - $n = n + \delta n$

   - Use these parameters as a guess for new ones

   - $E_{HF} = \min_{\{n\}} H_{HF}$

   - Does the filling $n=1$?

     - No

     - Yes

     - Use these parameters as a guess for new ones

End Minimisation

Chart 1: Showing complete schematic of the C++ code.
Chapter 6 Computational Method

The procedure \texttt{linmin} above finds the minimum of the function \texttt{Func}, and the procedure \texttt{qgaus} in Chart 3 integrates a function by Gaussian quadratures.
Chapter 6  Computational Method

As Chart 1 shows the code starts with an initialisation condition, setting all the trial parameters as follows:

1) The cell size
2) Respective Brillouin zone
3) The value of electron filling
4) The value of the Stoner parameter $U$
5) Number of quantisation k-points within the Brillouin Zone
6) Parameters to be minimised
7) The tolerance of the calculation, high tolerance meaning more computational time.

A secular equation is required for the cells before the bandstructure can be computed.
The Figures (1,2) above show an example of a super cell with 2 and 3 sites. Already the number of parameters required for minimisation is getting out of hand: this is where symmetry considerations must be taken into account. The number of parameters may then be reduced by the judicious use of symmetry. For the three-site case the number of parameters is 10, which includes the Z parameter, the angle between cells, assuming everything is coplanar.

We will recall from Chapter 2, where spin quantisation was transformed from the sites into the bonds; this transformation needs to be applied again for our many sites HF Hamiltonian. Previously we had the liberty of solving our Hamiltonian analytically for the one site case but in general, this is not the case. Only for very certain special configuration such as those discovered by Samson [4], the Double Spin Density Waves can one solve the secular equation analytically.

### 6.1 Two Sites

As Figure 1 above shows the number of parameters to minimise is seven assuming everything is coplanar.

\[
H_{HF} = -\sum_{ij} t_{ij} U^\dagger(i) \rho U(j) a_i^\dagger d_j - \sum_i \frac{1}{2} \Delta \sigma_{ij} ^{\dagger} b_{ia}^\dagger b_{ib} + \omega_i n_i
\]  

\[\vec{t}_{ij} = t_{ij} U^\dagger(i) U(j)\]  

The hopping matrices for each site can be written down explicitly,

For \( r \) even,

\[
\vec{t}_{r,r+1} = \begin{pmatrix}
\cos \frac{1}{2} (\theta_1 - \theta_2) & \sin \frac{1}{2} (\theta_1 - \theta_2) \\
-\sin \frac{1}{2} (\theta_1 - \theta_2) & \cos \frac{1}{2} (\theta_1 - \theta_2)
\end{pmatrix}
\]
\[ \tilde{\tau}_{r,r-1} = \begin{pmatrix} \cos \frac{1}{2}(\theta_1 - \theta_2 + Z) & \sin \frac{1}{2}(\theta_1 - \theta_2 + Z) \\ -\sin \frac{1}{2}(\theta_1 - \theta_2 + Z) & \cos \frac{1}{2}(\theta_1 - \theta_2 + Z) \end{pmatrix} \]  \quad (4)

For \( r \) odd.

\[ \tilde{\tau}_{r,r+1} = \begin{pmatrix} \cos \frac{1}{2}(\theta_2 - \theta_1 - Z) & \sin \frac{1}{2}(\theta_2 - \theta_1 - Z) \\ -\sin \frac{1}{2}(\theta_2 - \theta_1 - Z) & \cos \frac{1}{2}(\theta_2 - \theta_1 - Z) \end{pmatrix} \]  \quad (5)

\[ \tilde{\tau}_{r,r-1} = \begin{pmatrix} \cos \frac{1}{2}(\theta_2 - \theta_1) & \sin \frac{1}{2}(\theta_2 - \theta_1) \\ -\sin \frac{1}{2}(\theta_2 - \theta_1) & \cos \frac{1}{2}(\theta_2 - \theta_1) \end{pmatrix} \]  \quad (6)

Taking the Bloch states as,

\[ \Psi_k(r) = \begin{cases} \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} e^{ikr}, & r \text{ even} \\ \begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} e^{ikr}, & r \text{ odd} \end{cases} \]  \quad (7)

Our Schrödinger equation becomes:

(\text{r even})

\[ -\begin{pmatrix} \cos \frac{1}{2}(\theta_1 - \theta_2) & \sin \frac{1}{2}(\theta_1 - \theta_2) \\ -\sin \frac{1}{2}(\theta_1 - \theta_2) & \cos \frac{1}{2}(\theta_1 - \theta_2) \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} e^{ik(r+1)} \]

\[ -\begin{pmatrix} \cos \frac{1}{2}(\theta_1 - \theta_2 + Z) & \sin \frac{1}{2}(\theta_1 - \theta_2 + Z) \\ -\sin \frac{1}{2}(\theta_1 - \theta_2 + Z) & \cos \frac{1}{2}(\theta_1 - \theta_2 + Z) \end{pmatrix} \begin{pmatrix} c \\ d \end{pmatrix} e^{ik(r-1)} \]

\[ -\frac{1}{2} \Delta_k \begin{pmatrix} a \\ -b \end{pmatrix} e^{ikr} + w_k \begin{pmatrix} a \\ b \end{pmatrix} e^{ikr} = E \begin{pmatrix} a \\ b \end{pmatrix} e^{ikr} \]  \quad (8)

(\text{r odd})

\[ -\begin{pmatrix} \cos \frac{1}{2}(\theta_2 - \theta_1 - Z) & \sin \frac{1}{2}(\theta_2 - \theta_1 - Z) \\ -\sin \frac{1}{2}(\theta_2 - \theta_1 - Z) & \cos \frac{1}{2}(\theta_2 - \theta_1 - Z) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} e^{ik(r+1)} \]

\[ -\begin{pmatrix} \cos \frac{1}{2}(\theta_2 - \theta_1) & \sin \frac{1}{2}(\theta_2 - \theta_1) \\ -\sin \frac{1}{2}(\theta_2 - \theta_1) & \cos \frac{1}{2}(\theta_2 - \theta_1) \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} e^{ik(r-1)} \]

\[ -\frac{1}{2} \Delta_k \begin{pmatrix} c \\ -d \end{pmatrix} e^{ikr} + w_k \begin{pmatrix} c \\ d \end{pmatrix} e^{ikr} = E \begin{pmatrix} c \\ d \end{pmatrix} e^{ikr} \]  \quad (9)

both of these equations can be combined into single determinant matrix.
\[
\begin{pmatrix}
-\frac{1}{2}\Delta_1 + w_1 & 0 & -e^{ik}c_\alpha - e^{-ik}c_\beta & -e^{ik}s_\alpha - e^{-ik}s_\beta \\
0 & 1/2\Delta_1 + w_1 & e^{ik}s_\alpha + e^{-ik}s_\beta & -e^{ik}c_\alpha - e^{-ik}c_\beta \\
-e^{ik}c_\beta - e^{-ik}c_\alpha & e^{ik}s_\beta + e^{-ik}s_\alpha & -1/2\Delta_2 + w_2 & 0 \\
-e^{ik}s_\beta - e^{-ik}s_\alpha & -e^{ik}c_\beta - e^{-ik}c_\alpha & 0 & 1/2\Delta_2 + w_2
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
a \\
b \\
c \\
d
\end{pmatrix} = E
\begin{pmatrix}
a \\
b \\
c \\
d
\end{pmatrix}
\]

where \( c_\alpha = \cos \frac{1}{2}(\theta_1 - \theta_2) \), \( c_\beta = \cos \frac{1}{2}(\theta_1 - \theta_2 + Z) \),
\( s_\alpha = \sin \frac{1}{2}(\theta_1 - \theta_2) \), \( s_\beta = \sin \frac{1}{2}(\theta_1 - \theta_2 + Z) \).

