Master of Science Thesis

Deriving an extended one-band Hubbard model for cuprate superconductors

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April 2011

Abstract

The so-called three-band Hubbard model is generally believed to be a good model for fermions on a CuO_2 lattice and to contain key features allowing to understand high-temperature superconductivity in the cuprates. A simpler and more popular model is the one-band Hubbard model. In this thesis, an extended one-band Hubbard model is derived from the three-band model.

First, some mathematical background is given, as well as an introduction to Hubbard-like models. Then, to derive the extended one-band Hubbard model, the CuO_2 lattice is divided into clusters of one Cu and two O sites, and a variant of the Feshbach method is used to replace each such cluster by a single lattice site. To find a suitable one-band model, all Hamiltonian matrix elements are matched between the two models. Finally, different sets of three-band parameters are considered, and it is studied how this affects the parameters in the extended one-band Hubbard model.

Sammanfattning

Den så kallade treband-Hubbardmodellen antas allmänt vara en god modell för fermioner i ett CuO_2-gitter och innehålla viktiga egenskaper för förståelsen av högtemperatursupraledning i kuprater. En enklare och populärare modell är enband-Hubbardmodellen. I den här avhandlingen härleds en utökad enband-Hubbardmodell från treband-Hubbardmodellen.

Först diskuteras viss matematisk bakgrund och en introduktion till Hubbardmodellen ges. Sedan, för att härleda den utökade enband-Hubbardmodellen, delas CuO_2-gittret in i grupper om en Cu- och två O-atomer, och en variant av Feshbach-metoden används för att ersätta varje sådan grupp med en enda gitterpunkt. För att hitta en passande enband-modell matchas Hamiltonoperatorns alla matriselement mellan de två modellerna. Slutligen beaktas olika parametrar för treband-modellen, för att studera hur detta påverkar parametrarna i den utökade enband-Hubbardmodellen.

Acknowledgements

First and foremost I would like to thank my supervisor Edwin Langmann for his guiding and support throughout the work with this thesis. From him, I have gained valuable insight in what it is to do science. In particular, he has encouraged me to understand every step in the process as deeply as possible. In addition, I want to thank Per Håkan Lundow and Jonas de Woul, at the department of Theoretical Physics at the Royal Institute of Technology, for helping out with vital steps in my work. Last but not least, I would like to thank my friends Pontus Lans and Saddaf Shabbir, for saving me several hours each, providing their LaTex and Matlab skills, respectively.

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Chapter 1

Introduction and outline

Superconductivity, the phenomenon of vanishing resistivity at temperatures below a certain *critical temperature* T_c, was first observed in 1911 (see for example [8]). The so-called BCS theory, presented in 1957 [2], is a successful quantum theory for superconductivity in materials with $T_c \approx 30$ K and lower. One generally refers to superconductivity explained by BCS Theory as "conventional superconductivity".

During the 1980s materials were found in which superconductivity was observed at higher temperatures (a pioneering paper awarded by the Nobel Prize is [3]), and the term *high-temperature superconductivity* (HTSC) was introduced. Since then, superconducting materials with increasing T_c have been discovered. Notably, T_c values up to 138 K have been observed (see for example [8, p. 295]).

Until recent years and the discovery of iron-based superconductors (see for example [13]), all materials featuring HTSC were so-called *cuprates*. The common feature of these cuprates is that they consist of CuO_2 layers sandwiched between layers of other atoms. The layers in-between serve to dope the CuO_2 layers with either electrons or holes. The detailed structure of these CuO_2 layers is discussed in Chapter 4.

The so-called three-band Hubbard model is generally believed to be a good model for the fermions (electrons or holes) in a CuO_2 layer (see for example [14, p. 3759], [1, p. 2] and [6, p. 2794]), and thereby to contain the key features to understand HTSC in the cuprates. In this model, fermions reside on both Cu and O atoms in the CuO_2 layer. The three-band Hubbard model can be reduced to the less complex one-band Hubbard model or, simply, the Hubbard model. Here, fermions are considered only on the Cu sites, thereby removing the degrees of freedom associated with the O sites.

While the one-band Hubbard model is less detailed than the three-band model, it is easier for computational studies, with methods such as exact diagonalization or quantum Monte Carlo [1, p. 2], or with a restricted Hartree-Fock approach, as carried out in [5]. The Hubbard model can be extended to include additional terms, and we refer to this as extended one-band Hubbard models. Even though a large number of studies have been carried out on one-band Hubbard models, there is still much left to be understood regarding their behavior. Considerably fewer studies have been carried out for the more complex three-band Hubbard model.

It is often assumed that the terms of small magnitude, in an extended Hubbard model, can be ignored . However, there are indications [9, p. 1] that these "small terms" may play an important role, and it is therefore interesting to revisit how they are obtained. In this thesis, we derive an extended one-band Hubbard model from the three-band model, using a variant of the Feshbach method (see for example [10]).

Throughout the derivation, we will use the set of three-band model parameters in [1, p. 5]. The reader should be aware of the uncertainties of these values. After having derived the one-band model, we assume different sets of three-band parameters (guided by [11, Table VI] and [12, Section II]), and see how the extended one-band model parameters are changed.

In Chapter 2, we discuss some of the mathematical formalisms and techniques used in the thesis. In Chapter 3 we introduce the Hubbard model, and study it in some simple examples. In Chapter 4 and 5 we carry out the procedure of deriving an extended one-band Hubbard model, and we present the result in Chapter 6. In Appendix A, we fix our notation. Appendix B contains further mathematical details, and all Matlab programs are attached in Appendix C.

Chapter 2

Mathematical tools

2.1 Second quantization

The formalism used in this thesis is called second quantization. In this section, we give a brief introduction to second quantization, and in particular, we introduce the annihilation and creation operators. We recall that the central objects in a quantum theory are quantum states and operators. The states are represented by state vectors in a Hilbert space, and parallel vectors (i.e. differing only by a scale factor λ) represent the same states. All observable quantities – for example position, energy and momentum – are represented by operators acting on this Hilbert space.

In the first quantization formalism, also referred to as "quantum mechanics", the (time independent) quantum mechanical state of *one* particle is, in position representation, the complex-valued wave function $\psi(\mathbf{r})$. The absolute square of the wave function represents the probability density of the particle, i.e. $|\psi(\mathbf{r})|^2 d\mathbf{r}$ is the probability of finding the particle within the volume element $d\mathbf{r}$ around the coordinate $\mathbf{r}$. From this, it follows that one condition that has to be posed upon $\psi(\mathbf{r})$ is the normalization condition: $\int |\psi(\mathbf{r})|^2 d\mathbf{r} = 1$, where the integral is taken over the full space. The normalization conditions means that, with probability one, the particle will be found *anywhere* in space.

Now, consider a system of an arbitrary number N particles. The wave function now takes the form $\psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$, where $(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ is a vector in the 3N-dimensional space, and is such that $|\psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)|^2 \prod_{i=1}^{N} d\mathbf{r}_i$ is the probability of finding the N particles in the 3N-dimensional volume $\prod_{i=1}^{N} d\mathbf{r}_i$ around the coordinate $(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ in the 3N-dimensional space. Thus, the integral of $|\psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)|^2$ over all space is 1.

A fundamental concept in quantum mechanics is *indistinguishable particles*: If particles are characterized be the same quantum numbers, such as mass, charge and spin, they can be indistinguishable. Assume a state $\psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ representing N indistinguishable particles. Interchanging two coordinates in ψ corresponds to swapping two particle with each other. Since the particles are indistinguishable, this action must result in the same state, and thus the new wave function must differ from the original only by a scalar factor (this freedom pertains since parallel vectors represent the same state). Carrying out this procedure twice, we get

$$\psi(\mathbf{r}_1, \cdots, \mathbf{r}_j, \cdots, \mathbf{r}_k, \cdots, \mathbf{r}_N) = \lambda\psi(\mathbf{r}_1, \cdots, \mathbf{r}_k, \cdots, \mathbf{r}_j, \cdots, \mathbf{r}_N) = \\ = \lambda^2\psi(\mathbf{r}_1, \cdots, \mathbf{r}_j, \cdots, \mathbf{r}_k, \cdots, \mathbf{r}_N), \tag{2.1}$$

i.e. $\lambda^2 = 1$, and thus $\lambda = \pm 1$. This leads to the conclusion that there exist only two types of quantum mechanical particles: Those where $\lambda = 1$ (called *bosons*) and those where $\lambda = -1$ (called *fermions*). In this thesis, we are exclusively studying fermions (*electrons* or *holes*, i.e. the absence of electrons). A fundamental property of fermions is that it is not possible for more than one particle to occupy the same one-particle state: if $\mathbf{r}_j = \mathbf{r}_k$, then $\psi = 0$. This feature of fermions is referred to as the *Pauli exclusion principle*.

In the first quantization formalism we need to find a wave function $\psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N)$ obeying the relation $\lambda = -1$. It is in principle possible to construct such wave functions from one-particle wave functions $\psi_i(\mathbf{r}_i)$ as follows:

$$\psi(\mathbf{r}_1, \mathbf{r}_2, \cdots, \mathbf{r}_N) = \sum_{\nu_1, \cdots, \nu_N} A_{\nu_1, \nu_2, \cdots, \nu_N} \psi_{\nu_1}(\mathbf{r}_1)\psi_{\nu_2}(\mathbf{r}_2) \cdots \psi_{\nu_N}(\mathbf{r}_N),$$

where ν_i denotes the state of particle i, and $A_{\nu_1, \nu_2, \cdots, \nu_N}$ are certain complex numbers. The full process of constructing these states, including how the complex numbers $A_{\nu_1, \nu_2, \cdots, \nu_N}$ are determined, is found on for example in [4, Chapter 1.2]. Looking at the nature of the complex numbers $A_{\nu_1, \nu_2, \cdots, \nu_N}$, it becomes clear that this first quantization formalism will be very complex as the number of particles increases. A more convenient formalism is described below.

2.1.1 Fermion systems – annihilation and creation operators

The basic concept of the second quantization formalism is to define states in which the indistinguishable particles may be found, and to *count* how many particles there are in each state. Another name for second quantization is consequentially "occupation number representation". In this thesis, we will restrict ourselves to cases where there are a *finite* number L of states that may be occupied by one *fermion*. The reasoning is the following:

Assume that we have a collection of L single-particle quantum states that may be occupied by fermions: $\{\psi_1, \psi_2, \cdots, \psi_L\}$. Now, instead of constructing a many-particle wave function from these single-particle wave functions (as we did in the first quantization formalism), we define the following second quantization state:

$$|\mathbf{n}\rangle = |n_1, n_2, \cdots, n_L\rangle, \tag{2.2}$$

where $n_i \in \mathbb{N}$ is the number of particles in state ψ_i, and $\sum_j n_j = n$ is the total number of fermions.

In the following, we will need the *annihilation operator* a_i and the *creation operator* $a_i^\dagger$, the Hermitian adjoint [1] of a_i, associated with one-particle state ψ_i. We will now define these operators.

[1] The Hermitian adjoint $A^\dagger$ of any operator A on a Hilbert space $\mathcal{H}$ satisfies $\langle A^\dagger x|y\rangle = \langle x|Ay\rangle$ for any elements x and y in $\mathcal{H}$ with $\langle \cdots | \cdots \rangle$ the scalar product in $\mathcal{H}$.

First, we postulate the anti-commutator relations for a_i and $a_i^\dagger$:

$$\{a_j, a_k\} = 0, \quad \{a_j, a_k^\dagger\} = \delta_{jk} \quad \forall j,k \in \{1,2,\cdots,L\} \tag{2.3}$$

We show[2] below that (2.3) implies $\{a_j^\dagger, a_k^\dagger\} = 0$:

$$\{a_j^\dagger, a_k^\dagger\} = a_j^\dagger a_k^\dagger + a_k^\dagger a_j^\dagger = (a_k a_j)^\dagger + (a_j a_k)^\dagger = (a_k a_j + a_j a_k)^\dagger = (\{a_k, a_j\})^\dagger = 0^\dagger = 0 \tag{2.4}$$

Furthermore, we define the empty state Ω, and the action of any annihilation operator a_i upon this empty space:

$$\Omega = |n_1 = 0, n_2 = 0, \cdots, n_L = 0\rangle, \quad a_i\Omega = 0, \quad \langle\Omega|\Omega\rangle = 1 \tag{2.5}$$

The physical interpretation of (2.5) is that the empty state cannot be further emptied. (2.3) and (2.5) provide the full definition of the fermion system.

The action of the creation operator $a_i^\dagger$ on the empty state is

$$a_i^\dagger\Omega = |n_1 = 0, n_2 = 0, \cdots, n_i = 1, \cdots, n_L = 0\rangle, \tag{2.6}$$

i.e. a fermion is *created* in one-particle state ψ_i. Now, we can write any state (2.2) expressed in creation operators acting on the empty state:

$$\begin{aligned} |\mathbf{n}\rangle &\equiv (a_1^\dagger)^{n_1}(a_2^\dagger)^{n_2}\cdots(a_L^\dagger)^{n_L}\Omega \\ n_i &\in \{0,1\}. \end{aligned} \tag{2.7}$$

We refer to states such as (2.7) as *pure* states, and one can show that they provide a complete orthonormal basis, i.e. that any state can be written as a linear combination of states in (2.7).

The order in which the creations operators are applied in (2.7) is essential. One has to agree upon an unambiguous order convention, in this case "$i < j \Rightarrow a_i^\dagger$ is applied to the left of $a_j^\dagger$". This necessity is a consequence of the anti-commutator relations (2.4): since $a_i^\dagger a_j^\dagger = -a_j^\dagger a_i^\dagger$, the state $|\mathbf{n}\rangle$ is determined only up to a factor (-1) unless we specify the order.

We note that the Pauli exclusion principle follows directly from the anti-commutator relations: If one attempts to create a fermion in the single-particle state i, by applying $a_i^\dagger$ to a state $|\mathbf{n}\rangle$ where $n_i = 1$,

[2] We use the following properties of the Hermitian adjoint of the product and of the sum of two operators: $(\hat{A}\hat{B})^\dagger = \hat{B}^\dagger\hat{A}^\dagger$, and $(\hat{A}+\hat{B})^\dagger = \hat{A}^\dagger + \hat{B}^\dagger$

one will somewhere end up with the product $a_i^\dagger a_i^\dagger$. But (2.4) tells us that $\{a_i^\dagger, a_i^\dagger\} = 2a_i^\dagger a_i^\dagger = 0$, and the result would thus be zero. The conclusion is that, in a pure state, each single particle state can be occupied only by either zero or one particle.