For the simplified case of DSDW mentioned above, \( \theta_1 = 0 \) and \( Z = \pi \). The secular equation reduces to,

\[
\begin{pmatrix}
-\frac{1}{2}\Delta - E & 0 & -e^{ik}\widetilde{c} - e^{-ik}\widetilde{s} & e^{ik}\widetilde{s} - e^{-ik}\widetilde{c} \\
0 & \frac{1}{2}\Delta - E & -e^{ik}\widetilde{s} + e^{-ik}\widetilde{c} & e^{ik}\widetilde{c} - e^{-ik}\widetilde{s} \\
-e^{ik}\widetilde{s} - e^{-ik}\widetilde{c} & e^{ik}\widetilde{c} - e^{-ik}\widetilde{s} & -\frac{1}{2}\Delta - E & 0 \\
e^{ik}\widetilde{c} + e^{-ik}\widetilde{s} & -e^{ik}\widetilde{s} - e^{-ik}\widetilde{c} & 0 & \frac{1}{2}\Delta - E
\end{pmatrix}
\Rightarrow
\begin{pmatrix}
a \\
b \\
c \\
d
\end{pmatrix} = 0. \tag{11}
\]

where \( \widetilde{c} = \cos(\frac{\theta}{2}) \), and \( \widetilde{s} = \sin(\frac{\theta}{2}) \).

The four analytical bands can easily be found from the determinant.

\[
E = \pm \sqrt{\left(\frac{1}{4}\Delta^2 + 2\right) + \sqrt{\Delta^2 (1 + 2\cos 2k \sin \theta) + 4 \sin^2 2k}} \tag{12}
\]

\[-\frac{\pi}{2} \leq k \leq \frac{\pi}{2} \quad \text{(First Brillouin Zone)}\]

Similar procedure needs to be applied for any number of sites.
6.2 Three sites

For three sites the algebra is a little more involved, taking the Bloch fermion spinors as,

\[
\Psi_k(r) = \begin{pmatrix}
a \\
b \\
c \\
d \\
e \\
f
\end{pmatrix} e^{ikr}
\]

For \( r \) on the left of unit cell,

\[
\tilde{t}_{r,r+1} = \begin{pmatrix}
\cos \frac{1}{2} (\theta_1 - \theta_2) & \sin \frac{1}{2} (\theta_1 - \theta_2) \\
-\sin \frac{1}{2} (\theta_1 - \theta_2) & \cos \frac{1}{2} (\theta_1 - \theta_2)
\end{pmatrix} = \begin{pmatrix}
c_\alpha & s_\alpha \\
-s_\alpha & c_\alpha
\end{pmatrix}
\]

(13)

For \( r \) on the middle moment,

\[
\tilde{t}_{r,r+1} = \begin{pmatrix}
\cos \frac{1}{2} (\theta_1 - \theta_3 + Z) & \sin \frac{1}{2} (\theta_1 - \theta_3 + Z) \\
-\sin \frac{1}{2} (\theta_1 - \theta_3 + Z) & \cos \frac{1}{2} (\theta_1 - \theta_3 + Z)
\end{pmatrix} = \begin{pmatrix}
c_\beta & s_\beta \\
-s_\beta & c_\beta
\end{pmatrix}
\]

(14)

(15)

For \( r \) on the middle moment,

\[
\tilde{t}_{r,r+1} = \begin{pmatrix}
\cos \frac{1}{2} (\theta_2 - \theta_1) & \sin \frac{1}{2} (\theta_2 - \theta_1) \\
-\sin \frac{1}{2} (\theta_2 - \theta_1) & \cos \frac{1}{2} (\theta_2 - \theta_1)
\end{pmatrix} = \begin{pmatrix}
c_\alpha & -s_\alpha \\
s_\alpha & c_\alpha
\end{pmatrix},
\]

(16)

and

\[
\tilde{t}_{r,r+1} = \begin{pmatrix}
\cos \frac{1}{2} (\theta_2 - \theta_3) & \sin \frac{1}{2} (\theta_2 - \theta_3) \\
-\sin \frac{1}{2} (\theta_2 - \theta_3) & \cos \frac{1}{2} (\theta_2 - \theta_3)
\end{pmatrix} = \begin{pmatrix}
c_r & s_r \\
-s_r & c_r
\end{pmatrix}
\]

(17)
For \( r \) on the right moment,

\[
\begin{pmatrix}
\cos(-\frac{1}{2}(\theta_2 - \theta_3)) & \sin(-\frac{1}{2}(\theta_2 - \theta_3)) \\
-sin(-\frac{1}{2}(\theta_2 - \theta_3)) & \cos(-\frac{1}{2}(\theta_2 - \theta_3))
\end{pmatrix}
= \begin{pmatrix}
c_r & -s_r \\
s_r & c_r
\end{pmatrix}
\tag{18}
\]

\[
\begin{pmatrix}
\cos(-\frac{1}{2}(\theta_1 - \theta_3 + Z)) & \sin(-\frac{1}{2}(\theta_1 - \theta_3 + Z)) \\
-sin(-\frac{1}{2}(\theta_1 - \theta_3 + Z)) & \cos(-\frac{1}{2}(\theta_1 - \theta_3 + Z))
\end{pmatrix}
= \begin{pmatrix}
c_\beta & -s_\beta \\
s_\beta & c_\beta
\end{pmatrix}
\tag{19}
\]

So the complete Schrödinger equation becomes,

\[(r\text{-left})\]

\[
-\begin{pmatrix}
c_\alpha & s_\alpha \\
-s_\alpha & c_\alpha
\end{pmatrix}
\begin{pmatrix}
e \\
d
\end{pmatrix}e^{ik(r+1)}
- \begin{pmatrix}
c_\beta & s_\beta \\
-s_\beta & c_\beta
\end{pmatrix}
\begin{pmatrix}
e \\
f
\end{pmatrix}e^{ik(r-1)}
- \frac{1}{2}\Delta_1 \begin{pmatrix}
a \\
b
\end{pmatrix}e^{i\sigma_r} + w_1 \begin{pmatrix}
a \\
b
\end{pmatrix}e^{i\sigma_r} = E \begin{pmatrix}
a \\
b
\end{pmatrix}e^{i\sigma_r}
\tag{20}
\]

\[(r\text{-middle})\]

\[
-\begin{pmatrix}
c_\gamma & s_\gamma \\
-s_\gamma & c_\gamma
\end{pmatrix}
\begin{pmatrix}
e \\
f
\end{pmatrix}e^{ik(r+1)}
- \begin{pmatrix}
c_\alpha & s_\alpha \\
-s_\alpha & c_\alpha
\end{pmatrix}
\begin{pmatrix}
e \\
f
\end{pmatrix}e^{ik(r-1)}
- \frac{1}{2}\Delta_2 \begin{pmatrix}
c \\
d
\end{pmatrix}e^{i\sigma_r} + w_2 \begin{pmatrix}
c \\
d
\end{pmatrix}e^{i\sigma_r} = E \begin{pmatrix}
c \\
d
\end{pmatrix}e^{i\sigma_r}
\tag{21}
\]