From the definition in (2.3) and (2.5), it also follows what result one gets when acting with an annihilation operator $a_i^\dagger$ on a state $|\mathbf{n}\rangle$. We look separately on the cases where $n_i = 0$ and $n_i = 1$, i.e. when the single-particle state ψ_i is non-occupied and occupied, respectively:

$$
\begin{aligned}
&\text{If } n_i = 0: \\
&\quad a_i|\mathbf{n}\rangle = a_i(a_1^\dagger)^{n_1}\cdots(a_i^\dagger)^0\cdots(a_N^\dagger)^{n_N}|\Omega\rangle = a_i(a_1^\dagger)^{n_1}\cdots I\cdots(a_N^\dagger)^{n_N}|\Omega\rangle = \\
&\qquad = (-1)^{\xi_0}(a_1^\dagger)^{n_1}\cdots(a_N^\dagger)^{n_N}\underbrace{a_i\Omega}_{=0} = 0 \qquad (2.8) \\
&\text{If } n_i = 1: \\
&\quad a_i|\mathbf{n}\rangle = a_i(a_1^\dagger)^{n_1}\cdots a_i^\dagger\cdots(a_N^\dagger)^{n_N}\Omega = (-1)^{\xi_1}(a_1^\dagger)^{n_1}\cdots a_i a_i^\dagger\cdots(a_N^\dagger)^{n_N}\Omega = \\
&\qquad = (-1)^{\xi_1}(a_1^\dagger)^{n_1}\cdots(1 - a_i^\dagger a_i)\cdots(a_N^\dagger)^{n_N}\Omega = \\
&\qquad = (-1)^{\xi_1}(a_1^\dagger)^{n_1}\cdots I\cdots(a_N^\dagger)^{n_N}\Omega - (-1)^{\xi_1}(a_1^\dagger)^{n_1}\cdots a_i^\dagger(-1)^{\xi_2}\cdots(a_N^\dagger)^{n_N}\underbrace{a_i\Omega}_{=0} = \\
&\qquad = (-1)^{\xi_1}|\mathbf{n}'\rangle \qquad (2.9) \\
&\quad \xi_0 = \sum_{k\neq i} n_k; \quad \xi_1 = \sum_{k=1}^{i-1} n_k; \quad \xi_2 = \xi_0 - \xi_1
\end{aligned}
$$

When there is no particle in state ψ_i, acting with a_i on $|\mathbf{n}\rangle$ results in zero. When there is a particle in ψ_i, acting with a_i on $|\mathbf{n}\rangle$ yields (with a possible factor -1) $|\mathbf{n}'\rangle$, the same state except that the particle in state ψ_i has been annihilated.

2.1.2 The number operator $\hat{N}$

We define the number operator on the system of L sites as follows:

$$\hat{N} = \sum_{i=1}^{L} \hat{N}_i; \quad \hat{N}_i = a_i^\dagger a_i \qquad (2.10)$$

Acting with $\hat{N}_i$ on the state $|\mathbf{n}\rangle$, using (2.8) and (2.9), gives

$$\begin{aligned}\hat{N}_i|\mathbf{n}\rangle =& a_i^\dagger a_i (a_1^\dagger)^{n_1}\cdots(a_i^\dagger)^{n_i}\cdots(a_N^\dagger)^{n_N}\Omega = a_i^\dagger(-1)^{\xi_1}(a_1^\dagger)^{n_1}\cdots a_i(a_i^\dagger)^{n_i}\cdots(a_N^\dagger)^{n_N}\Omega = \\ &= \left\{ \begin{array}{l} a_i^\dagger 0 = 0, \text{ if } n_i = 0 \\ a_i^\dagger(-1)^{\xi_1}(a_1^\dagger)^{n_1}\cdots I\cdots(a_N^\dagger)^{n_N}\Omega, \text{ if } n_i = 1 \end{array} \right\} = \\ &= \left\{ \begin{array}{l} a_i^\dagger 0 = 0, \text{ if } n_i = 0 \\ (-1)^{2\xi_1}(a_1^\dagger)^{n_1}\cdots a_i^\dagger\cdots(a_N^\dagger)^{n_N}\Omega = |\mathbf{n}\rangle, \text{ if } n_i = 1 \end{array} \right\},\end{aligned}$$

which shows that the states $|\mathbf{n}\rangle$ are eigenstates to $\hat{N}_i$ with eigenvalue n_i: $\hat{N}_i|\mathbf{n}\rangle = n_i|\mathbf{n}\rangle$. We may now extend to the full operator $\hat{N}$, acting on $|\mathbf{n}\rangle$:

$$\begin{aligned}\hat{N}|\mathbf{n}\rangle = \sum_{i=1}^{L}\hat{N}_i|\mathbf{n}\rangle = \sum_{i=1}^{L} n_i|\mathbf{n}\rangle = n|\mathbf{n}\rangle \\ n = n_1 + n_2 + \cdots + n_L\end{aligned} \tag{2.11}$$

The states $|\mathbf{n}\rangle$ are eigenstates to $\hat{N}$, with eigenvalue n, the total particle number.

2.1.3 Fock spaces and tensor products

We now look closer into the mathematical formalism used when single-particle systems are combined to a larger system.

Consider a fermion system with a single one-particle state. For a second quantized quantum mechanical state to be well defined, we require that it is an eigenstate to the number operator $\hat{N}$, with an eigenvalue that is zero or a positive integer. This requirement demands that we have an integer number of particles in our system. As we have previously discussed, a fermion state may be occupied by at most one fermion. In other words, the eigenvalue n may be only 0 or 1. Our states are thus vectors a Hilbert space $\mathcal{H}_{one}$, which is of dimension two: there are only two possible states in the Hilbert space.

Now consider a system of two single-particle fermion states ψ_i and ψ_j, that both may be either empty or occupied. We realise that there are four different situations where both n_i and n_j are well defined: $\{n_i = 0, n_j = 0\}, \{n_i = 1, n_j = 0\}, \{n_i = 0, n_j = 1\}$ and $\{n_i = 1, n_j = 1\}$. These four states span[1] the Hilbert space $\mathcal{H}_{two}$: Any state in $\mathcal{H}_{two}$ may be obtained by a linear combination of these four pure states. We thus conclude that $\mathcal{H}_{two}$ is of dimenstion four[2]. By repeating this reasoning, we can see that adding another single particle fermion state to our system will always double the number of pure states. The general conclusion is that states in a system with L single-particle states will be represented by vectors in a Hilbert space $\mathcal{H}_L$ of dimension 2^L.

A formal way to combine the Hilbert spaces of L single-particle systems is the *tensor product* $\otimes$:

[1] We use the word "span" in this context as synonymous to "provide a complete orthonormal basis to"

[2] The dimension of any Hilbert space $\mathcal{H}$ is equal to the number of states in a complete basis of $\mathcal{H}$.

$$\mathcal{H}_L = \underbrace{\mathcal{H}_{one} \otimes \cdots \otimes \mathcal{H}_{one}}_{L \text{ times}} \tag{2.12}$$

We refer to $\mathcal{H}_L$ as the *Fock space*, and introducing the direct sum[1] $\oplus$ we may also write

$$\mathcal{H}_L = \mathcal{F}_0 \oplus \mathcal{F}_1 \oplus \cdots \oplus \mathcal{F}_L, \tag{2.13}$$

where $\mathcal{F}_k$ is the subspace of $\mathcal{H}_L$ spanned by all pure states states with particle number $n = k$.

In this thesis we will use tensor product both between Hilbert spaces (as above) and between vectors. Below, we state two useful properties of the tensor product between vectors:

$$(v_1 \otimes v_2)(w_1 \otimes w_2) = v_1 v_2 \otimes w_1 w_2 \tag{2.14}$$

$$\langle v_1 \otimes v_2 | w_1 \otimes w_2 \rangle_{(\mathcal{H}_1 \otimes \mathcal{H}_2)} = \langle v_1 | w_1 \rangle_{\mathcal{H}_1} \langle v_2 | w_2 \rangle_{\mathcal{H}_2}, \text{ where:} \tag{2.15}$$

$v_1, w_1 \in \mathcal{H}_1; \quad v_2, w_2 \in \mathcal{H}_2; \quad (v_1 \otimes v_2) \in (\mathcal{H}_1 \otimes \mathcal{H}_2)$
$\langle \cdots | \cdots \rangle_{(\dots)}$ is the inner product in respective Hilbert space.

2.2 Matrix representation in quantum physics

Throughout the thesis, we will associate *operators* with *matrices* and *states* with *vectors*. In this section, we therefore give some background to this matrix formulation of quantum physics. For a more exthausive introduction, see for example [7, p. 146-153]. In Section 2.2.3, we also give a concrete vector and matrix representation of the fermion system described in Section 2.1.1. This representation will be of use when we carry out numerical calculations in Matlab.

Consider a Hilbert space $\mathcal{H}$ representing a quantum system, and assume that we have defined a complete orthonormal basis of states $|n\rangle$ on $\mathcal{H}$. Then, any operator[2] $\hat{O}$ on $\mathcal{H}$ may be represented by a matrix, whose elements are

$$O_{nm} = \langle n | \hat{O} | m \rangle, \tag{2.16}$$

i.e. the inner product (as defined on $\mathcal{H}$) between the state $|n\rangle$ and the state resulting from acting with $\hat{O}$ on $|m\rangle$. In this manner, the O matrix representation is constructed:

[1] The direct sum $U \oplus V$ of two vector spaces is defined as the sum of subspaces in which U and V have only the zero vector in common

[2] Our general notation convention is that operators $\hat{A}$ are written with a hat, and their matrix representation A, in some basis, is written without hat. However, in Chapters 4 and 5 we will write the Hamiltonian operators H without hat, as well as their matrix representation.

$$O = \begin{pmatrix} O_{1,1} & O_{1,2} & \cdots & O_{1,L} \\ O_{2,1} & O_{2,2} & \cdots & O_{2,L} \\ \vdots & \vdots & \ddots & \vdots \\ O_{L,1} & O_{L,2} & \cdots & O_{L,L} \end{pmatrix}, \tag{2.17}$$

where $L = dim(\mathcal{H})$.

2.2.1 Observables and eigenvalues

We call an *observable* a measurable physical quantity of a system. It is a fundamental postulate of quantum mechanics that *all physical observables are represented by self-adjoint* [1] [2] *operators on a Hilbert space $\mathcal{H}$, and the expectation value of an operator $\hat{A}$ in a state $\Psi \in \mathcal{H}$ is $\langle\Psi|\hat{A}|\Psi\rangle$.* In matrix formulation, this postulate means that all physical observables are represented by self-adjoint matrices[3]. Self-adjoint matrices have real eigenvalues.

The explicit elements in the matrix representation O, as in (2.17), of any operator $\hat{O}$ depend on the choice of basis $|n\rangle$. We will be interested in finding the matrix' eigenvalues, an inherent property of the operator $\hat{O}$, independent of the choice of basis.

2.2.2 Commutating operators – block diagonal matrices

The eigenvalue problem in matrix representation,

$$O\mathbf{v} = E\mathbf{v}, \tag{2.18}$$

can be simplified in an interesting special case which we will discuss in this section. We remind ourselves that, given the matrix O, the task is to find vectors $\mathbf{v_i}$ and corresponding scalars E_i such that (2.18) holds. Now, let's assume that in a certain basis, O can be written as follows:

$$O = \begin{pmatrix} O_{1,1} & \cdots & O_{1,a} & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ O_{a,1} & \cdots & O_{a,a} & 0 & \cdots & 0 \\ 0 & \cdots & 0 & O_{a+1,a+1} & \cdots & O_{a+1,L} \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ 0 & \cdots & 0 & O_{L,a+1} & \cdots & O_{L,L} \end{pmatrix} \tag{2.19}$$

If we just use regular matrix multiplication, Equation (2.18) can in this case be re-written as follows:

[1] A self-adjoint operator $\hat{O}$ is equal to its adjoint $\hat{O}^\dagger$

[2] An example of an operator that is not self adjoint is the annihilation operator a_i. Its adjoint is the creation operator $a_i^\dagger$, and we clearly have $a_i \neq a_i^\dagger$. From this it follows that the eigenvalues of a_i do not correspond to any physical observable, and nor do those of $a_i^\dagger$.

[3] A self-adjoint matrix is equal to its conjugate transpose, meaning that for every matrix element O_{nm} it holds that $O_{mn} = (O_{nm})^*$, the * denoting usual complex conjugate.

$$\begin{pmatrix} \sum_{i=1}^{a} O_{1,i}v_i + 0 + \cdots + 0 \\ \sum_{i=1}^{a} O_{2,i}v_i + 0 + \cdots + 0 \\ \vdots \\ \sum_{i=1}^{a} O_{a,i}v_i + 0 + \cdots + 0 \\ 0 + \cdots + 0 + \sum_{i=a+1}^{L} O_{a+1,i}v_i \\ 0 + \cdots + 0 + \sum_{i=a+1}^{L} O_{a+2,i}v_i \\ \vdots \\ 0 + \cdots + 0 + \sum_{i=a+1}^{L} O_{L,i}v_i \end{pmatrix} = E \begin{pmatrix} v_1 \\ v_2 \\ \vdots \\ v_a \\ v_{a+1} \\ v_{a+2} \\ \vdots \\ v_L \end{pmatrix} \tag{2.20}$$

In (2.20), there are L equations to simultaneously be solved. However, we note that the a first equations are decoupled[1] from the $(L-a)$ last equation. Therefore, solving (2.20) is equivalent to solving two equations:

$$\begin{pmatrix} \sum_{i=1}^{a} O_{1,i}v_i \\ \sum_{i=1}^{a} O_{2,i}v_i \\ \vdots \\ \sum_{i=1}^{a} O_{a,i}v_i \end{pmatrix} = E \begin{pmatrix} v_1 \\ \vdots \\ v_a \end{pmatrix} \text{ and } \begin{pmatrix} \sum_{i=a+1}^{L} O_{a+1,i}v_i \\ \sum_{i=a+1}^{L} O_{a+2,i}v_i \\ \vdots \\ \sum_{i=a+1}^{L} O_{L,i}v_i \end{pmatrix} = E \begin{pmatrix} v_a + 1 \\ \vdots \\ v_L \end{pmatrix}, \tag{2.21}$$

which, rewritten on matrix form is:

$$\begin{aligned} &O_1^a \mathbf{v}_1^a = \mathbf{v}_1^a \text{ and } O_{a+1}^L \mathbf{v}_{a+1}^L = \mathbf{v}_{a+1}^L \\ &O_i^j \equiv \{O_{k,l}\}_{i \le k,l \le j};\ \mathbf{v}_i^j = (v_i, v_{i+1}, \cdots, v_j) \end{aligned} \tag{2.22}$$

The first equation in (2.22) has a solutions – eigenvalues E_k with corresponding eigenvectors $(\mathbf{v}_1^a)_k$ – and the second equation has $(L-a)$ solutions.