\[(r\text{-right})\]

\[
-\begin{pmatrix}
c_\beta & s_\beta \\
-s_\beta & c_\beta
\end{pmatrix}
\begin{pmatrix}
a \\
b
\end{pmatrix}e^{ik(r+1)}
- \begin{pmatrix}
c_\gamma & s_\gamma \\
-s_\gamma & c_\gamma
\end{pmatrix}
\begin{pmatrix}
e \\
d
\end{pmatrix}e^{ik(r-1)}
- \frac{1}{2}\Delta_2 \begin{pmatrix}
e \\
f
\end{pmatrix}e^{i\sigma_r} + w_2 \begin{pmatrix}
e \\
f
\end{pmatrix}e^{i\sigma_r} = E \begin{pmatrix}
e \\
f
\end{pmatrix}e^{i\sigma_r}
\tag{22}
\]

where \( c_\alpha = \cos\frac{1}{2}(\theta_1 - \theta_2) \), \( c_\beta = \cos\frac{1}{2}(\theta_1 - \theta_3 + Z) \), \( c_\gamma = \cos\frac{1}{2}(\theta_2 - \theta_3) \)
\[ s_\alpha = \sin \left( \frac{1}{2}(\theta_1 - \theta_2) \right), \quad s_\beta = \sin \left( \frac{1}{2}(\theta_1 - \theta_3 + Z) \right), \quad s_\gamma = \sin \left( \frac{1}{2}(\theta_2 - \theta_3) \right), \text{and setting } t_{ij} = 1. \]

The secular equation for the three-site case can now be written down as,

\[
\begin{pmatrix}
-\frac{1}{2}\Delta_1 + w_1 & 0 & -e^{ik}c_\alpha & -e^{ik}s_\alpha & -e^{-ik}c_\beta & -e^{-ik}s_\beta \\
0 & \frac{1}{2}\Delta_1 + w_1 & e^{ik}s_\alpha & -e^{ik}c_\alpha & e^{-ik}s_\beta & -e^{-ik}c_\beta \\
-e^{-ik}c_\alpha & e^{-ik}s_\alpha & -\frac{1}{2}\Delta_2 + w_2 & 0 & -e^{ik}c_\gamma & -e^{-ik}s_\gamma \\
-e^{-ik}s_\alpha & -e^{-ik}c_\alpha & 0 & \frac{1}{2}\Delta_2 + w_2 & e^{ik}s_\gamma & -e^{-ik}c_\gamma \\
-e^{ik}c_\beta & e^{ik}s_\beta & -e^{-ik}c_\gamma & e^{-ik}s_\gamma & -\frac{1}{2}\Delta_3 + w_3 & 0 \\
-e^{ik}s_\beta & -e^{ik}c_\beta & -e^{-ik}s_\gamma & -e^{-ik}c_\gamma & 0 & \frac{1}{2}\Delta_3 + w_3 \\
\end{pmatrix}
\begin{pmatrix}
a \\
b \\
c \\
d \\
e \\
f \\
\end{pmatrix}
= E
\begin{pmatrix}
a \\
b \\
c \\
d \\
e \\
f \\
\end{pmatrix}
\]

(23)

### 6.3 Four and more sites

Following exactly the same procedure as above we can write down the secular equations for any number of sites. These matrices are then directly implemented into the computational code, where appropriate diagonalisation of these matrices is carried out to obtain the bandstructure.
Chapter 6

Computational Method

Chart 3. Energy Evaluation

Charts 2 and 3 highlight the bare essentials of the C++ minimisation code. Certainly one can always find an equation for a general electronic configuration, but it cannot be solved analytically, frequently one has to resort to numerical approximations for the band structures. The function VHF also has the crucial task of evaluating the Fermi Surface, thereby giving the limits of the integration. A closer examination of the function VHF will reveal its complexity in form and structure.

In the first instance VHF(a) was implemented in the code, however even though this approach of guessing initial $E_F$ was very fast, it ran into difficulties at certain values
of electron density $n$. So another more robust method was devised which evaluated $E_F$ by sorting procedure (VHF(b)).

The initialisation procedure calculates the bandstructures for particular values of $(\{\Delta_i, w_i\}, \theta_i)$ related to the size of the cell with $i$ sites.

![Diagram](image1)

**Figure 3** Example of two site cell containing two electrons DSDW

![Diagram](image2)

**Figure 4.** Paramagnetic Bandstructure

We use the paramagnetic case as an example to illustrate the computational procedure. Symmetry of the system is fully utilised in order to simplify the calculations, as Figure (4) shows only one of the quadrant needs to be considered, hence the lower right hand quadrant is chosen (Figure 5). This may not be true for two- and three-site supercells in which case we need to consider the whole of the Brillouin zone.
Chapter 6  Computational Method

Figure 5. Two lowest bands

For the configuration in Figure 1, the secular equation may be calculated in the usual manner as described in chapter 2. We set $n$ the electron density to some value and then evaluate the corresponding Fermi surface. The intercept of the Fermi surface immediately gives the wavevectors $k_{\alpha,\beta}$ so that one is able to integrate the area bound by the bands to evaluate the energy $VHF$ Figure 6.

Figure 6. Integration of the lowest band.

As $n$ is increased incrementally, the Fermi surface rises into the neighbouring band. One has to be very careful as not to miss out the lower band in the integration, which
could lead to spurious result. The process of determining which region(s) to include in the integration can be very delicate as the complexity of the cell increases, hence increasing the number of bands. The code has to cleverly distinguish this feature without costing too much in computational time.

In cases where there is an overlap of the bands shaded region in Figure 7 represents the integration area, the darker shade is where there is an overlap of curve one and two. Notice how the integration limits have changed in Figure 7.

![Figure 7. Integration of two bands.](image)

Once the correct region is selected then VHF is found by integrating the area. The Hartree Fock energy is calculated from the equations developed in chapter 2, namely

\[
E_{HF} = V_{HF} + \frac{1}{N_a} \sum_i \frac{\Delta^2_i}{4U} + \frac{1}{N_a} \sum_i w_i n_i + \frac{1}{N_a} \sum_i \frac{U}{4} n_i^2 \tag{24}
\]

Most of the computational power is used in the next step, where the minimisation of the above function is carried out meticulously. Literally many days even weeks can pass before one can get a meaningful result. This is beauty of the one-dimensional problem, it is extremely rich with a large number of local minima packed closely together. It is enough for us that the algorithm represents an upper bound to the actual ground state.
The computational procedure amounts to that of discretisation of a general analytical secular equation, hence with an increasing number of points of discretisation the greater the accuracy is achieved. There is of course a trade off between the degree of accuracy and the time taken for the computation, which is the usual computational scenario for any realistic physical problem one tries to tackle.
6.4 Reference:


Chapter 7

In this Chapter we report the results of our calculations, and give a general discussion on the results.

7 Spin texture selection in the one-dimensional Hubbard Model

The Hartree-Fock (HF) approximation to the Hubbard model is not a perturbative technique but a variational mean-field approximation. This both its greatest strength and greatest weakness. As will be shown, HF predicts magnetism, which is non-perturbative phenomenon. In dimension $d>1$ there are no exact solutions, it can be difficult to quantify errors involved and therefore decide whether it is a good approximation or not. For the one-dimensional case, Lieb and Wu [1] have obtained an exact solution, based on which other workers have obtained exact correlation functions in the one-dimensional Hubbard model [2] [3].