If a matrix O has the form described in (2.19), we say that it has *block-diagonal* form. We introduce the notation of the direct sum $\oplus$ of matrices to describe a block-diagonal matrix with M blocks:

$$\oplus_{i=1}^{M} O_i = \begin{pmatrix} O_1 & & & \\ & O_2 & & \\ & & \ddots & \\ & & & O_M \end{pmatrix}, \tag{2.23}$$

where the matrices O_i are square matrices diagonally located in O, and all other elements of O are zero. The reasoning for separating equation $O\mathbf{v} = E\mathbf{v}$ may be extended to the case where O has M blocks, as in (2.23):

[1] More precisely, we mean that if an element v_i appears with a non-zero coefficient in the first a equations, it does not appear in the $L-a$ last equations, and vice versa.

$$O = \oplus_{i=1}^{M} O_i \Longrightarrow O\mathbf{v} = E\mathbf{v} \Leftrightarrow \begin{cases} O_1 \mathbf{v}_1^{D_1} = E\mathbf{v}_1^{D_1} \\ O_2 \mathbf{v}_{D_1+1}^{D_2} = E\mathbf{v}_{D_1+1}^{D_2} \\ \vdots \\ O_M \mathbf{v}_{D_{M-1}+1}^{M} = E\mathbf{v}_{D_{M-1}+1}^{M} \end{cases} \tag{2.24}$$

where $D_i - D_{i-1}$ is the number of rows (and columns) in O_i (with $D_0 \equiv 0$)

Diagonal blocks in a matrix O on a Hilbert space $\mathcal{H}$ have a physical interpretation: They correspond to subspaces of $\mathcal{H}$ in which all states share a common eigenvalue, unique to that block, with respect to an operator $\hat{P}$ that commute with $\hat{O}$: $[\hat{O}, \hat{P}] = 0$. We say that such an operator $\hat{P}$ represents a *symmetry* of $\hat{O}$, and we may use the following result to find a basis in which O, the matrix representation of $\hat{O}$ is block-diagonal:

Proposition 2.2.1 *Consider $\hat{O}$, an observable on a Hilbert space $\mathcal{H}$, and a complete orthonormal basis $\{\psi_n\}$ in $\mathcal{H}$, such that each ψ_n is an eigenstate to another observable $\hat{P}$ on $\mathcal{H}$, $\hat{P}\psi_n = p_n\psi_n$, ordered such that $p_1 = p_2 = \cdots = p_{D_1}, p_{D_1+1} = p_{D_1+2} = \cdots = p_{D_2}, \cdots, p_{D_{M-1}} = \cdots = p_{D_M}$, with $p_{D_j} \neq p_{D_k}$ for $j \neq k$ and $0 \equiv D_0 < D_1 < D_2 < \cdots < D_M \equiv dim(\mathcal{H})$.*

Then, $O = \oplus_{i=1}^{M} O_i$ is the matrix representation of $\hat{O}$, O_i expressed in the basis $\{\psi_k\}_{D_{i-1}<k\leq D_i}$; $i \in \{1, \cdots, M\}$.

Proof Choose any two basis states ψ_n and ψ_m such that $p_n \neq p_m$. Then, since $[\hat{P}, \hat{O}] = 0$, we have

$$\hat{P}\hat{O}\psi_n = \hat{O}\hat{P}\psi_n = \hat{O}p_n\psi_n = p_n\hat{O}\psi_n,$$

and $\hat{O}\psi_n$ is thus also an eigenstate to $\hat{P}$ with the same eigenvalue p_n as ψ_n. Thus, $\hat{O}\psi_n$ may be written as a linear combination of basis states $\{\psi_k\}_{D_{i-1}<k\leq D_i}$, with $p_{D_i} = p_n$. All these states ψ_k are orthogonal to ψ_m, and thus the matrix element $O_{m,n} = \langle\psi_m|\hat{O}|\psi_n\rangle$ is zero. ψ_n and ψ_m are arbitrarily chosen basis states possessing different eigenvalues p_n and p_m, and we conclude that the matrix representation O, expressed in $\{\psi_n\}$,must be block-diagonal. □

In practice, given an operator $\hat{P}$ such as above, the challenge will often be to find a suitable basis $\{\psi_n\}$ such as described above.

Proposition 2.2.1 may be used for several symmetries to the same operator: If there exists another operator $\hat{P}'$ such that $[\hat{P}', \hat{O}] = 0$, we may regard every subspace $\mathcal{H}_i$ in the above reasoning as consisting of yet smaller subspaces, each corresponding to unique eigenvalues p_i' of $\hat{P}'$, and find a basis $\{\psi_n'\}$ such as described above, and carry out the same procedure in order to make the O matrix consist of an even larger number of even smaller blocks.

Later, we will use Proposition 2.2.1 to find a basis in which the Hamiltonian matrix is block-diagonal. We will use, among others, the number operator $\hat{N}$, representing the symmetry.

2.2.3 Matrix representation of fermion systems

We will now define a vector and matrix representation of the fermion system discussed in Section 2.1.1, defined by the annihilation and creation operators a_i and $a_i^\dagger$, and the empty space Ω. In the Hilbert space $\mathcal{H}_L$ representing the system of L single particle states (that may be either empty or occupied with a fermion), we will represent the annihilation and creation operators with matrices. We make the following definitions:

$$I_2 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}; \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}; \quad \sigma_+ = \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}; \quad \sigma_- = \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \quad e_0 = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \tag{2.25}$$

and define the following representations:

$$\begin{aligned} a_i &= \underbrace{\sigma_3 \otimes \cdots \otimes \sigma_3}_{i-1 \text{ times}} \otimes \sigma_- \otimes \underbrace{I_2 \otimes \cdots \otimes I_2}_{L-i \text{ times}} \\ a_i^\dagger &= \underbrace{\sigma_3 \otimes \cdots \otimes \sigma_3}_{i-1 \text{ times}} \otimes \sigma_+ \otimes \underbrace{I_2 \otimes \cdots \otimes I_2}_{L-i \text{ times}} \\ \Omega &= \underbrace{e_0 \otimes \cdots \otimes e_0}_{L \text{ times}} \end{aligned} \tag{2.26}$$

One can show, using the rules for multiplications of tensor products in (2.14), that the identifications (2.26) preserve the following essential properties of the fermion system:

- $(a_i)^\dagger = a_i^\dagger$: (i.e. $a_i^\dagger$ is the hermitian adjoint of a_i)
- $\{a_i, a_j^\dagger\} = \delta_{i,j}$
- $\{a_i, a_j\} = 0 \quad \forall\, i, j$
- $a_i \Omega = 0$

We will use the above representation when using Matlab to calculate numerical values of Hamiltonian matrix elements.

2.3 Feshbach Method

In this section, we present and discuss the Feshbach technique, which can be used to "partition" eigenvalue problems. For a more extensive discussion of this method, see for example [10]. In Section 5.1.1, we will use this technique to eliminate high-energy states in the three-band Hubbard model.

Consider the Schrödinger equation on a Hilbert space $\mathcal{H}$ of dimension[1] $\mathcal{M}$:

$$\hat{H}\Psi = E\Psi \tag{2.27}$$

With a given complete orthonormal basis $\{f_i\}_{i\in\{1,2,\cdots,\mathcal{M}\}}$, (2.27) may be expressed as

$$\begin{aligned} H\mathbf{c} &= E\mathbf{c} \\ \mathbf{c} = (c_1, \cdots, c_{\mathcal{M}}); &\qquad \Psi = \sum_{i=1}^{\mathcal{M}} c_i f_i, \end{aligned} \tag{2.28}$$

with H the matrix of expectation values of $\hat{H}$ in f_i: $H_{ij} = \langle f_i|\hat{H}|f_j\rangle$.

Now consider a subspace $\mathcal{H}_A \subset \mathcal{H}$, spanned by the following subset to $\{f_i\}$: $\{f_i\}_{i=1}^{\mathcal{M}_A}$; $\mathcal{M}_A < \mathcal{M}$, and let $\mathcal{H}_B = \mathcal{H} \setminus \mathcal{H}_A$, spanned by $\{f_i\}_{i=\mathcal{M}_A+1}^{\mathcal{M}}$. Using this notation, we can now rewrite (2.28) as

$$\begin{pmatrix} H_{AA} & H_{AB} \\ \\ H_{BA} & H_{BB} \end{pmatrix} \begin{pmatrix} \mathbf{c}_A \\ \mathbf{c}_B \end{pmatrix} = E \begin{pmatrix} \mathbf{c}_A \\ \mathbf{c}_B \end{pmatrix} \tag{2.29}$$

Using regular matrix multiplication, we can rewrite equation (2.29) into two equations

$$\begin{aligned} H_{AA}\mathbf{c}_A + H_{AB}\mathbf{c}_B &= E\mathbf{c}_A \\ H_{BA}\mathbf{c}_A + H_{BB}\mathbf{c}_B &= E\mathbf{c}_B \end{aligned} \tag{2.30}$$

From the second equation in (2.30) we get[2] $\mathbf{c}_B = (EI_{BB} - H_{BB})^{-1}H_{BA}\mathbf{c}_A$ which, inserted into the first equation, gives an effective Hamiltonian

$$H_{eff} = H_{AA} + H_{AB}(EI_{BB} - H_{BB})^{-1}H_{BA}, \tag{2.31}$$

and an equation

$$H_{eff}(E)\,\mathbf{c}_A = E\,\mathbf{c}_A \tag{2.32}$$

Equation (2.32) has exactly the same form as (2.28) [10, p. 971], but instead of an equation in $\mathcal{M}$ dimensions we now have an equation in $\mathcal{M}_A < \mathcal{M}$ dimensions. This reduction of dimensions,

[1] We will in this thesis be concerned only with finite-dimensional Hilbert spaces. However, for the technique outlined in this section, it would not be a problem if $\mathcal{H}$ would be an infinite Hilbert space.

[2] Provided that $(EI_{BB} - H_{BB})^{-1}$ exists See [10] for more discussion on the existence of this inverse matrix.

however, comes at the cost that the linear equation in (2.28) is replaced by a an equation (2.32) where the left hand side depends on E in a non-trivial way.

There are several[3] techniques to solve equation (2.32) by, for example, iteration procedures. When using this technique in Section 5.1.1 we will, however, do the approximation that $H_{eff}(E) \approx H_{AA}$, avoiding the dependence of E. This is equivalent to setting all elements in H_{AB} to zero.[4] It would be interesting to take also into account the terms $H_{AB}(EI_{BB} - H_{BB})^{-1}H_{BA}$, but this is left to future work.

Looking at the form of H_{eff} in (2.31), we can see that the accuracy of our approximation depends both on the magnitude (preferably small) of the elements in the off-diagonal matrices H_{AB} and H_{BA}, and on the difference (preferably large) between the energy E and the elements of H_{BB}.

[3] See for example [10, p. 970].

[4] In the case where H is self-adjoint this implies that all elements in H_{BA} are zero, too.

Chapter 3

The Hubbard model on small clusters

In this chapter, we introduce the Hubbard model, and study it in simple examples. We will first consider a two-sites system, and thereafter study how the complexity grows with the number of sites in the system.

3.1 Solving the Hubbard model on two sites

Consider two sites on which fermions can reside (See Figure 3.1). A fermion with spin $\sigma \in \{\uparrow, \downarrow\}$ is annihilated (created) on site i by the annihilation (creation) operator $a_{i,\sigma}^{(\dagger)}$. To get an understanding of the Hubbard model, we now want to study it in this simple case. We will define the Hamiltonian matrix in some basis, and diagonalize it to find the energy eigenvalues. The Hubbard Hamiltonian on the two-sites system is defined as

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (a_{2,\sigma}^{\dagger} a_{1,\sigma} + a_{1,\sigma}^{\dagger} a_{2,\sigma}) + \sum_{i=1,2} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}, \tag{3.1}$$

where $\hat{n}_{i,\sigma} = a_{i,\sigma}^{\dagger} a_{i,\sigma}$, t is the amplitude of the energy for a fermion hopping from one site to the other and U corresponds to the Coulomb interaction between two fermions residing on the same site. Note that "hopping" is, in the second quantization formalism, manifested as annihilating a fermion on one site and creating one on the other.

Including spin, there are four single-particle states that may either be occupied or empty. Thus, there are 16 pure states, all eigenstates to the particle number operator $\hat{N}$ with eigenvalue ranging from 0 (both sites empty) to 4 (both sides occupied with one $\uparrow$ and one $\downarrow$ fermion).

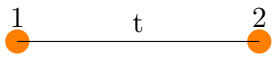

Figure 3.1: Two sites system. Fermions may reside either on site 1 or 2, and it is possible to hop from one site to the other.

As discussed in Section 2.2.2, we want to find operators that commute with $\hat{H}$ to help find a basis in which the matrix representation of $\hat{H}$ is block-diagonal with as many and as small blocks as possible. Since $[a_{i,\sigma}, \hat{n}_{j,\sigma'}] = [a^\dagger_{i,\sigma}, \hat{n}_{j,\sigma'}] = 0 \; \forall \; i, j, \sigma, \sigma'$, and since on this system the total particle number operator $\hat{N} = \hat{n}_{1,\uparrow} + \hat{n}_{1,\downarrow} + \hat{n}_{2,\uparrow} + \hat{n}_{2,\downarrow}$ and the total spin operator $\hat{S}^z = \frac{1}{2}(\hat{n}_{1,\uparrow} + \hat{n}_{2,\uparrow}) - \frac{1}{2}(\hat{n}_{1,\downarrow} + \hat{n}_{2,\downarrow})$, we can conclude that $[\hat{N}, H] = [\hat{S}^z, H] = 0$ holds. Guided by the structure of the Hamiltonian in (3.1) [1], we define the following operator $\hat{T}$ and show that it commutes with H:

$$\hat{T}\hat{T}^\dagger = \hat{T}^\dagger\hat{T} = I; \quad \hat{T}a_{i,\sigma}\hat{T}^\dagger = a_{i+1,\sigma}; \quad \hat{T}\Omega = \Omega; \quad 2 + 1 \equiv 1 \tag{3.2}$$

To show that $[\hat{T}, H] = 0$, we treat each term individually:

1) $\hat{T}\left(a^\dagger_{2,\sigma}a_{1,\sigma} + a^\dagger_{1,\sigma}a_{2,\sigma}\right) = \hat{T}a^\dagger_{2,\sigma}\hat{T}^\dagger\hat{T}a_{1,\sigma}\hat{T}^\dagger\hat{T} + \hat{T}a^\dagger_{1,\sigma}\hat{T}^\dagger\hat{T}a_{2,\sigma}\hat{T}^\dagger\hat{T} =$
$= a^\dagger_{1,\sigma}a_{2,\sigma}\hat{T} + a^\dagger_{2,\sigma}a_{1,\sigma}\hat{T} = \left(a^\dagger_{1,\sigma}a_{2,\sigma} + a^\dagger_{2,\sigma}a_{1,\sigma}\right)\hat{T}$

2) $\hat{T}\hat{n}_{i,\sigma} = \hat{T}a^\dagger_{i,\sigma}\hat{T}^\dagger\hat{T}a_{i,\sigma}\hat{T}^\dagger\hat{T} = a^\dagger_{i+1,\sigma}a_{i+1,\sigma}\hat{T} = \hat{n}_{i+1,\sigma}\hat{T}$, and thus:
$\hat{T}\left(\hat{n}_{1,\uparrow}\hat{n}_{1,\downarrow} + \hat{n}_{2,\uparrow}\hat{n}_{2,\downarrow}\right) = \left(\hat{n}_{2,\uparrow}\hat{n}_{2,\downarrow} + \hat{n}_{1,\uparrow}\hat{n}_{1,\downarrow}\right)\hat{T}$ and we conclude that:
$[\hat{T}, \hat{H}] = 0$

We use the three symmetries of $\hat{H}$ represented by the operators $\hat{N}$, $\hat{S}^z$ and $\hat{T}$ to define a complete orthonormal basis in which the states are eigenstates to these three operators, and with different eigenvalues. Below we present this basis, along with the eigenvalues[2] for each of the states:

[1] More precisely, the fact that it seems equivalent for any fermion to reside on site 1 as on site 2

[2] Our standard notation is that we use lowercase letters for eigenvalues (for example n and s^z), but to avoid confusion with the hopping amplitude, we let T be the eigenvalues associated with $\hat{T}$