In spite of the existence of these exact results, our HF mean-field is instructive and meaningful, because it allows us to obtain a more direct physical picture of the many-body correlations. While at the same time it determines the limitations of the HF approximation under the extreme conditions of one-dimensionality. This puts the HF approximation on a firmer basis in two and three dimensions where no exact results are available. At least on a qualitative level there is a general tendency for the mean-field theories to be independent of dimensionality, which means our results can give some indications on what to expect in higher dimension.

To date a lot of effort has been expended in determining the correct ground state spin configurations of the one-band Hubbard model. One can not find a systematic study of the phase diagram at $T=0$ including the effects of a charge and spin correlations, within the unrestricted HF method. The exact results [8] shows that the ground state has zero total magnetic moment with short-range antiferromagnetic (AF) and charge correlations.
Andriotis et al [19] have studied the one-dimensional Hubbard model on a periodic lattice. They performed similar supercell calculations with collinear spins with low doping. As we have shown above, they also find a phase separation with ferromagnetic and antiferromagnetic regions of the supercell. Kishigi et al [20] look at coexistence of CDW and SDW in the one-dimensional quarter filled Hubbard model, their findings support our results. Caprara et al [21] study the effects of a chemically or deformation induced CDW on the SDW ground state of the Hubbard model at half-filling using the slave-boson approach.

Majority of the literature surveyed concentrates on the two-dimensional Hubbard model, many groups employing the unrestricted HF calculations. Chu [22] looks at the square lattice Hubbard model with low doping and collinear spins, and finds a soliton lattice formed by antiferromagnetic domains with periodic discommensurations. The excess holes are localised at the discommensurations, and the periodicity opens a gap at the Fermi level. Yang et al [23] show that the holes coalesce into lines or other one-dimensional structures forming so-called spin bags [24]. A nearest-neighbour repulsion term suppresses the alignment. Kato et al [9] and Poilblanc et al [25] obtain similar results.

Fujita et al [27] find the soliton lattices in the two-dimensional Hubbard model more stable than the SDW near the half filling. For quarter filled case they find a windmill type structure where the spins are point towards each other, which resembles the case of DSDW obtained here. Magnetic polarons, domain walls and vortices are among the numerous configurations found by Vergés et al [12]. These vortices are metastable, thus giving a lot of nearly degenerate states. Schulz [31] finds for small U that the linearly polarised incommensurate SDW is stable.

There have been various other studies of the instability of the uniform SDW. Chubukov et al [13] look at the stability of the $(\theta, \theta)$ spiral fluctuations and show that it breaks up into domain walls. The $(\pi, \theta)$ spiral is unstable to non-coplanar spin configuration. Arrigoni et al [15] show that phase separation occurs for the SDW according to Maxwell construction, between hole-rich and hole-poor phases. This is due to an anomalous decrease in chemical potential with doping. Zhou et al [28] look at the excitations of the SDW, which can lead to an instability of the soliton lattice.
They don’t find any non-coplanar states. A slave-boson study is done by Fréesard et al [26] their results are refinement of HF approximations. Similar approach is taken by Auerbach et al [29] in their study of the t-J model, they show that the SDW is unstable to fluctuations. Sarker et al [30] perform a HF analysis on the Hubbard model they find domain walls and spiral states with phase separation.

A comparative study of collinear and spiral SDW in a free electron model by Kotani [32] has shown that the collinear states are more stable and stabilise further when harmonics are taken into account. Ichimura et al [33] consider the soliton lattice as well as vortex lattices, and show that the vortex lattices are less favoured apart from the windmill lattice.

### 7.1 Spin Spirals

The spin direction is assumed unique (say the $z$-direction), and the possibility of non-coplanar spin arrangements is discarded based on the literature survey. This justified, since the stability of spin spiral density wave outweighs that of helical modulation [9][11], although one can not rule out the non-collinear spin arrangements altogether. Experimentally spin spirals have been observed in the $V_2O_{3-x}$ compounds [7]. One has the advantage of only taking the diagonal terms of the Pauli spin matrices along with $\sigma_x$, in contrast to the non-collinear case considered by Crockford et al [10].

### 7.2 Single site supercells.

The results for a single site unit cell show that only spin spirals of the type shown in Chapter 2 exist, computational they are easiest to calculate since only a single cell is involved. The addition of a field term $w$ merely adjusts the Fermi level, and it becomes zero upon minimisation, hence the only spin textures to survive are the spin spiral density wave (SS).

The ground state energy is show in Figure 1. $U = 4t$ is chosen so that a comparison may be made with other researchers [4][5]. The self-consistent order parameter $\Delta$ is
shown in Figure 2. The critical onset of the angle between the sites is shown in Figure 3. The magnetisation is shown in Figure 4.

Figure 1. Ground state energy for $U=4t$ in the one-site approximation.

Figure 2. Variation of $\Delta$ with electron filling.

Figure 3. The magnetisation is shown in Figure 4.
These results are in exact agreement with those obtained by Samson [6]. We find for a simple single site, the ground state configurations are coplanar. Most studies done in the two-dimensional Hubbard model also find coplanar spin textures. Verges et al [12] have pointed out the interesting fact about the self-consistent solutions of the HF approximations explicitly the spins either lie along a single direction or are completely coplanar. However, Chubukov et al [13] find some evidence for the non-coplanar textures.

7.3 Two-sites

For the two-site problem, we could ask the following questions:

1) Is there a non-uniform charge density wave (NCDW) which is lower in energy than the ground state energy of the SSDW?
2) Are there any new ground state configurations?
To our surprise, only a DSDW type of configuration was found, similar to one found by Samson [6] for the two-site case. The main quantitative difference being that our ground state shows a continuous change from a metallic SS to insulating DSDW state. The other differences are because of quantisation of the k-space, where each energy band is divided between 300 to 4000 points. Increasing the number of points increases the accuracy at the detriment of computational time.
A comparison of the ground state energy with that of the paramagnetic HF state, shows the paramagnetic state is always unstable for $U>0$ in one dimensions. Perfect nesting ensures that the band susceptibility diverges at the Fermi wave vector $2k_F$, like the spin Peierls system discussed in Chapter 5. A collinear spin density wave represents the electrons with a spatially varying potential, which opens a gap at the Fermi energy thus stabilising the SS and DSDW collinear configurations.

For very large number of points (4000) per band as the Figure 5 below shows, we can reproduce the results to high degree of accuracy.

Figure 5. Ground state energy of the one-dimensional Hubbard model with $U=4t$

Notice the kink in the SS energy curve it occurs at exactly $n=0.5$ filling. The same is true for $n=1.5$ due to electron-hole symmetry of the system. It is for this reason we restrict ourselves to the range $0 \leq n \leq 1$. The collinear DSDW phases live around this region of the kink, and clearly they are lower in energy than the SS. The top curve is
for the paramagnetic phase \( (\Delta = 0) \). The curve emerging from the paramagnetic phase is that of the DSDW phase obtained by Samson, it agrees exceedingly well with ours.

The exchange coupling \( \Delta \) is modified likewise.

![Graph: Delta on both sites vs. Electron density](image)

**Figure 6. Variation of the Delta band gaps on both sites.**

We can take an explicit glance at the ground state energies for various configurations in order to make sure we are seeing the correct picture.