State	Eigenvalue n	Eigenvalue s^z	Eigenvalue T
$f_1 = \Omega$	0	0	1
$f_2 = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow} + a^\dagger_{2,\uparrow}\right)\Omega$	1	$+1/2$	1
$f_3 = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow} - a^\dagger_{2,\uparrow}\right)\Omega$	1	$+1/2$	-1
$f_4 = 1/\sqrt{2}\left(a^\dagger_{1,\downarrow} + a^\dagger_{2,\downarrow}\right)\Omega$	1	$-1/2$	1
$f_5 = 1/\sqrt{2}\left(a^\dagger_{1,\downarrow} - a^\dagger_{2,\downarrow}\right)\Omega$	1	$-1/2$	-1
$f_6 = a^\dagger_{1,\uparrow}a^\dagger_{2,\uparrow}\Omega$	2	$+1$	-1
$f_7 = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow}a^\dagger_{1,\downarrow} + a^\dagger_{2,\uparrow}a^\dagger_{2,\downarrow}\right)\Omega$	2	0	1
$f_8 = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow}a^\dagger_{2,\downarrow} + a^\dagger_{2,\uparrow}a^\dagger_{1,\downarrow}\right)\Omega$	2	0	1
$f_9 = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow}a^\dagger_{1,\downarrow} - a^\dagger_{2,\uparrow}a^\dagger_{2,\downarrow}\right)\Omega$	2	0	-1
$f_{10} = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow}a^\dagger_{2,\downarrow} - a^\dagger_{2,\uparrow}a^\dagger_{1,\downarrow}\right)\Omega$	2	0	-1
$f_{11} = a^\dagger_{1,\downarrow}a^\dagger_{2,\downarrow}\Omega$	2	-1	-1
$f_{12} = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow}a^\dagger_{1,\downarrow}a^\dagger_{2,\uparrow} + a^\dagger_{1,\uparrow}a^\dagger_{2,\uparrow}a^\dagger_{2,\downarrow}\right)\Omega$	3	$+1/2$	1
$f_{13} = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow}a^\dagger_{1,\downarrow}a^\dagger_{2,\uparrow} - a^\dagger_{1,\uparrow}a^\dagger_{2,\uparrow}a^\dagger_{2,\downarrow}\right)\Omega$	3	$+1/2$	-1
$f_{14} = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow}a^\dagger_{1,\downarrow}a^\dagger_{2,\downarrow} + a^\dagger_{1,\downarrow}a^\dagger_{2,\uparrow}a^\dagger_{2,\downarrow}\right)\Omega$	3	$-1/2$	1
$f_{15} = 1/\sqrt{2}\left(a^\dagger_{1,\uparrow}a^\dagger_{1,\downarrow}a^\dagger_{2,\downarrow} - a^\dagger_{1,\downarrow}a^\dagger_{2,\uparrow}a^\dagger_{2,\downarrow}\right)\Omega$	3	$-1/2$	-1
$f_{16} = a^\dagger_{1,\uparrow}a^\dagger_{1,\downarrow}a^\dagger_{2,\uparrow}a^\dagger_{2,\downarrow}\Omega$	4	0	1

Creating the Hamiltonian matrix in this basis, $H_{ij} = \langle f_i|\hat{H}|f_j\rangle$, we get the 16×16 matrix

$$H = \begin{pmatrix}
0 & 0 & \dots & & & & & & & & & & & & & \\
0 & -t & \ddots & & & & & & & & & & & & & \\
\vdots & \ddots & +t & & & & & & & & & & & & & \\
 & & & -t & & & & & & & & & & & & \\
 & & & & +t & & & & & & & & & & & \\
 & & & & & 0 & & & & & & & & & & \\
 & & & & & & U & -2t & & & & & & & & \\
 & & & & & & -2t & 0 & & & & & & & & \\
 & & & & & & & & U & 0 & & & & & & \\
 & & & & & & & & 0 & 0 & & & & & & \\
 & & & & & & & & & & 0 & & & & & \\
 & & & & & & & & & & & U+t & & & & \\
 & & & & & & & & & & & & U-t & & & \\
 & & & & & & & & & & & & & U+t & & \\
 & & & & & & & & & & & & & & U-t & \\
 & & & & & & & & & & & & & & & 2U
\end{pmatrix}, \quad (3.3)$$

where the only nonzero off-diagonal elements are found in the $\{n = 2, s^z = 0, T = 1\}$ sector. Thus, to find all energy eigenvalues, we only need to solve one characteristic equation; all other eigenvalues

are directly found on the diagonal. We solve the characteristic equation $(U-E)(-E)-(-2t)(-2t) = 0 \Rightarrow E = \frac{U}{2} \pm \sqrt{\frac{U^2}{4} + 4t^2}$, and then list all eigenvalues of H, in the order of appearance in the matrix:

$$E = 0, -t, t, -t, t, 0, \frac{U}{2} + \sqrt{\frac{U^2}{4} + 4t^2}, \frac{U}{2} - \sqrt{\frac{U^2}{4} - 4t^2}, U, 0, 0, U + t, U - t, U + t, U - t, 2U \quad (3.4)$$

We may now assign some values to the parameters t and U to get an idea of the energies. We choose $t = 1$ eV and $U = 3$ eV and get the following energies, sorted by the particle number of their respective eigenstate (all energies in eV):

$$\begin{aligned} n = 0: &\quad E = 0 \\ n = 1: &\quad E = -1, -1, 1, 1 \\ n = 2: &\quad E = -1, 0, 0, 0, 3, 4 \\ n = 3: &\quad E = 2, 2, 4, 4 \\ n = 4: &\quad E = 6 \end{aligned} \quad (3.5)$$

We see that the ground level energy -1 eV is three-fold degenerate: Two eigenstates with $n = 1$ and one with $n = 2$ share this energy eigenvalue. We keep t fixed at 1 eV, vary U such that $U/t \in \{0, 1, \cdots, 8\}$, and plot the energies found in Figure 3.2. We find, for example, that for $t/U < 3$, the ground state has particle number $n = 2$, and for $t/U > 3$ it has particle number $n = 1$.

3.2 Complexity increases rapidly

One may generalize the Hamiltonian in (3.1) to apply to systems consisting of more than two sites. A natural extension is to let the system be a ring of L sites, where the fermions may hop to both "neighbor" sites in the ring. See Figure 3.3 for the cases where $L = 3, 4, 5$. A natural extension of the Hamiltonian in (3.1) to a fermion system on a ring of L sites is:

$$\hat{H} = -t \sum_{i=1}^{L} \sum_{\sigma} (a^{\dagger}_{i+1,\sigma} a_{i,\sigma} + a^{\dagger}_{i,\sigma} a_{i+1,\sigma}) + \sum_{i=1}^{L} \hat{n}_{i,\uparrow} \hat{n}_{i,\downarrow}; \qquad L + 1 \equiv 1 \quad (3.6)$$

When adding one site to the ring, we add two available single-fermion states (including spin), and it thus increases the dimension of the Hilbert space by a factor $2^2 = 4$. For a ring with L sites, the Hilbert space of the fermion states is of dimension 4^L. We realize that the complexity of finding the fermion energies, i.e. diagonalizing the Hamiltonian matrix, grows rapidly. To illustrate this, we let Matlab solve the Hubbard problem for a ring of L sites, and observe the calculation time that the program needs to build the matrix and find its energies. The full code is found in Appendix C.1.2. We have adapted the code such that it handles the case treated in Section 3.1 (where $L = 2$), too. Inserting $t = 1$ eV and $U = 3$ eV, we verify that the Matlab program yields the same energies as we found analytically in Section 3.1.

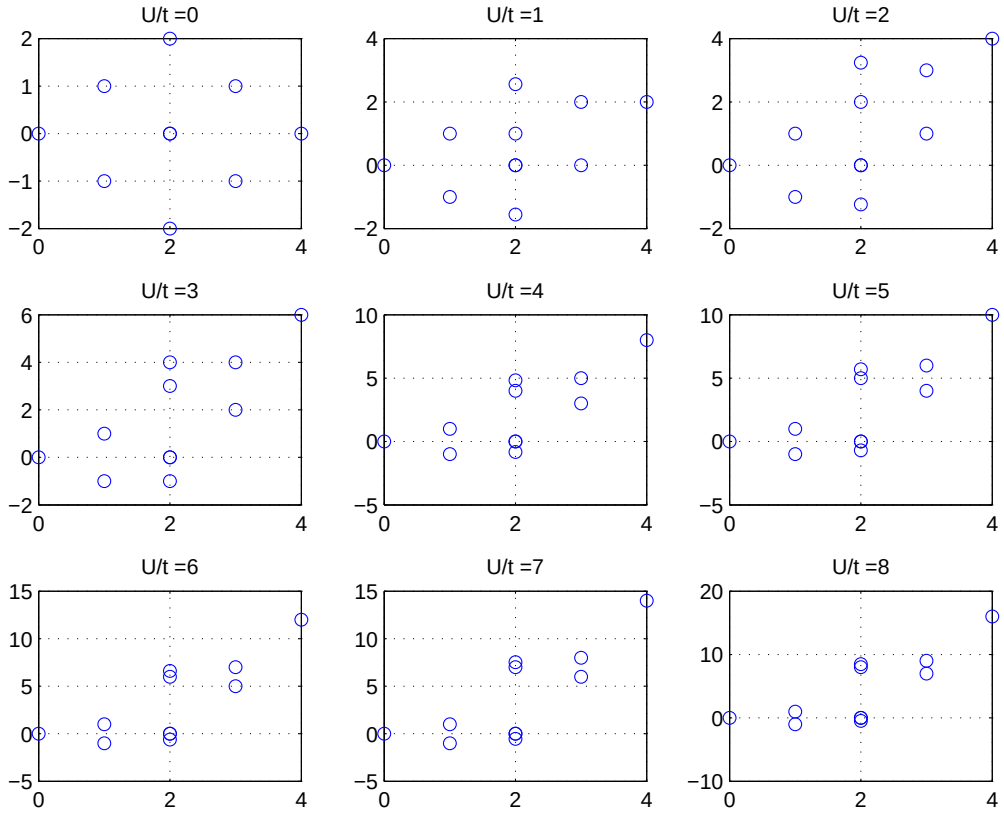

Figure 3.2: Fermion energies in the Hubbard model on a two sites system, with $t = 1$ eV and U varying from 0 to 8 eV. Each circle represents an eigenstates to H, its energy (in eV) is marked on the y-axis, and its particle number $0 - 4$ on the x-axis. Note that the scale on the y-axis varies between the different plots.

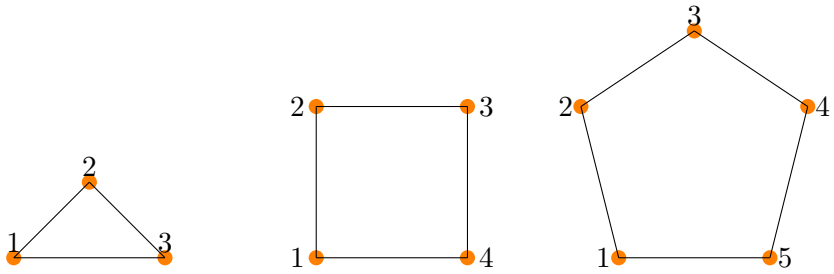

Figure 3.3: Rings with 3, 4 and 5 sites. Fermions can hop according to the black lines.

Below, we present the times that Matlab needs to solve the Hubbard problem on a ring of L sites, for different L:

L	Size of H matrix	**Time to solve**	Lowest energy (with $t = 1$ eV and $U = 3$ eV)
2	16×16	2.2 s	$-1\, eV$
3	64×64	4.3 s	$-2\, eV$
4	256×256	30 s	$-3.50(9)\, eV$
5	1024×1024	Out of memory	- -
6	4096×4096	- -	- -

Admittedly, one can write a more efficient Matlab code and/or use a more powerful computer. As an example, it is worth mentioning that our code doesn't use any symmetry to obtain a block-diagonal matrix form of H. However, this example shows that it soon becomes unmanageable for any hardware to solve the problem, as the number of sites increases. As one is often interested in systems with a large number of sites (thermodynamic limit) it is clear that the method described above is very restricted and other methods should be found.

Chapter 4

Three-band Hubbard model

We intend to find all elements in the matrix representation of the three-band Hubbard Hamiltonian H[1], representing the energy of fermions on a CuO_2 lattice of the type found in the cuprates. The structure of this lattice is described in Figure 4.1. In the next chapter, we will match each of these matrix elements to a corresponding matrix element in an extended one-band Hubbard Hamiltonian.

In line with [1, p. 4], it is assumed that a fermion on a Cu site will be in the $3d_{x^2-y^2}$ orbital, and on an oxygen site in a $2p_\delta$ orbital, $\delta = x$ or $\delta = y$. [2]. Further, we assume that there are L Cu sites, each assigned with a label $i \in \{1, \cdots L\}$. The three-band Hamiltonian is then [3]

$$\begin{aligned} H = & (\epsilon_d - \mu) \sum_{i,\sigma} \hat{n}^d_{i,\sigma} + (\epsilon_p - \mu) \sum_{l,\sigma} \hat{n}^p_{l,\sigma} + \\ & + t_{pd} \sum_{\langle i,l \rangle, \sigma} \alpha^{pd}_{i,l} (p^\dagger_{l,\sigma} d_{i,\sigma} + d^\dagger_{i,\sigma} p_{l,\sigma}) + t_{pp} \sum_{\langle l,l' \rangle, \sigma} \alpha^{pp}_{l,l'} (p^\dagger_{l,\sigma} p_{l',\sigma} + p^\dagger_{l',\sigma} p_{l,\sigma}) + \\ & + U_{dd} \sum_i \hat{n}^d_{i,\uparrow} \hat{n}^d_{i,\downarrow} + U_{pd} \sum_{\langle i,l \rangle, \sigma, \sigma'} \hat{n}^d_{i,\sigma} \hat{n}^p_{l,\sigma'} + \\ & + U_{pp} \sum_l \hat{n}^p_{l,\uparrow} \hat{n}^p_{l,\downarrow}, \end{aligned} \tag{4.1}$$

where l runs over all O sites, $\langle i,l \rangle$ over all nearest-neighbor Cu-O pairs and $\langle l,l' \rangle$ over all nearest-neighbor O-O pairs, and $\sigma, \sigma' \in \{\uparrow, \downarrow\}$.

[1] From now, we will omit the hat over the three-band Hubbard Hamiltonian. The reason is that in Chapter 5, we will match it to an extended one-band model denoted $\tilde{H}$, and to keep the hat it would thus not be practical. It will be made clear when we refer to the operator H, or its matrix representation in a certain basis.

[2] $\delta = x, y$ depending on the position with respect to the Cu site: O atoms having their nearest-neighbor Cu sites above and below are in the $2p_y$ orbital, and O atoms with the nearest Cu sites on both sides are in $2p_x$ orbital, x being the horizontal and y the vertical axis in Figure 4.1.

[3] We us the following notation: $d^{(\dagger)}_{i,\sigma}$ annihilates (creates) a fermion on a Cu site i and $p^{(\dagger)}_{l,\sigma}$ annihilates (creates) a fermion on an O site. $\hat{n}^d_{i,\sigma} = d^\dagger_{i,\sigma} d_{i,\sigma}$ and $\hat{n}^p_{l,\sigma} = p^\dagger_{l,\sigma} p_{l,\sigma}$. See Appendix A for notation conventions

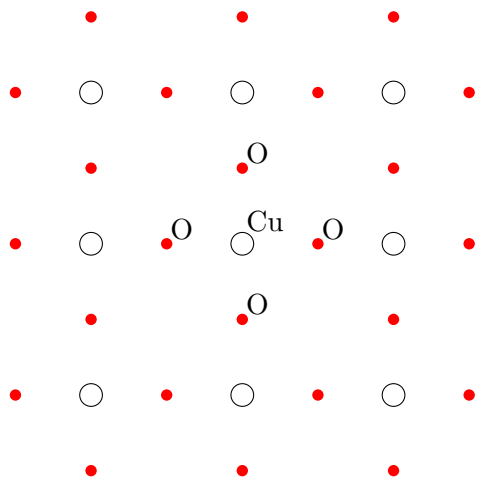

Figure 4.1: Structure of the CuO_2 lattice. Cu sites are black circles and O sites are red bullets. O sites are found on half the distance between any two Cu sites. We let the unit distance be the shortest distance between two Cu sites, and note that given a Cu site at $\mathbf{i} = (i_x, i_y)$, next-neighboring Cu sites are found at $\mathbf{i}+\hat{\mathbf{x}}$, $\mathbf{i}-\hat{\mathbf{x}}$, $\mathbf{i}+\hat{\mathbf{y}}$ and $\mathbf{i}-\hat{\mathbf{y}}$, where $\hat{\mathbf{x}}$ and $\hat{\mathbf{y}}$ are the unit vectors in the horizontal and vertical directions, respectively.

ϵ_d and ϵ_p are the on-site energies on Cu and O sites, respectively. U_{dd}, U_{pp} and U_{pd} measure the Coulomb repulsion between two electrons sitting either on the same site (U_{dd} and U_{pp}) or on two nearest-neighbor Cu-O sites (U_{pd}).

t_{pd} and t_{pp} are the amplitudes of Cu-O and O-O hopping, respectively. $\alpha_{i,l}^{pd} \in \{-1, 1\}$ and $\alpha_{l,l'} \in \{-1, 1\}$ are sign factors [1], as illustrated in Figure 4.2. We choose the chemical potential to be zero, and use the parameter values in [1, p. 5] as our reference: $\epsilon_d = 0, \epsilon_p - \epsilon_d = 3.0, t_{pd} = 1, U_{dd} = 8.0, U_{pd} = 0.5, U_{pp} = 3.0$, all energies in eV [2] [3]

Our strategy is to divide the lattice into smaller clusters, and consider the Hamiltonian acting only on that subspace. We will find the eigenvalues and corresponding eigenstates to this subspace Hamiltonian, and thereafter combine these states and energies for all the clusters on the lattice. This will give the full Hamiltonian matrix in the Hilbert space of the whole CuO_2 lattice.

We choose each cluster to consist of one Cu atom and two neighboring O atoms. There will be two types of such clusters: horizontally oriented and vertically oriented. As a consequence, Cu-O hopping to the left within horizontal clusters, and downwards within vertical clusters, will have $\alpha_{pd} = 1$, whereas hopping to the right and upwards will have $\alpha_{pd} = -1$. We also note that there is no O-O hopping within a cluster. Finally, we note that this choice of clusters leads to that only nearest-neighbor clusters are coupled in the global Hamiltonian, and that each cluster interior in the lattice has four nearest-neighbors. See Figure 4.3 for an illustration.

[1] The magnitude t_{pd} and t_{pp} is determined by the integral of the overlapping wave functions. The differing signs are due to the structure of the $2p_x$, $2p_y$ and $3d_{x^2y^2}$ orbitals. We use the same sign convention as [1]

[2] It only has an interesting physical meaning to define the *difference* $\epsilon_p - \epsilon_d$ between the on-site energies. To equally vary the magnitudes of both ϵ_p and ϵ_d is equivalent to merely choosing the zero energy level

[3] The fact that $\epsilon_p - \epsilon_d > 0$ tells us that we are considering a system dopes with *holes*, and not electrons. For electrons, we would have $\epsilon_d > \epsilon_p$ [6, p. 2794].

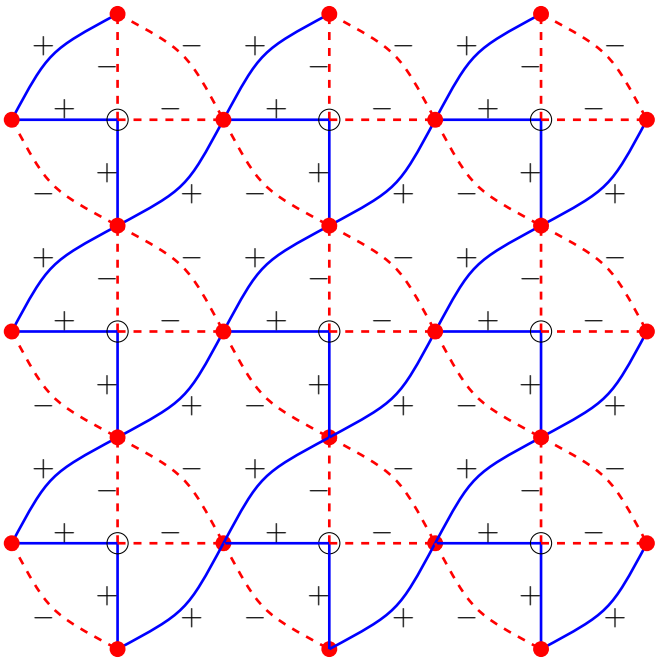

Figure 4.2: Hopping sign convention. Cu sites are black circles and O sites are red bullets. $\alpha^{pd}_{i,l} = 1$ *for Cu-O connections drawn in full blue lines and along which there is a plus sign, and* $\alpha^{pd}_{i,l} = -1$ *for dashed red lines with a minus sign. Accordingly for* $\alpha^{pp}_{l,l'}$ *and O-O connections.*

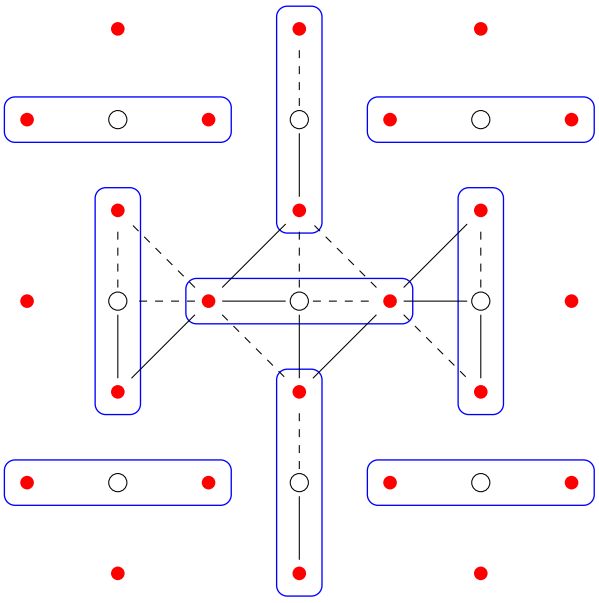

Figure 4.3: Part of lattice divided into clusters. Cu atoms are black circles and and O atoms are red bullets. Full lines represent $\alpha^{pd}_{i,l} = 1$ *for Cu-O connections and* $\alpha^{pp}_{l,l'} = 1$ *for O-O connections, while dashed lines represent* $\alpha^{pd}_{i,l} = -1$ *or* $\alpha^{pp}_{l,l'} = -1$.

4.1 One-cluster energies and states

We associate with each cluster the label i, the index of the Cu site which is part of the cluster.

To find a suitable notation for the Hamiltonian acting on one cluster, we associate with the horizontal and the vertical clusters, the unit vectors $\mathbf{n} = (1, 0)$ and $\mathbf{n} = (0, 1)$ (where $\mathbf{n} = (n_x, n_y)$), respectively, the unit being the smallest distance between two Cu atoms, as described in Figure 4.1. Further, we denote $d_{i,\sigma} \equiv d_{i,0,\sigma}$ and $p_{i\mp\mathbf{n}/2,\sigma} \equiv p_{i,\pm,\sigma}$. This way, we may express the Hamiltonian H_i, acting on cluster i, with a formula valid for both horizontal and vertical clusters:

$$\begin{aligned} H_i =& \epsilon_d \sum_\sigma \hat{n}^d_{0,\sigma} + \epsilon_p \sum_\sigma \left(\hat{n}^p_{+,\sigma} + \hat{n}^p_{-,\sigma}\right) \\ &+ t_{pd} \sum_\sigma (p^\dagger_{+,\sigma} - p^\dagger_{-,\sigma}) d_{0,\sigma} + d^\dagger_{0,\sigma}(p_{+,\sigma} - p_{-,\sigma}) + \\ &+ U_{dd} \hat{n}^d_{0,\uparrow} \hat{n}^d_{0,\downarrow} + U_{pp}(\hat{n}^p_{+,\uparrow} \hat{n}^p_{+,\downarrow} + \hat{n}^p_{-,\uparrow} \hat{n}^p_{-,\downarrow}) + U_{pd} \sum_{\sigma,\sigma'} \hat{n}^d_{0,\sigma}(\hat{n}^p_{+,\sigma'} + \hat{n}^p_{-,\sigma'}), \end{aligned} \tag{4.2}$$

where we on the right hand side have suppressed the index i, common to all operators.

The states in one cluster are vectors in a Hilbert space of dimension $2^6 = 64$. To find the energies and states amounts to finding the 64 eigenvalues and 64 eigenstates of the $\{64 \times 64\}$ Hamiltonian matrix. The fact that H_i commutes with $\hat{N}$ and $\hat{S}^z$ will allow us to define a basis in which the matrix will be block-diagonal. In fact, it is possible to define operators representing further symmetries that simplifies the matrix even more. We carry out the solution of the one cluster problem in Appendix B.1; we give details about the analytical solution in the subspaces where $\{n = 0, 1, 2\}$, and we use Matlab to find all energies.

For reasons that soon will become clear, we focus on the four (normalized) eigenstates $A^\dagger_{i,a_i}\Omega$ to H_i having the lowest energies E_{a_i}. They are (energies in eV): [2]

$A^\dagger_{i,1}\Omega$, $E_1 = 0$; $A^\dagger_{i,2}\Omega$, $E_2 = -0.56(2)$; $A^\dagger_{i,3}\Omega$, $E_3 = -0.56(2)$ and $A^\dagger_{i,4}\Omega$, $E_4 = 2.03(7)$, where we have defined the following operators:

$$\begin{aligned} A^\dagger_{i,1} =& I \\ A^\dagger_{i,2} =& -0.92(9) d_{0,\uparrow} + 0.26(1)\left(p^\dagger_{+,\uparrow} - p^\dagger_{-,\uparrow}\right) \\ A^\dagger_{i,3} =& -0.92(9) d_{0,\downarrow} + 0.26(1)\left(p^\dagger_{+,\downarrow} - p^\dagger_{-,\downarrow}\right) \\ A^\dagger_{i,4} =& 0.44(2)\left[d^\dagger_{0,\uparrow}\left(p^\dagger_{-,\downarrow} - p^\dagger_{+,\downarrow}\right) + \left(p^\dagger_{-,\downarrow} - p^\dagger_{+,\downarrow}\right) d^\dagger_{0,\downarrow}\right] + 0.12(7)\left(p^\dagger_{+,\uparrow} p^\dagger_{+,\downarrow} + p^\dagger_{-,\uparrow} p^\dagger_{-,\downarrow}\right) - \\ &- 0.22(3)\left(p^\dagger_{+,\uparrow} p^\dagger_{-,\downarrow} + p^\dagger_{-,\uparrow} p^\dagger_{+,\downarrow}\right) + 0.29(6) d^\dagger_{0,\uparrow} d^\dagger_{0,\downarrow}, \end{aligned} \tag{4.3}$$

[2] In accordance with our notation convention (see Appendix A), the last significant digit is surrounded by a parenthesis. For example: $-0.5625 < -0.56(2) < -0.5615$

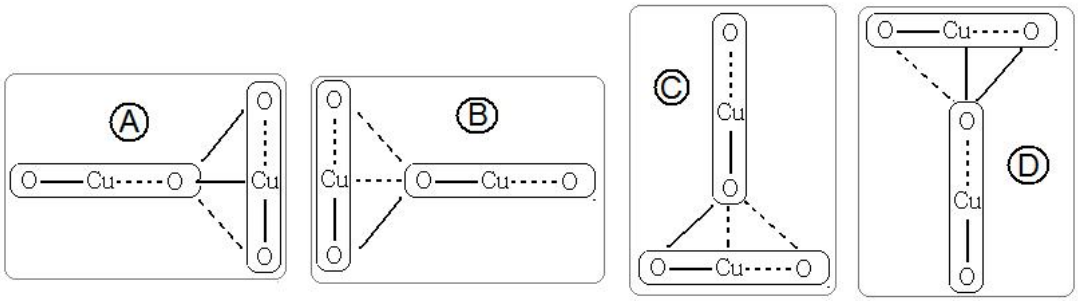

Figure 4.4: The four cluster combinations. Full lines represent hopping where $\alpha^{pd} = 1$ (For Cu-O hopping) or $\alpha^{pp} = 1$ (For O-O hopping), and dotted lines represent $\alpha^{pd} = -1$ or $\alpha^{pp} = -1$

where the common index i again has been suppressed on the right hand sides. While we have presented only the four lowest-energy states here, we computed 64 eigenstates $\{A^\dagger_{i,a_i}\Omega\})_{a_i\in\{1,2,\cdots,64\}}$ to H_i, constituting a complete orthonormal basis in the subspace of cluster i.

4.2 The full Hamiltonian

The sum of the operators in (4.2), $\sum_{i=1}^{L} H_i$, represents the sum of energies in all clusters, isolated from each other. To get the full Hamiltonian, (4.1), the terms that constitute the interaction between neighboring clusters need to be added in. There are four different types of cluster pairs $\langle i,j\rangle$, as illustrated in Figure 4.4.

We let H_{ij} be the interaction Hamiltonian between clusters i and j, which gives the full Hamiltonian

$$H = \sum_i H_i + \sum_{\langle i,j\rangle} H_{ij} \tag{4.4}$$

The explicit expression for each $H_{i,j}$ will depend not only on i and j, but also what type A-D of cluster pair $\langle i,j\rangle$ is. We note, however, that all H_{ij}:s contain terms that depend on U_{pd}, t_{pd} and t_{pp}.

The full Hamiltonian in matrix notation is a $64^L \times 64^L$ matrix, whose elements are $H_{n,m} = \langle\Psi_n|H|\Psi_m\rangle$ in some basis $|\Psi_n\rangle$.

We could construct a complete orthonormal basis in $\mathcal{H}$, the Hilbert space of the fermion states on the whole lattice, by combining the one-cluster states $(A^\dagger_{a_i}\Omega)_{a_i\in\{1,2,\cdots,64\}}$. The fact that the states $A^\dagger_{a_i}\Omega$ are eigenstates to their respective H_i simplifies this procedure. To find the energies representing the full system amounts to diagonalizing this $64^L \times 64^L$ matrix. The complexity of this task grows very fast with the size L of the lattice, and it soon becomes unmanageable. (See Section 3.2 for an example of how the complexity grows in a similar system.) In Chapter 5, we show how each element in the matrix representation of the three-band Hamiltonian can be reproduced by an extended one-band model.