Electron filling \( n=0.3 \) and \( Z=0 \) we get the following:
Chapter 7 Spin Texture Selection in the 1D Hubbard Model

\[ Z = 0 \quad \theta_1 = 0 \quad \theta_2 = \theta \]

Figure 7 Ground state energy for \( U=4t \)

\[ Z = \pi \quad \theta_1 = 0 \quad \theta_2 = \theta \]

Figure 8. Ground state energy for \( U=4t \)

Bandstructure \( Z = 0, \theta = 0 \)

Figure 9. Bandstructure for \( n=0.3 \) \( \Delta_{1,2} = 1.2005 \) \( \nu_{1,2} = 0 \) \( \theta_{1,2} = 0 \) \( Z = 0 \)
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The lowest energy is achieved when $Z = 0$ and $\theta = 0$, we then have saturated ferromagnetism $\uparrow \uparrow \uparrow \uparrow$. The upper bands are above the Fermi surface (Figure 9), only the lowest band contributes to the ground state energy. The band structure gives a simple two-point Fermi surface. Further investigations will allow us to calculate the FM and SS phase boundary. We know from Chapter 2, the dispersion energy of the SS is given by when $\theta = Q$:

$$E(k) = -2\cos k \cos \frac{1}{2}Q \pm \sqrt{\frac{1}{4} \Delta^2 + 4(\sin^2 k \sin^2 \frac{1}{2}Q)}$$

For the lowest band we can use binomial expansion and expand in terms of the exchange splitting $\Delta$ and wave vector $Q$ up to fourth order in $Q$.

$$E(k) = -2\cos k(1 - \frac{1}{8}Q^2 + \frac{1}{384}Q^4 + \ldots) - \frac{1}{2}\Delta(1 + \frac{1}{16} \sin^2 k(\frac{1}{4}Q^2 - \frac{1}{48}Q^4 + \ldots)$$

$$- \frac{1}{8} \frac{\Delta^2}{\Delta^2} \sin^4 k(\frac{1}{16}Q^4 + \ldots)$$

$$E(k) = -\frac{1}{2}\Delta - 2\cos k + (\frac{1}{4}\cos k - \frac{1}{8}\sin^2 k)Q^2$$

$$+ (-\frac{1}{192}\cos k + \frac{1}{16}\sin^2 k - \frac{1}{8}\sin^4 k)Q^4 + O(Q^6)$$

Now the HF energy $E_{HF}$ is given by,

$$E_{HF} = \frac{1}{2\pi} \int_{-\pi}^{\pi} dk E(k) + \frac{\Delta^2}{4U} + \frac{Un^2}{4}$$

$$E_{HF} = \frac{\Delta^2}{4U} + \frac{Un^2}{4} + (-\frac{1}{2}\Delta n - \frac{2}{\pi}\sin n\pi)$$

$$+ (\frac{1}{4\pi}\sin n\pi + \frac{1}{8}(\sin 2n\pi - \frac{1}{2}n))Q^2$$

$$+ (-\frac{1}{192\pi}\sin n\pi + \frac{1}{16\pi}\sin 2n\pi + \frac{1}{4\pi}\sin 4n\pi))Q^4 + O(Q^6)$$

Saturated ferromagnetism has $Q = 0$, and writing $\Delta = Un - \xi$ then the HF energy can be written as:
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\[ E_{HF} = \frac{\xi^2}{4U} - \frac{2}{\pi} \sin n\pi \]  

(4)

Which implies that if FM exists, it is saturated i.e. \( \xi = 0 \). This independence of the energy follows from the fact that double occupancy is forbidden in the saturated FM. To calculate the stability of FM state, we need to only consider the second partial derivative with respect to \( Q \).

\[ \frac{\partial^2 E_{HF}}{\partial Q^2} \bigg|_{\xi=0, Q=0} > 0 \]  

(5)

\[ \frac{\partial^2 E_{HF}}{\partial Q^2} \bigg|_{\xi=0, Q=0} = \frac{2}{\pi} \sin n\pi + \frac{1}{Un} \left( \frac{1}{2\pi} \sin 2n\pi - n \right) \]  

(6)

\[ \Rightarrow \frac{2}{\pi} \sin n\pi + \frac{1}{Un} \left( \frac{1}{2\pi} \sin 2n\pi - n \right) > 0 \]  

(7)

\[ \Rightarrow U > U_e(n) = \frac{2\pi n - \sin 2n\pi}{n \sin \pi n} \]  

(8)


---

**Figure 10. FM Phase boundaries**
For the minimum ground state energy around quarter filling \( n=0.5 \). Figures 11 and 12 show that the saturated spin spirals have given way to DSDW phase. Since the minimum occurs for \( Z=\pi \) both \( \theta_1, \theta_2 = 0 \); this type of configuration takes place \( \uparrow \uparrow \downarrow \downarrow \).

\[
\begin{align*}
Z = \pi & \quad \theta_1 = 0 \quad \theta_2 = \theta \\
-0.67 & \quad -0.672 & \quad -0.674 & \quad -0.676 & \quad -0.678 & \quad -0.68 & \quad -0.682 \\
0 & \quad 90 & \quad 180 \\
\end{align*}
\]

Figure 11. Ground state energy \( U=4t \)

\[
\begin{align*}
Z = 0 & \quad \theta \\
-0.59 & \quad -0.6 & \quad -0.61 & \quad -0.62 & \quad -0.63 & \quad -0.64 & \quad -0.65 \\
0 & \quad 90 & \quad 180 \\
\end{align*}
\]

Figure 12. Ground state energy for \( U=4t \)
Chapter 7  
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Band structure for double antiferromagnet (DSDW)

Figure 13. \( n=0.5 \ \Delta_{1,2} = 1.3606 \ \omega_{1,2} = 0 \ \theta_{1,2} = 0 \ Z = \pi \)

For filling \( n=1 \) and \( Z = \pi \)

\[ Z = \pi \]

Figure 14. Ground state energy

\[ Z = 0 \]

Figure 15. Ground state energy
Here the minimum is at exactly $\theta = \pi$ and $Z = 0$. The two-sites are equivalent to one site AFM when $\theta_1 = \theta$ and $Z = \pi$.

We wish to calculate the complete phase diagram for the two-site case.

### 7.4 Phase Separation within the Hubbard Model

Phase separation happens if the ground state energy in Figure 5 is not convex. Marder et al [14] give a concise illustration of the Maxwell construction in their mean-field calculations of the t-J model. Marder et al [14] predict that for low $U$ the ground state of the system can be phase separated state consisting of one antiferromagnetic (AF) domain and another canted state. We must emphasis the facts that the exact results of the one-dimensional Hubbard model do not show such phase separations, the 1D results give a unique phase over the whole $U - n$ phase [8][15].