Chapter 5

Matching the Hubbard models

We want to replace the clusters, each consisting of one Cu site and two O sites, with one single lattice site. This procedure is illustrated in Figure 5.1: Each cluster, with a Cu site labeled $i \in \{1, 2, \cdots, L\}$, is replaced with a site labeled i. For this new one-band model, with an Hamiltonian $\tilde{H}$, to represent the low-energy states of the three-band model, with Hamiltonian H as in Equation (4.1), appropriately, it is necessary that it is done in such a way that every matrix element $H_{n,m}$ is reproduced in the matrix element $\tilde{H}_{n,m}$. The matrix elements depend not only on the operators, but also on the choice of basis states. Consequentially, we have to find a matching both between the basis states, and between the operators H and $\tilde{H}$.

We will first define an association of basis states, and thereafter find the one-band Hubbard model Hamiltonian $\tilde{H}$.

5.1 Associating states

As illustrated in Figure 5.1, we want to replace the state in each cluster with a state on one single site. Taking spin into account, we want to replace the system with six accessible single-particle states by a system with two accessible single-particle states. In other words, we want to replace, in each cluster, the Hilbert space $\mathcal{H}_i$ of dimension $2^6 = 64$ with a reduced Hilbert space $\mathcal{H}_{i,red}$ of dimension $2^2 = 4$.

In Section 5.1.1, we will make the approximation that the states in each cluster i will be in either of the following four states: $A^\dagger_{i,1}\Omega, A^\dagger_{i,2}\Omega, A^\dagger_{i,3}\Omega$ or $A^\dagger_{i,4}\Omega$, with $A^\dagger_{i,a_i}$ as in Equation (4.3).

5.1.1 Ignoring high-energy three-band states

In Section 4.1, we solved the isolated problem of each cluster. That is, we found states $A^\dagger_{i,a_i}\Omega$ with corresponding energies E_{a_i} ($a_i \in \{1, 2, \cdots, 64\}$), such that H_i is diagonal in the basis $\{A^\dagger_{i,a_i}\Omega\}$. Using these states, we may construct a complete orthonormal basis in $\mathcal{H}$, the Hilbert space spanned by *all* possible pure fermion states on the whole CuO_2 lattice:

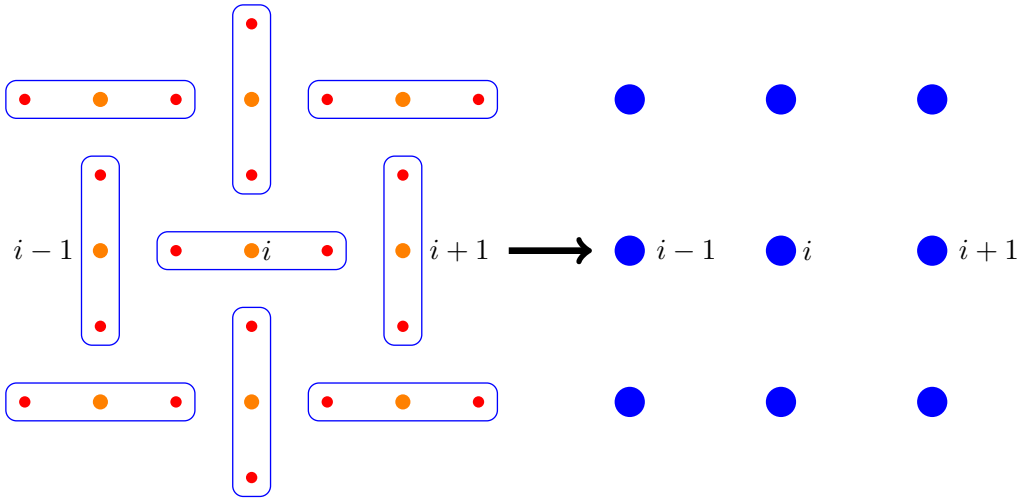

Figure 5.1: Clusters collapsed to sites. To the left: a part of the CuO_2 lattice, with the division into nine clusters. To the right: Each cluster is replaced by a single site, the state on which will replace the state in the corresponding cluster, when we match the two models. The cluster whose Cu-atom has index i is replaced by site i. (The index assignment is arbitrarily chosen here, and only to illustrate the matching principle.)

$$|\mathbf{a}_{Full}\rangle = \prod_{i=1}^{L} A^{\dagger}_{i,a_i}\Omega \tag{5.1}$$
$$\mathbf{a}_{Full} = (a_1, a_2, \cdots, a_L);\ a_i \in \{1, 2, \cdots, 64\}$$

Now consider $\mathcal{H}_A \subset \mathcal{H}$, spanned by the following basis:

$$|\mathbf{a}\rangle = \prod_{i=1}^{L} A^{\dagger}_{i,a_i}\Omega \tag{5.2}$$
$$\mathbf{a} = (a_1, a_2, \cdots, a_L);\ a_i \in \{1, 2, 3, 4\}$$

We apply the partitioning method outlined in Section 2.3:

$H|\Psi\rangle = E|\Psi\rangle$ on $\mathcal{H}$ is equivalent to $H_{eff}|\Psi_A\rangle = E\Psi_A$ on $\mathcal{H}_A$, with the effective Hamiltonian:

$$H_{eff} = H_{AA} + H_{AB}(E - H_{BB})^{-1}H_{BA} \tag{5.3}$$

We make our key approximation:

$$H_{eff} = H_{AA} \tag{5.4}$$

This approximation amounts to treating the terms linking different CuO_2-clusters in leading order perturbation theory. We stress that the approximation (5.4) is highly non-trivial. It would be of great interest to examine the validity of this approximation in greater detail. That is, however, beyond the scope of this project.

5.1.2 Associating states between the models

We have now determined a basis that spans $\mathcal{H}_A$, and we have assumed that this is the regime that we are interested in, by approximating $H_{eff} = H_{AA}$.

We now observe that the four states in which we are interested have the following quantum numbers, respectively: $\{n = 0, s^z = 0\}, \{n = 1, s^z = \frac{1}{2}\}, \{n = 1, s^z = -\frac{1}{2}\}, \{n = 2, s^z = 0\}$. This allows us to make the following identification: three-band model operators in cluster i are identified with the one-band operators on site i [1]

$$\begin{aligned} A^\dagger_{i,1} &\longleftrightarrow \tilde{A}^\dagger_{i,1} = I \\ A^\dagger_{i,2} &\longleftrightarrow \tilde{A}^\dagger_{i,2} = a^\dagger_{i,\uparrow} \\ A^\dagger_{i,3} &\longleftrightarrow \tilde{A}^\dagger_{i,3} = a^\dagger_{i,\downarrow} \\ A^\dagger_{i,4} &\longleftrightarrow \tilde{A}^\dagger_{i,4} = a^\dagger_{i,\uparrow} a^\dagger_{i,\downarrow} \end{aligned} \tag{5.5}$$

Note that each identification preserves n and s^z . By the straightforward analogy of the basis in (5.2), a complete orthonormal basis in the one-band Hilbert space $\tilde{\mathcal{H}}$ is constituted by the states:

$$\begin{aligned} |\tilde{\mathbf{a}}\rangle &= \prod_{i=1}^{L} \tilde{A}^\dagger_{i,a_i} \Omega \\ \tilde{\mathbf{a}} &= (a_1, a_2, \cdots, a_L);\ a_i \in \{1, 2, 3, 4\} \end{aligned} \tag{5.6}$$

5.2 Finding the one-band Hubbard Hamiltonian

Equation (5.5) now defines how three-band model states are associated with states in the extended one-band model. To ensure that each matrix element is exactly reproduced, it remains to define an extended one-band Hubbard Hamiltonian $\tilde{H}$.

[1] In each of the identifications (5.5), we could add an arbitrary phase factor $e^{i\theta_{a_i}}$; $\theta_{a_i} \in \mathbb{R}$. We have, implicitly in (5.5), set $\theta_{a_i} = 0 \,\forall\, a_i$. Other choices of θ_{a_i} would give an equivalent identification, as long as we take the phase factor into account when matching the three-band to one-band matrix elements in Section (5.2.2). For the same reason, when we calculate the three-band matrix elements using Matlab, we make sure that Matlab uses the correct phases. (See Appendix C.2.2 for the code.)

We remind ourselves that the task is to find a one-band Hamiltonian $\tilde{H}$ such that *all* elements in the three-band matrix H are exactly reproduced. The following proposition considerably simplifies this task:

Proposition 5.2.1 *Consider the three-band Hamiltonian $H = \sum_i H_i + \sum_{\langle i,j\rangle} H_{ij}$ on $\mathcal{H}$, the Hilbert space of fermion states on the CuO_2 lattice. Assume that the choice of division into clusters defined in Figure 4.3 and the identification (5.5) between three-band and one-band creation operators are used. Furthermore, assume that the the same ordering is used for both models: let the cluster with the Cu site labeled i in the three-band model be associated with the site labeled i in the one-band model. To find a one-band Hubbard model Hamiltonian $\tilde{H}$, such that every matrix element $\langle \mathbf{a}'|H|\mathbf{a}\rangle$ equals the corresponding matrix element $\langle \tilde{\mathbf{a}}'|\tilde{H}|\tilde{\mathbf{a}}\rangle$, it is then sufficent to match the following matrix elements, for all nearest-neighbor pairs $\langle i,j\rangle$ of clusters/sites:*
$\langle \Omega A_{j,a'_j} A_{i,a'_i} | \frac{1}{T_i} H_i + \frac{1}{T_j} H_j + H_{ij} | A^\dagger_{i,a_i} A^\dagger_{j,a_j} \Omega\rangle =$
$= \langle \Omega \tilde{A}_{j,a'_j} \tilde{A}_{i,a'_i} | \frac{1}{T_i} \tilde{H}_i + \frac{1}{T_j} \tilde{H}_j + \tilde{H}_{ij} | \tilde{A}^\dagger_{i,a_i} \tilde{A}^\dagger_{j,a_j} \Omega\rangle,$
where T_i is the number of $\langle i,j\rangle$ pairs in which cluster/site i takes part ($T_i = 4$ for interior lattice clusters/sites), H_i and $\tilde{H}_i$ are the parts of the Hamiltonians acting only on cluster/site i, and H_{ij} and $\tilde{H}_{ij}$ are the parts of the Hamiltonians representing the interaction energy between clusters/sites i and j.

Proof See Appendix B.2

Since we have assumed that each cluster i can be found in one of only four different states $A^\dagger_{i,a_i}\Omega$, the state on two clusters i and j, whose combined Hilbert space is the tensor product $h_i \otimes h_j$, is one of the following 16 cases: $A^\dagger_{i,a_i}\Omega \otimes A^\dagger_{j,a_j}\Omega = A^\dagger_{i,a_i} A^\dagger_{j,a_j}\Omega$. We now want to find all elements in the 16×16 matrix representing the three-band Hamiltonian, and match them to the 16×16 elements in the one-band Hamiltonian matrix. Due to that H and $\tilde{H}$ (as we will choose it in our ansatz) conserve particle number and spin, the number of nonzero elements is considerably reduced. We label the 16 states as follows, in order to obtain a matrix with a block-diagonal form:

$$\begin{aligned}
&\Psi_1 = A^\dagger_{i,1}A^\dagger_{j,1}\Omega; \Psi_2 = A^\dagger_{i,2}A^\dagger_{j,1}\Omega; \Psi_3 = A^\dagger_{i,1}A^\dagger_{j,2}\Omega; \Psi_4 = A^\dagger_{i,3}A^\dagger_{j,1}\Omega; \Psi_5 = A^\dagger_{i,1}A^\dagger_{j,3}\Omega;\\
&\Psi_6 = A^\dagger_{i,2}A^\dagger_{j,2}\Omega; \Psi_7 = A^\dagger_{i,4}A^\dagger_{j,1}\Omega; \Psi_8 = A^\dagger_{i,2}A^\dagger_{j,3}\Omega; \Psi_9 = A^\dagger_{i,3}A^\dagger_{j,2}\Omega; \Psi_{10} = A^\dagger_{i,1}A^\dagger_{j,4}\Omega;\\
&\Psi_{11} = A^\dagger_{i,3}A^\dagger_{j,3}\Omega; \Psi_{12} = A^\dagger_{i,4}A^\dagger_{j,2}\Omega; \Psi_{13} = A^\dagger_{i,2}A^\dagger_{j,4}\Omega;\\
&\Psi_{14} = A^\dagger_{i,4}A^\dagger_{j,3}\Omega; \Psi_{15} = A^\dagger_{i,3}A^\dagger_{j,4}\Omega; \Psi_{16} = A^\dagger_{i,4}A^\dagger_{j,4}\Omega
\end{aligned} \tag{5.7}$$

It follows from the matching (5.5) that each three-band two-clusters states in (5.7) are identified with the corresponding one-band two-cluster state $\tilde{\Psi}_k = \tilde{A}^\dagger_{i,a_i}\tilde{A}^\dagger_{j,a_j}\Omega$.

5.2.1 Ansatz for the one-band Hubbard Hamiltonian

We propose the following ansatz for an extended one-band Hubbard model Hamiltonian on two sites i and j [1]. Assume that the operator that we want to find satisfies particle number and spin conservation, and that it is invariant under the transformations $\uparrow\leftrightarrow\downarrow$ (swapping all spins) and $i \leftrightarrow j$ (interchanging sites i and$j$):

$$\tilde{H} = \tilde{H}_{\text{Hopping}} + \tilde{H}_{\mu} + \tilde{H}_{U} + \tilde{H}_{\text{Interaction}},$$

where

$$\begin{aligned}
\tilde{H}_{\text{Hopping}} &= -\sum_{\sigma=\uparrow,\downarrow} (a^{\dagger}_{i,\sigma} a_{j,\sigma} + a^{\dagger}_{j,\sigma} a_{i,\sigma}) \left[t + X(\hat{n}_{i,-\sigma} + \hat{n}_{j,-\sigma}) + Z\hat{n}_{i,-\sigma}\hat{n}_{j,-\sigma}\right] \\
\tilde{H}_{\mu} &= -\mu(\hat{n}_i + \hat{n}_j) \\
\tilde{H}_{U} &= U(\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}) \\
\tilde{H}_{\text{Interaction}} &= \frac{V}{2}\hat{n}_i\hat{n}_j + \sum_{\sigma} W\left(\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}\hat{n}_{j,\sigma} + \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}\hat{n}_{i,\sigma}\right) + W''\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}\hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}
\end{aligned}$$

When trying to match all elements, it turns out that we need to add terms to the hopping and interaction parts of $\tilde{H}$ that measure the difference between the particle numbers on site i and j, and thereby break the $i \leftrightarrow j$ interchange invariance:

$$\begin{aligned}
&\sum_{\sigma} \epsilon_{ij} W'\left(\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}\hat{n}_{j,\sigma} - \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}\hat{n}_{i,\sigma}\right) \\
&- \sum_{\sigma=\uparrow,\downarrow} (a^{\dagger}_{i,\sigma} a_{j,\sigma} + a^{\dagger}_{j,\sigma} a_{i,\sigma}) \epsilon_{ij} X'((\hat{n}_{i,-\sigma} - \hat{n}_{j,-\sigma})),
\end{aligned}$$

where $\epsilon_{ij} \in \{-1, 1\}$[2]. The full one-band Hamiltonian ansatz on two sites i and j thus reads:

$$\begin{aligned}
\tilde{H} = &-\sum_{\sigma=\uparrow,\downarrow} (a^{\dagger}_{i,\sigma} a_{j,\sigma} + a^{\dagger}_{j,\sigma} a_{i,\sigma}) \left[t + (X + \epsilon_{ij}X')\hat{n}_{i,-\sigma} + (X - \epsilon_{ij}X')\hat{n}_{j,-\sigma}) + Z\hat{n}_{i,-\sigma}\hat{n}_{j,-\sigma}\right] - \\
&- \mu(\hat{n}_i + \hat{n}_j) + U(\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + \hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}) + \\
&+ \frac{V}{2}\hat{n}_i\hat{n}_j + \sum_{\sigma=\uparrow,\downarrow} (W + \epsilon_{ij}W')\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}\hat{n}_{j,\sigma} + (W - \epsilon_{ij}W')\hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}\hat{n}_{i,\sigma} + W''\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}\hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}
\end{aligned} \tag{5.8}$$

[1] Throughout this chapter, we call the one-band operator on two sites $\tilde{H}$, avoiding indexes i and j. We do so to be able to separate between the parts $\tilde{H}_i$ and $\tilde{H}_j$ of $\tilde{H}$ that act only on site i or j and the part $\tilde{H}_{ij}$ which couples i with site j. In Chapter 6, $\tilde{H}$ is the extended one-band Hamiltonian on the whole CuO_2 lattice

[2] ϵ_{ij} is introduced in order to take account for the arbitrary assignments of i and j in a given nearest-neighbors pair of clusters. The role of this sign factor becomes clearer in Section 5.2.2

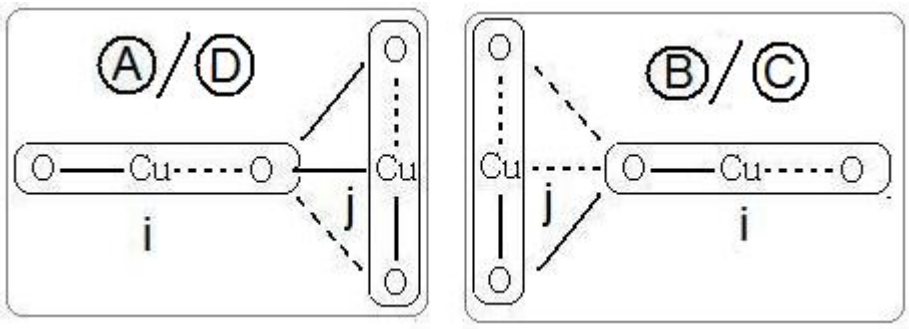

Figure 5.2: Labelling convention i and j for cluster combination types A/D and B/C. Full lines represent hopping where $\alpha^{pd} = 1$ (For Cu-O hopping) or $\alpha^{pp} = 1$ (For O-O hopping), and dotted lines represent $\alpha^{pd} = -1$ or $\alpha^{pp} = -1$

Below we make clear which parts of $\tilde{H}$ that act on one cluster only ($\tilde{H}_i$ and $\tilde{H}_j$), and which parts ($\tilde{H}_{ij}$)that couple two clusters:

$$\begin{aligned} \tilde{H} &= \tilde{H}_i + \tilde{H}_j + \tilde{H}_{ij}, \text{ where:} \\ \tilde{H}_i + \tilde{H}_j &= \tilde{H}_\mu + \tilde{H}_U \\ \tilde{H}_{ij} &= \tilde{H}_V + \tilde{H}_W + \tilde{H}'_W + \tilde{H}_{W''} + \tilde{H}_t + \tilde{H}_X + \tilde{H}_{X'} + \tilde{H}_Z, \end{aligned} \tag{5.9}$$

where we use an obvious short-hand notation for the different terms of the Hamiltonian in (5.8).

5.2.2 Matching matrix elements – finding the parameters

In this section, we construct the 16×16 one-band Hamiltonian matrix h whose elements are

$$h_{k,l} = \langle \tilde{\Psi}_k | \frac{\tilde{H}_i}{T_i} + \frac{\tilde{H}_j}{T_j} + \tilde{H}_{ij} | \tilde{\Psi}_l \rangle$$

where T_i is the number of next-neighbor pairs in which site i takes place (see Proposition 5.2.1). We will consider only cases where both i and j are interior lattice sites, each surrounded by four other sites, and thus $T_i = T_j = 4$.[1] As previously discussed, there are four types of cluster combinations in the three-band model (see Figure 4.4). However, studying these different types, we find that type A is equivalent to type D, and type B is equivalent to type C (this is more easily seen if rotating A and B by 90 degrees). Thus, it is sufficient to carry out the matching for the type A and type B cluster combinations. We also have to decide upon an assignment of labels i and j to each of the clusters in the pair under consideration. We choose the convention illustrated in Figure 5.2.

[1] In the thermodynamique limit of number of lattice sites, the fraction between interior site and border sites approaches one. Furthermore, when carrying out the numerical calculation, we find that the one-band parameter values found do not change when we set $T_i = 3$ (sites on the border) or $T_i = 2$ (corner sites).

The ordering of the states $\tilde{\Psi}_k$ in (5.7) is chosen such that h will be block-diagonal, where the diagonally oriented blocks with nonzero elements are the following: h_1^1 (where $n = s^z = 0$); h_2^3 ($n = 1, s^z = \frac{1}{2}$); h_4^5 ($n = 1, s^z = -\frac{1}{2}$); h_6^6 ($n = 2, s^z = 1$); h_7^{10} ($n = 2, s^z = 0$); h_{11}^{11} ($n = 2, s^z = -1$); h_{12}^{13} ($n = 3, s^z = \frac{1}{2}$); h_{14}^{15} ($n = 3, s^z = -\frac{1}{2}$); h_{16}^{16} ($n = 4, s^z = 0$), where $h_m^n \equiv \{h_{k,l}\}_{m \le k,l \le n}$

We get the following results[2]:

$$
\begin{aligned}
h_1^1 &= 0 \\
h_2^3 = h_4^5 &= \begin{pmatrix} -\mu/T_i & -t \\ -t & -\mu/T_i \end{pmatrix} \\
h_6^6 = h_{11}^{11} &= -2\mu/T_i + V/2 \\
h_7^{10} &= \begin{pmatrix} (-2\mu+U)/T_i & -(t+X+X') & (t+X+X') & 0 \\ -(t+X+X') & -2\mu/T_i + V/2 & 0 & -(t+X-X') \\ (t+X+X') & 0 & -2\mu/T_i + V/2 & (t+X-X') \\ 0 & -(t+X-X') & (t+X-X') & (-2\mu+U)/T_i \end{pmatrix} \\
h_{12}^{13} = h_{14}^{15} &= \begin{pmatrix} (-3\mu+U)/T_i + V + (W+W') & (t+2X+Z) \\ (t+2X+Z) & (-3\mu+U)/T_i + V + (W-W') \end{pmatrix} \\
h_{16}^{16} &= (-4\mu+2U)/T_i + 2V + 4W + W''
\end{aligned}
\tag{5.10}
$$

We use Matlab to calculate numerical values of the corresponding three-band model parameters, and find the one-band parameters from the following equations:

$$
\begin{aligned}
\mu &= -h_{2,2} \\
t &= -h_{2,3} \\
V &= h_{6,6} + 2\mu \\
U &= h_{7,7} + 2\mu \\
X &= (h_{7,9} + h_{9,10})/2 - t \\
X' &= (h_{7,9} - h_{9,10})/2 \\
W &= (h_{12,12} + h_{13,13})/2 + 3\mu - U - 2V \\
W' &= (h_{12,12} - h_{13,13})/2 \\
W'' &= h_{16,16} + 4\mu - 2U - 4V - 4W
\end{aligned}
\tag{5.11}
$$

Inserting the values found with Matlab [3] we find the following parameters for *both* type A and B cluster combinations: [4]

[2] For clarity, we use T_i in for all matrix elements, keeping in mind that $T_i = T_j = 4$.

[3] The full code for cluster combinations of type A/D and type B/C is found in Appendix C.2.2

[4] We also verify that the numerical results satisfy the additional constraints that follow from the form of h: $h_{1,1} = 0$; $h_{2,2} = h_{3,3} = h_{4,4} = h_{5,5}$; $h_{6,6} = h_{8,8} = h_{9,9} = h_{11,11}$; $h_{7,7} = h_{10,10}$; $h_{7,8} = -h_{7,9}$; $h_{7,10} = h_{8,9} = 0$; $h_{8,10} = -h_{9,10}$; $h_{12,12} = h_{14,14}$; $h_{13,13} = h_{15,15}$; $h_{12,13} = h_{13,13}$ and $h_{k,l} = h_{l,k}\ \forall k, l$

$$\begin{aligned}
\mu &= 0.56(2) \\
U &= 3.16(0) \\
t &= -0.31(1) \\
X &= -0.12(0) \\
X' &= -0.16(7) \\
Z &= 0.04(4) \\
V &= 0.05(9) \\
W &= 0.07(0) \\
W' &= 0.09(6) \\
W'' &= -0.14(9)
\end{aligned} \tag{5.12}$$

We do the same procedure again, but with the labelling conversed from Figure 5.2: $i \to j$ and $j \to i$. We find the same result as in (5.12), expect that $X' \to -X'$ and $W' \to -W'$. This confirms our expectation: The only terms in $\tilde{H}$ that depend on the assignment of labels i and j, for a given cluster pair $\langle i, j \rangle$, are $\tilde{H}_{X'}$ and $\tilde{H}_{W'}$. The pattern of horizontal and vertical clusters, together with the above results from matching cluster combinations of type A, B, C and D now allows us to define ϵ_{ij} as follows: In the below figure, the sign of ϵ_{ij}, in the extended one-band Hamiltonian (5.8) acting on two sites i and j, is $\epsilon_{ij} = 1$ if the arrow points from i to j, and $\epsilon_{ij} = -1$ if the arrow points from j to i:

$$\begin{array}{ccccccccccc}
 & & \uparrow & & \downarrow & & \uparrow & & \downarrow & & \uparrow \\
\rightarrow & \bullet & \leftarrow & \circ & \rightarrow & \bullet & \leftarrow & \circ & \rightarrow & \bullet & \leftarrow \\
 & & \downarrow & & \uparrow & & \downarrow & & \uparrow & & \downarrow \\
\leftarrow & \circ & \rightarrow & \bullet & \leftarrow & \circ & \rightarrow & \bullet & \leftarrow & \circ & \rightarrow \\
 & & \uparrow & & \downarrow & & \uparrow & & \downarrow & & \uparrow \\
\rightarrow & \bullet & \leftarrow & \circ & \rightarrow & \bullet & \leftarrow & \circ & \rightarrow & \bullet & \leftarrow \\
 & & \downarrow & & \uparrow & & \downarrow & & \uparrow & & \downarrow \\
\leftarrow & \circ & \rightarrow & \bullet & \leftarrow & \circ & \rightarrow & \bullet & \leftarrow & \circ & \rightarrow \\
 & & \uparrow & & \downarrow & & \uparrow & & \downarrow & & \uparrow
\end{array} \tag{5.13}$$

In the above, circles are sites i where the Cu site labeled i (in the three-band model) is part of a horizontally oriented cluster, and bullets are sites i where the Cu site with label i appears in a vertically oriented cluster.

We write down the expression for the extended one-band Hubbard model on the full CuO_2 lattice in Chapter 6.

5.3 Varying the three-band model parameters

The values of the parameters in the three-band Hubbard model are not precisely determined. Throughout our calculations, we have used the values given in [1, p. 5], and the one-band parameter values in (5.12) correspond to that specific choice of three-band parameters.

In this section, we study how the one-band parameters are varied are obtained when using other parameter values in the three-band model.

5.3.1 Other sets of three-band parameters

In this section, we use one set of three-band parameters found in [12, Section II]) and three sets of parameters from [11, Table VI]. More precisely, we take, from [11, Table VI], the sets of parameters referred to as "Present", "HSC" and "SJ". In the below table, the complete sets of three-band parameters are listed. We call the parameters used previously in our calculations, from [1, p. 5], "Arrigoni", and the parameters from [12, Section II] "Raimondi", while the three parameter sets from [11, Table VI] are named "McMahan" (called "Present" in [11, Table VI]), "HSC" and "SJ". Note that in these calculations, we set the chemical potential μ to zero. (All energies in eV)

Parameter	Arrigoni	Raimondi	McMahan	HSC	SJ
$\epsilon_p - \epsilon_d$	3.0	3.51	3.5	3.6	1.5
t_{pd}	1.0	1.3	1.5	1.3	1.07
t_{pp}	0.5	0.65	0.6	0.65	0.53
U_{dd}	8.0	9.1	9.4	10.5	9.0
U_{pd}	0.5	1.3	0.8	1.5	1.5
U_{pp}	3.0	3.9	4.7	3.6	6.0
μ	0	0	0	0	0

Below, we present the values of the one-band parameters obtained when using each of the above sets of three-band parameters. Note that the first row corresponds to [1], and the one-band parameters are the same as listed in (5.12).

Three-band parameters used	μ	U	t	X	X'	Z
Arrigoni	0.56(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)
Raimondi	0.78(7)	4.17(3)	-0.43(3)	-0.14(4)	-0.19(8)	0.04(3)
McMahan1990	1.00(0)	3.79(7)	-0.51(8)	-0.12(9)	-0.21(2)	0.05(4)
HSC	0.77(3)	4.51(7)	-0.42(6)	-0.14(8)	-0.21(3)	0.05(5)
SJ	0.93(9)	2.87(6)	-0.48(6)	-0.04(8)	-0.14(4)	0.03(8)

Three-band parameters used	V	W	W'	W''
Arrigoni	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
Raimondi	0.17(0)	0.16(5)	0.23(9)	-0.35(1)
Present	0.11(9)	0.08(6)	0.13(6)	−0.18(4)
HSC	0.19(2)	0.20(8)	0.29(7)	−0.47(0)
SJ	0.30(1)	0.12(7)	0.28(6)	-0.43(7)

5.3.2 Varying each three-band parameter separately

In this section, we start off with the three-band parameters from [1, p. 5]. We then vary one of the parameters, while keeping the others fixed, and study what happens to the one-band parameters. The results are presented both graphically, and by listing the results in tables.

Varying $\epsilon_p - \epsilon_d$

We fix all three-band parameters except $\epsilon_p - \epsilon_d$ at the values from [1, p. 5]: $t_{pd} = 1$, $t_{pp} = 0.5$, $U_{dd} = 8$, $U_{pd} = 0.5$, $U_{pp} = 3$ and $\mu = 0$. The table below gives the one-band parameters that result from setting ϵ_p to each of the values in the far left column (and $\epsilon_d = 0$). Figure 5.3 plots all one-band parameters in units of $t = 1$ (t is not plotted).