Given a band filling $n$, and taking the values $n_\alpha < n < n_\beta$, then the homogeneous state is unstable if the following relations apply:
\[ E(n) > aE(n_\alpha) + bE(n_\beta), \]

where \( a + b = 1 \) and \( an_\alpha + bn_\beta = n \).

\[ a = \frac{n_\beta - n}{n_\beta - n_\alpha} \]

\[ b = \frac{n - n_\alpha}{n_\beta - n_\alpha} \]

\[ E_{ps}(n) = \frac{(n_\beta - n)E(n_\alpha) + (n - n_\alpha)E(n_\beta)}{n_\beta - n_\alpha} \]

Suppose that the metallic ferromagnetic (FM) phase with band filling \( n_1 \) coexists with an antiferromagnetic (AFM) phase with \( n = 1 \) and there is a gap at the Fermi surface then the above Figure 17 depicts the picture of such coexistence. The domain wall moves either to the left or to the right depending on whether an electron is added or taken away. This is equivalent to imagining liquid-gas equilibrium; as the pressure (chemical potential) is varied, the system changes from liquid (AFM) to gas (FM) at a certain pressure. This scenario is an artefact of the HF approximation; it is not prevalent in the exact solution since there is no gap.
Figure 18. Phase Separation

Figure 18 shows a schematic behaviour of $E(n)$ curve. Table 1 gives the phase boundaries for the phase separation ($n_{\alpha}$) and ferromagnetism ($n_{FM}$) calculated numerically.

<table>
<thead>
<tr>
<th>$U$</th>
<th>$n_{\alpha}$</th>
<th>$n_{\beta}$</th>
<th>$n_{FM}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>1</td>
<td>1</td>
<td>0</td>
</tr>
<tr>
<td>1</td>
<td>0.9975</td>
<td>1</td>
<td>0.09</td>
</tr>
<tr>
<td>2</td>
<td>0.95</td>
<td>1</td>
<td>0.16</td>
</tr>
<tr>
<td>3</td>
<td>0.88</td>
<td>1</td>
<td>0.24</td>
</tr>
<tr>
<td>4</td>
<td>0.81</td>
<td>1</td>
<td>0.32</td>
</tr>
<tr>
<td>5</td>
<td>0.77</td>
<td>1</td>
<td>0.41</td>
</tr>
<tr>
<td>10</td>
<td>0.69</td>
<td>1</td>
<td>0.75</td>
</tr>
<tr>
<td>20</td>
<td>0.73</td>
<td>1</td>
<td>0.89</td>
</tr>
<tr>
<td>1000</td>
<td>1</td>
<td>1</td>
<td>1</td>
</tr>
</tbody>
</table>

Table 1. Phase boundaries
Chapter 7  
Spin Texture Selection in the 1D Hubbard Model

Figure 19 Phase separation

SS-DSDW

Figure 20 The ground state energy for $U=4t$
Chapter 7 Spin Texture Selection in the 1D Hubbard Model

We can calculate the DSDW phase from Figure 20, the width of the phase is given by the onset of the kink to its departure. Results for two-sites are fairly accurate (5 decimal places or more) and compare well with those obtained by Samson [6] see Table 2. However as mentioned earlier computational speed is greatly affected by increase in the number of points in the k-space. Therefore, a compromise is inevitable, as we shall see for larger super-cells the number points in k-space have to be reduced.

<table>
<thead>
<tr>
<th>n</th>
<th>E(4000)</th>
<th>Samson</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.49</td>
<td>-0.671523</td>
<td>-0.671521</td>
</tr>
<tr>
<td>0.5</td>
<td>-0.680945</td>
<td>-0.680944</td>
</tr>
<tr>
<td>0.51</td>
<td>-0.681689</td>
<td>-0.681687</td>
</tr>
<tr>
<td>0.52</td>
<td>-0.682914</td>
<td>-0.682911</td>
</tr>
</tbody>
</table>

Table 2. Just a sample of points around the kink, $U=4t$.

Table 3 below shows the calculations of the DSDW tongue

<table>
<thead>
<tr>
<th>U</th>
<th>$n_{\text{min}}$</th>
<th>$n_{\text{max}}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.0</td>
<td>0.500</td>
<td>0.500</td>
</tr>
<tr>
<td>1.0</td>
<td>0.504</td>
<td>0.505</td>
</tr>
<tr>
<td>1.5</td>
<td>0.504</td>
<td>0.506</td>
</tr>
<tr>
<td>2.0</td>
<td>0.500</td>
<td>0.509</td>
</tr>
<tr>
<td>2.5</td>
<td>0.495</td>
<td>0.519</td>
</tr>
<tr>
<td>3.0</td>
<td>0.492</td>
<td>0.529</td>
</tr>
<tr>
<td>3.5</td>
<td>0.490</td>
<td>0.542</td>
</tr>
<tr>
<td>4.0</td>
<td>0.485</td>
<td>0.534</td>
</tr>
<tr>
<td>4.5</td>
<td>0.493</td>
<td>0.530</td>
</tr>
<tr>
<td>5.0</td>
<td>0.427</td>
<td>0.518</td>
</tr>
<tr>
<td>5.5</td>
<td>0.504</td>
<td>0.507</td>
</tr>
<tr>
<td>6.0</td>
<td>-</td>
<td>-</td>
</tr>
</tbody>
</table>

Table 3. The DSDW tongue.
Incidentally the appearance of tongues is not a unique feature of the HF approximation; these tongues are quite similar to Arnold tongues for the circle map \[16\]. See Figure 21 below.

![Arnold tongues](image)

Figure 21 Arnold tongues

Suzumura \textit{et al} \[18\] have reported similar results to ours on the HF ground state and excitations of the quarter-filled Hubbard model. They considered collinear \(Q = \frac{\pi}{2}\) spin density waves. At \(U=4t\) with a phase factor of \(\frac{\pi}{2}\) they obtain the equivalent DSDW ground state. They find a mixed state of \(Q = \pi\) charge density wave (CDW) and spin density wave with a minimum energy of \(-0.6786\), corresponding to a magnetic configuration. This minimum is a lot higher than our DSDW state, tables below show a comparison of ground state energies for different spin configurations at the quarter filling for \(U=4t\).

<table>
<thead>
<tr>
<th>HF-Approximation</th>
<th>Samson</th>
<th>Suzumura \textit{et al}</th>
</tr>
</thead>
<tbody>
<tr>
<td>E=0.67878</td>
<td>-</td>
<td>E=0.6786</td>
</tr>
</tbody>
</table>
We can deduce from above that there is some commensurability energy gain in going from the SS to a coexisting CDW/SDW state. However, the minimisation procedure has show that the energy gain in forming a CDW/SDW mixed state is less than that of spin spiral density wave (SS), but much higher than the DSDW ground state for the two-site case.

Within the HF approximation, we can see that the effect of the field \( w \) is merely to encourage CDW, if \( w \) is sizeable, without any doubt CDW will be favoured, thus suppressing SDW. However, the other players in the equation, namely the interaction \( U \) and the exchange coupling \( \Delta \), as we have mentioned earlier, open a gap for the spins. Our calculations show that the SS are dominant over CDW in all of the phase space for the two-site case. For three-sites and more sites the situation may not be the same because various new configurations will come into play which previously were not possible due to the size of the cell.
7.5 Three-sites

The minimisation algorithm amounts to self-consistent procedure, which imposes a complicated interdependence of the spins density and charge density, this can give rise to discontinuous phase transitions between magnetic and non-magnetic phases. Although we did not see any CDW for the two-site case, we expect to see non-uniform charge distribution for the three-site case especially at the \( n = \frac{1}{3} \) filling and multiples thereof.

Figure 22, below shows the ground state energy for \( U=4t \).

![Graph showing ground state energy for three-site supercell. Notice the very small notch appearing around \( n=0.67 \), the notch around 0.33 is too small to be noticed.](image_url)
As we expected, the opening of a gap at the Fermi level on the Brillouin zone boundary due to perfect nesting of the Fermi surface has lowered the ground state from SS phase to a CDW phase. The charge density wave (CDW) has the form given below in Figure 23. The long arrows show high electron density and the short arrows show low electron density.

\[ \Delta_1 = -0.14177t, \Delta_2 = -0.08686t, \Delta_3 = -0.08991t, w_1 = 0.077561t \text{ and } w_2 = 0.075163t \]

Electron densities per site, near the CDW the electrons pile up on the third site.
Figure 25. Plot of the summation of the densities in Figure 24, as expected an exact overlap is observed.

Figure 26. By application of symmetry we can set $w_3 = 0$.

The spin configuration drastically changes from the one shown in Figure 23, to the one where the first two spins are at 90 degree to one another (see Figure 27 below), this happens for all the $U$ values tested up till $U=U_{\text{critical}}$, when FM overpowers the CDW.

Figure 27 Stable configuration around the minimum kink until SS take over.
Figure 28. At low doping FM prevents any charge from developing except at \( n=0.33 \), this metastable charge density only appears for low \( U \).

Figure 29. The exchange splitting for \( U=1 \). Notice the peaks around \( n=0.33 \) and \( n=0.66 \).
Band structures for the three-sites for parameters near the minimum values:

\[ \Delta_1 = \Delta_2 = 0.11t \quad \Delta_3 = 0.09 \]
\[ Z = \frac{\pi}{2} \quad \theta_1 = 0 \quad \theta_2 = \frac{\pi}{2} \quad \theta_3 = \pi \]

\[ \Delta_1 = \Delta_2 = t \quad \Delta_3 = 0.09 \]
\[ Z = \frac{\pi}{2} \quad \theta_1 = 0 \quad \theta_2 = \frac{\pi}{2} \quad \theta_3 = \pi \]
\[ w_1 = 0, w_2 = 0 \quad \text{and} \quad w_3 = 0 \]

Figure 30(a) The Delta's are too small to open a gap

(b) very small gap

Bandstructure around the minimum.

Figure 31. Bands at the minimum \( n=0.66 \)
\[ \Delta_1 = -0.14177t, \Delta_2 = -0.08686t \quad \text{and} \quad \Delta_3 = 0.09 \]
\[ w_1 = 0.077561t \quad w_2 = 0.075163t \quad w_3 = 0 \]
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\[ Z = 0 \quad \theta_1 = 0 \quad \theta_2 = \frac{\pi}{2} \quad \theta_3 = \pi \] with small delta’s

\[ \begin{align*}
25 \\
20 \\
15 \\
10 \\
5 \\
0 \\
-5 \\
-10 \\
-15 \\
-20 \\
-25
\end{align*} \]

\[ \frac{\pi}{3} \]

Figure 32

7.6 Fermi surfaces

Fermi surface for the 4 site, we capture the DSDW kink again, at \( n=0.25 \) and \( n=0.75 \) the kinks are quite small by comparison.

\[ \begin{align*}
0.25 \\
0.75 \\
\text{Figure 33a Fermi energy for four-sites. } U=4t
\end{align*} \]

\[ \begin{align*}
0.29 \\
0.29 \\
0.39 \\
0.49 \\
0.59 \\
0.69 \\
\text{Figure 34b Fermi energy for three-sites.}
\end{align*} \]
The Fermi surface for the SS shows the absence of these kinks.

For Ferromagnetism the Fermi energy is given by \( E_F = -2t \cos(k_F) \).

Adding \( E_F \) as the energy for the ferromagnetic case in order to illustrate the transition point from FM to SS. The straight line is an excellent fit for the spin spiral. \( \frac{dE_F}{dn} < 0 \) is a sign of instability against phase separation.

Figure 35. Fermi energy for the SS phase

Figure 36. Superimposition of \( E_F \) (the top curve) show excellent agreement with the FM phase.
Ground state for different values of $U$ are shown in Figure 37 below, calculations similar to the two-site can now be carried out. The Maxwell construction can be applied numerically and hence the phase separation can be calculated. CDW tongue is not as large as the DSDW tongue as Figure shows.

![Figure 37 Ground state energies for various $U$.](image)

The field $w$ has major effect on the minimisation procedure except at and around the development of the non-uniform states at $n=\frac{2}{3}$, we must handle it with great care in order to achieve convergence. In order not to complicate the Figure 37 too much we have not shown the full curves. The kinks are so small as hardly to be noticed except for $U=4$, nevertheless kinks are there, the CDW tongues can easily be extracted from these curves, Tables 3 and 4 below show the boundary values for the onset of CDW. These phases are stable or at least metastable in comparison with the SDW and DSDW. One may argue that these new phases are as result of our initial assumptions of artificial periodicity of the system which favours Peierls instability and a lowering of the total energy. Since for rational filling $n = \frac{2p}{q}$, where $p, q \in \mathbb{Z}$, this must be so
for a finite system, we can always expect a stable state for some integer value of \( p \) given \( \frac{q}{2} \) is equal to the number of sites per unit cell.

The above line of reasoning may be true, but we cannot rule out the stability or instability of such states. The state at \( n=\frac{1}{2} \) is extremely small and hardly shows up on the graph, however the charge density state at \( n=\frac{2}{3} \) is rather more pronounced and most likely to be stable. Figure 44 shows the various stable tongues.

We can show the effect of \( w \) on the band structure for the minimum configuration at \( n=\frac{2}{3} \).

Figure 38. \( \Delta_1=-0.14177t, \Delta_2=-0.08686t \) and \( \Delta_3=0.09 \) \( w_1=0.077561t \) and \( w_2=0.075163t \) \( w_3=0 \)

\( w_1=1 \) and the rest of the values are the same as last Figure 31.

Figure 39. \( \Delta_1=-0.14177t, \Delta_2=-0.08686t \) and \( \Delta_3=0.09 \) \( w_1=1t \) and \( w_2=0.075163t \) \( w_3=0 \)
$w_1 = 1 \quad w_2 = 1$

Figure 40. $w_1 = 1 \quad w_2 = 1$ Notice how the bands have been raised

<table>
<thead>
<tr>
<th>$U$</th>
<th>$n_1$</th>
<th>$n_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.66</td>
<td>0.66</td>
</tr>
<tr>
<td>1</td>
<td>0.659</td>
<td>0.66</td>
</tr>
<tr>
<td>1.5</td>
<td>0.659</td>
<td>0.661</td>
</tr>
<tr>
<td>2</td>
<td>0.656</td>
<td>0.658</td>
</tr>
<tr>
<td>2.5</td>
<td>0.651</td>
<td>0.668</td>
</tr>
<tr>
<td>3</td>
<td>0.647</td>
<td>0.676</td>
</tr>
<tr>
<td>3.5</td>
<td>0.645</td>
<td>0.686</td>
</tr>
<tr>
<td>4</td>
<td>0.641</td>
<td>0.683</td>
</tr>
<tr>
<td>4.5</td>
<td>0.642</td>
<td>0.685</td>
</tr>
<tr>
<td>5</td>
<td>0.643</td>
<td>0.667</td>
</tr>
<tr>
<td>5.1</td>
<td>0.656</td>
<td>0.664</td>
</tr>
<tr>
<td>5.2</td>
<td>0.66</td>
<td>0.66</td>
</tr>
<tr>
<td>5.2</td>
<td>0.66</td>
<td>0.66</td>
</tr>
</tbody>
</table>