ϵ_p	μ	U	t	X	X'	Z	V	W	W'	W''
2	0.73(2)	2.41(1)	-0.39(4)	-0.08(6)	-0.15(0)	0.03(8)	0.08(3)	0.05(2)	0.09(0)	-0.12(9)
2.5	0.63(8)	2.77(9)	-0.34(9)	-0.10(5)	-0.16(0)	0.04(2)	0.07(0)	0.06(2)	0.09(4)	-0.14(1)
3	0.56(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
3.5	0.50(0)	3.54(9)	-0.27(8)	-0.13(2)	-0.17(2)	0.04(4)	0.04(9)	0.07(6)	0.09(8)	-0.15(2)
4	0.45(0)	3.93(8)	-0.25(0)	-0.14(1)	-0.17(4)	0.04(1)	0.04(2)	0.07(9)	0.09(7)	-0.15(1)

Varying t_{pd}

We fix all parameters except t_{pd}: $\epsilon_p - \epsilon_d = 3$, $t_{pp} = 0.5$, $U_{dd} = 8$, $U_{pd} = 0.5$, $U_{pp} = 3$ and $\mu = 0$. The table below gives the one-band parameters that result from setting t_{pd} to the values in the far left column. Figure 5.4 plots all one-band parameters in units of $t = 1$.

t_{pd}	μ	U	t	X	X'	Z	V	W	W'	W''
0.8	0.37(9)	3.23(5)	-0.22(1)	-0.12(2)	-0.14(9)	0.03(3)	0.04(5)	0.08(4)	0.10(5)	-0.17(6)
1	0.56(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.1488
1.3	0.87(3)	3.07(0)	-0.44(8)	-0.11(0)	-0.18(5)	0.04(9)	0.07(5)	0.05(3)	0.08(5)	-0.1144
1.5	1.09(8)	3.02(2)	-0.53(9)	-0.10(3)	-0.19(2)	0.04(9)	0.08(3)	0.04(5)	0.07(8)	-0.09(6)
1.7	1.33(4)	2.98(1)	-0.62(8)	-0.09(6)	-0.19(8)	0.04(8)	0.09(0)	0.03(8)	0.07(1)	-0.08(1)

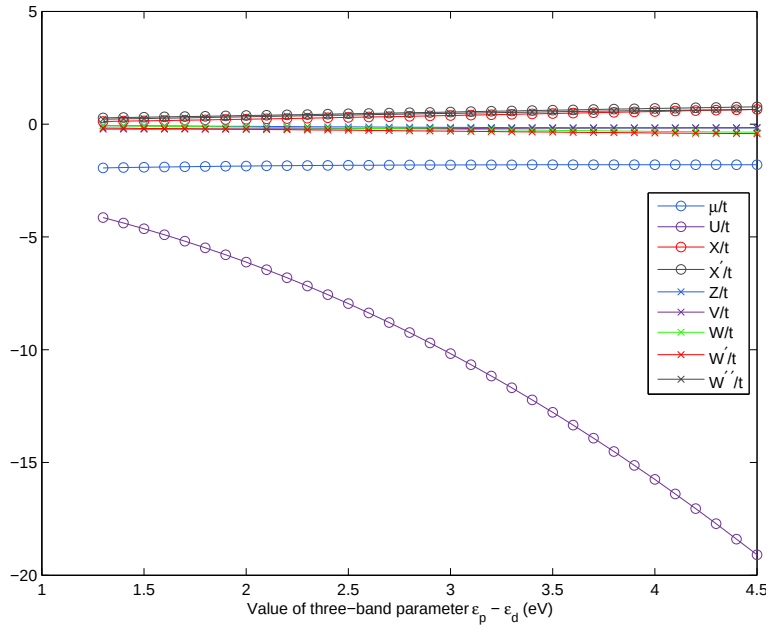

Figure 5.3: Plots of one-band parameter in units of $t = 1$, when varying the three-band parameter $\epsilon_p - \epsilon_d$. (Colors in electronic version)

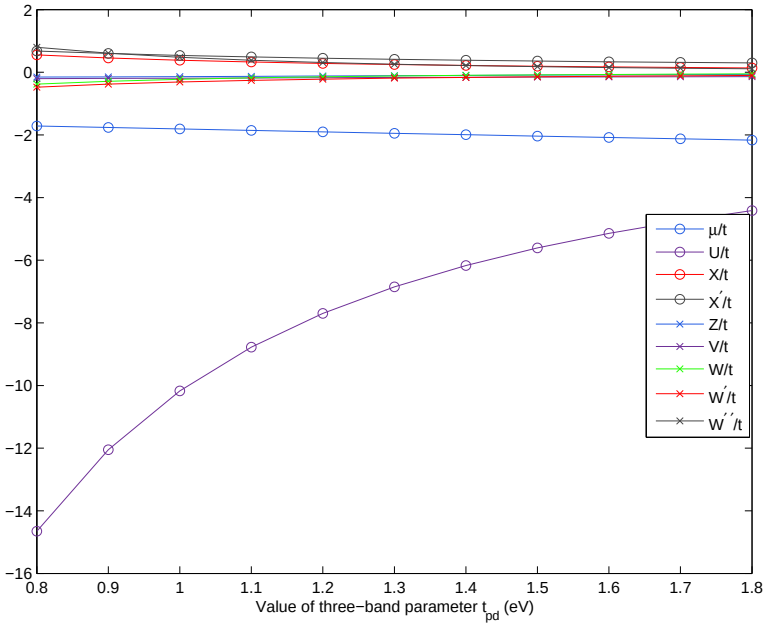

Figure 5.4: Plots of one-band parameter in units of $t = 1$, when varying the three-band parameter t_{pd}, (Colors in electronic version)

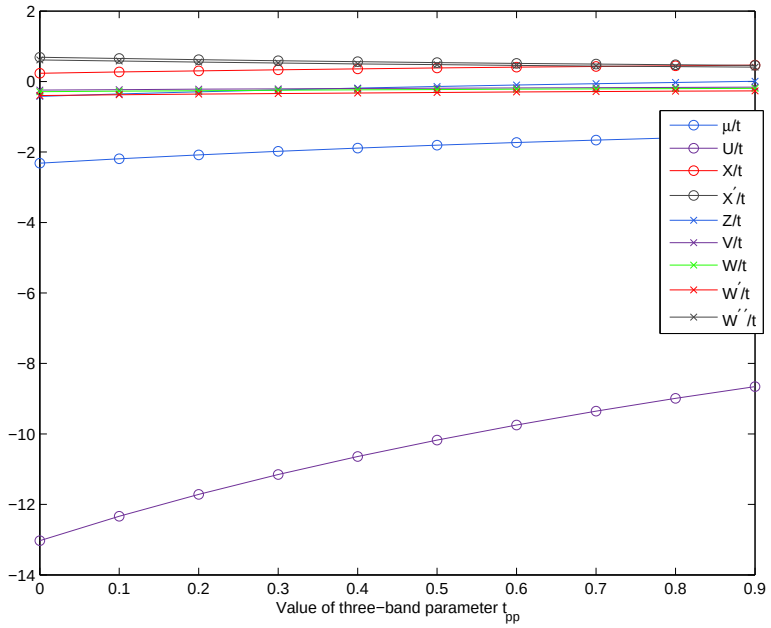

Figure 5.5: Plots of one-band parameter in units of $t = 1$, when varying the three-band parameter t_{pp} (Colors in electronic version)

Varying t_{pp}

We fix all parameters except t_{pp}: $\epsilon_p - \epsilon_d = 3$, $t_{pd} = 1$, $U_{dd} = 8$, $U_{pd} = 0.5$, $U_{pp} = 3$ and $\mu = 0$. The table below gives the one-band parameters that result from setting t_{pp} to the values in the far left column. Figure 5.5 plots all one-band parameters in units of $t = 1$.

t_{pp}	μ	U	t	X	X'	Z	V	W	W'	W''
0	0.56(2)	3.16(0)	-0.24(3)	-0.05(7)	-0.16(7)	0.10(2)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
0.2	0.56(2)	3.16(0)	-0.27(0)	-0.08(2)	-0.16(7)	0.07(9)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
0.5	0.56(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
0.8	0.56(2)	3.16(0)	-0.35(2)	-0.15(7)	-0.16(7)	0.00(9)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)

Varying U_{dd}

We fix all parameters except U_{dd}: $\epsilon_p - \epsilon_d = 3$, $t_{pd} = 1$, $t_{pp} = 0.5$, $U_{pd} = 0.5$, $U_{pp} = 3$ and $\mu = 0$. The table below gives the one-band parameters that result from setting U_{dd} to the values in the far left column. Figure 5.6 plots all one-band parameters in units of $t = 1$.

U_{dd}	μ	U	t	X	X'	Z	V	W	W'	W''
8	0.56(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
8.6	0.56(2)	3.20(9)	-0.31(1)	-0.12(0)	-0.17(2)	0.04(9)	0.05(9)	0.07(2)	0.09(9)	-0.15(6)
9.6	0.56(2)	3.27(4)	-0.31(1)	-0.11(9)	-0.17(8)	0.05(6)	0.05(9)	0.07(4)	0.10(2)	-0.16(5)
10.4	0.56(2)	3.31(7)	-0.31(1)	-0.11(9)	-0.18(1)	0.06(0)	0.05(9)	0.07(5)	0.10(3)	-0.17(1)

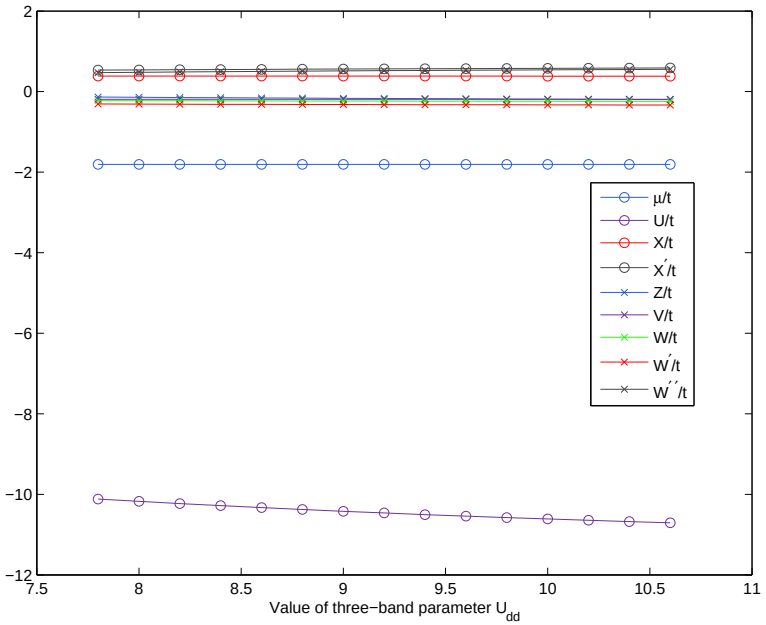

Figure 5.6: Plots of one-band parameter in units of $t = 1$, when varying the three-band parameter U_{dd} (Colors in electronic version)

Varying U_{pd}

We fix all parameters except U_{pd}: $\epsilon_p - \epsilon_d = 3$, $t_{pd} = 1$, $t_{pp} = 0.5$, $U_{dd} = 8$, $U_{pp} = 3$ and $\mu = 0$. The table below gives the one-band parameters that result from setting U_{pd} to the values in the far left column. Figure 5.7 plots all one-band parameters in units of $t = 1$.

U_{pd}	μ	U	t	X	X'	Z	V	W	W'	W''
0	0.56(2)	2.76(4)	-0.31(1)	-0.11(9)	-0.16(9)	0.04(6)	0	0	0	0
0.5	0.56(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
1	0.56(2)	3.54(4)	-0.31(1)	-0.12(0)	-0.16(5)	0.04(2)	0.11(8)	0.14(2)	0.19(6)	-0.30(7)
1.5	0.56(2)	3.91(1)	-0.31(1)	-0.11(9)	-0.16(3)	0.04(0)	0.17(7)	0.21(8)	0.29(9)	-0.47(8)

Varying U_{pp}

We fix all parameters except U_{pp}: $\epsilon_p - \epsilon_d = 3$, $t_{pd} = 1$, $t_{pp} = 0.5$, $U_{dd} = 8$, $U_{pd} = 0.5$ and $\mu = 0$. The table below gives the one-band parameters that result from setting U_{pp} to the values in the far left column. Figure 5.8 plots all one-band parameters in units of $t = 1$.

U_{pp}	μ	U	t	X	X'	Z	V	W	W'	W''
3.	0.56(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
3.6	0.56(2)	3.17(8)	-0.31(1)	-0.11(9)	-0.16(6)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(7)
4.2	0.56(2)	3.19(4)	-0.31(1)	-0.11(8)	-0.16(6)	0.04(3)	0.05(9)	0.07(0)	0.09(6)	-0.14(6)
4.8	0.56(2)	3.20(7)	-0.31(1)	-0.11(7)	-0.16(5)	0.04(3)	0.05(9)	0.06(9)	0.09(5)	-0.14(5)

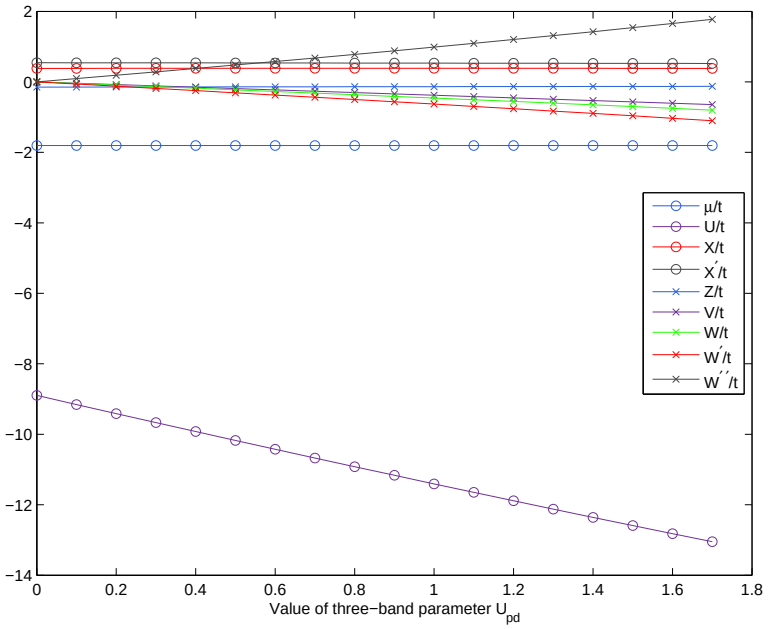

Figure 5.7: Plots of one-band parameter in units of $t = 1$, when varying the three-band parameter U_{pd} (Colors in electronic version)

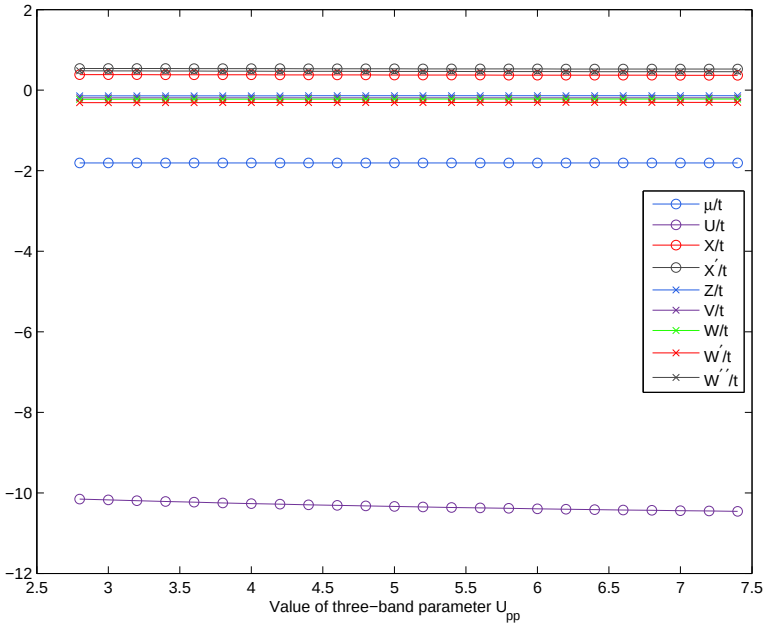

Figure 5.8: Plots of one-band parameter in units of $t = 1$, when varying the three-band parameter U_{pp} (Colors in electronic version)