Table 4. Stable non-uniform charge density wave tongue for the three-sites

<table>
<thead>
<tr>
<th>$U$</th>
<th>$n_1$</th>
<th>$n_2$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>0.33</td>
<td>0.33</td>
</tr>
<tr>
<td>0.3</td>
<td>0.33</td>
<td>0.33</td>
</tr>
<tr>
<td>0.5</td>
<td>0.325</td>
<td>0.337</td>
</tr>
<tr>
<td>1</td>
<td>0.326</td>
<td>0.337</td>
</tr>
<tr>
<td>1.5</td>
<td>0.327</td>
<td>0.338</td>
</tr>
<tr>
<td>2</td>
<td>0.328</td>
<td>0.331</td>
</tr>
<tr>
<td>2.1</td>
<td>0.329</td>
<td>0.331</td>
</tr>
<tr>
<td>2.4</td>
<td>0.33</td>
<td>0.33</td>
</tr>
</tbody>
</table>

Table 5. The Metastable small tongue for the three-sites
7.7 Four sites

We find a stable state equivalent to the DSDW state at $n = \frac{1}{2}$. Even though the Fermi surface shows a jump the intermediate state at $n = \frac{1}{2}$ does not appear in the ground state. This can be explained by the fact that at low electron concentrations only the lower band is involved, furthermore FM states are highly favoured for any $U > 0$, this suppresses any charge density likely to take place for low $n$.

The Fermi level, for our case is equivalent to the chemical potential. For a large N-site system we would get a complicated graph for the chemical potential with a large number of steps of varying width. If we plot the chemical potential against the winding number we would get a similar plot to the one below, produced by Jensen et al [36] for a one dimensional circle map a devil's staircase.

![Figure 41 The Complete Devil's staircase for a circle map.](image)

7.8 Bandstructure for four-sites.
Four-sites have similar band structure to the two-sites. The DSDW band structure is show below, the only difference being the Brillouin zone is folded up again and the wavevector $k$ runs from $-\pi/4$ to $\pi/4$. 

\[ E(k) \]

\[ 3 \]
\[ 2 \]
\[ 1 \]
\[ 0 \]
\[ -1 \]
\[ -2 \]
\[ -3 \]

Figure 42 DSDW for four-sites. Bands are superimposed in pairs

For quadruple spin density wave given below the bandstructure with all the $\Delta$'s=1 and $w=0$ is given below Figure 43.

\[ \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \downarrow \]

\[ E(k) \]
\[ 3 \]
\[ 2 \]
\[ 1 \]
\[ 0 \]
\[ -1 \]
\[ -2 \]
\[ -3 \]

Figure 43 Quadruple spin density wave.
After extremely lengthy calculations we can put everything into perspective by putting all the tongues for different phase separation in one Figure. Figure 44 shows all the uniform phases along non-uniform charge density wave phases.

Figure 44. The complete Hartree-Fock phase diagram showing both uniform and non-uniform phases.
Chapter 7  Spin Texture Selection in the 1D Hubbard Model

7.9 Reference:


Chapter 7  Spin Texture Selection in the 1D Hubbard Model


[16]  Ott E *Chaos in Dynamical systems*  (Cambridge University Press, 1993)


[29]  Auerbach A and Larson B E *Phys. Rev.* **B 43** 7800-9


Chapter 8

8 Conclusions and further research

We have used the unrestricted self-consistent Hartree-Fock mean-field approximation to the one-dimensional periodic Hubbard model, to study the effects of spin and charge correlations, as well as the effects of spin charge fluctuations on the ground state of the Hubbard model. We have found that, for certain range of values of the parameters of the system, the ground state of the Hubbard model favours non-metallic domains. We have proven that in the case of two sites per unit cell, the ground state energy does not have a non-uniform charge density wave state, however we recover the results obtained by Samson for the uniform charge density.

With three sites, we found the one-dimensional system has instability towards a non-uniform state that opens a gap at the Fermi energy. Our findings are consistent with the results obtained by Samson [1], Zhou et al [2], Auerbach et al [3], and Tanemura et al [4] Andriotis et al [9].

For three sites, we have found a new metastable state near the \( n = \frac{1}{2} \) filling and a stable non-uniform charge density wave at \( n = \frac{3}{2} \). For four sites, similar results as two sites were found, except that the computational time was huge. A small DSDW type tongue around \( n = \frac{1}{2} \) was found and \( n = \frac{3}{2} \). At \( n = \frac{1}{2} \) filled case we recover the two-site DSDW.

We conjecture that studying systems with larger unit cells, will increase the number of lowest-lying states that exhibit spin configurations which differ very little in energy from each other. Our finds make it explicit that, as \( N \) the size of the unit cell increases, it will become prohibitively expensive, if at all possible, to obtain a computationally unique ground-state configuration of the system. An exhaustive search of the solutions of HF equations is then not only impractical, but global minima which are generally hard to find depend heavily on the boundary condition.
Inherent to all one-dimensional systems is the fact that quantum fluctuations can destroy any long-range order. So most of the long-range orders of ferromagnetism, antiferromagnetism, spin spiral density waves, and charge density waves would be destroyed. However, the system could retain short-range correlations of the form found to exist as the ground state of the system. The ground state energies found are much higher than the exact ground state energies found by Shiba [5].

In higher dimensions we expect the quantum fluctuations to be weaker in strength, and hence may not be able to overcome the short-range order clustering effects, at least near low temperatures. This may allow a phase transition to exist. Therefore our results are more relevant to 2D and 3D cases, although they do not give definitive answers, they do provide a model in which many of the physical processes underlying state selection operate in a transparent way.

The appreciable value of charge fluctuation $\delta n$ at certain fillings may allow the possibility of a superconducting state even after quantum fluctuations are taken into account. It could happen that the quantum fluctuations in 2D either stabilise the system to a charge-density state (as our results show), or they drive the system in to a superconducting state. If the charges are made mobile in a correlated way, in another words a charge density wave.

We have presented a U-n phase diagram, which shows all the possible tongues that can exist for systems up to four-sites, it is not hard to visualise that increasing the system size will produce more tongues. These tongues will inevitably start to overlap one another, as N the size of the supercells becomes very large, the whole of the phase space can be occupied with different types of spin orders. Then one can employ further Hartree-Fock higher accuracy calculations to establish which of the over lapping tongues is lower in energy and hence more stable. This evidently brings in the concept of fractals to mind, but that would take us outside the subject of discussion.
8.1 Further work

This area is by no means closed the next step would be to move into higher dimensions, where one could look at chains coupled together. Research in higher dimensions is already very active [6][7]. Finite and zero temperature studies of these systems in 2D with similar parameters applied would give insight into newly discovered materials of high temperature superconductors, heavy fermions and other strongly correlated materials.

Another interesting project would be to introduce phonons within the system, and then minimise the model within the unrestricted HF approximation taking into account \( \{\theta, \Delta, \omega\} \) per site. This should provide a link to polaron problem [8]. Alternatively, instead of taking positive-U we could look at negative-U Hubbard model. This can be obtained by particle-hole transformation, where the chemical potential turns into a magnetic field. Many of the above results should carry over, we would get more insight about superconducting phases.

One could look at the degenerate N-band Hubbard model, with three interaction parameters, repulsion between two electrons on the same orbital, repulsion between two electrons on different orbitals, and Hund’s rule exchange interaction between orbitals that tries to align the spin, HF should become exact as \( N \to \infty \). A different type of mean field theory such as the Slave boson method may be tried, one could look for excitations.
8.2 Reference:


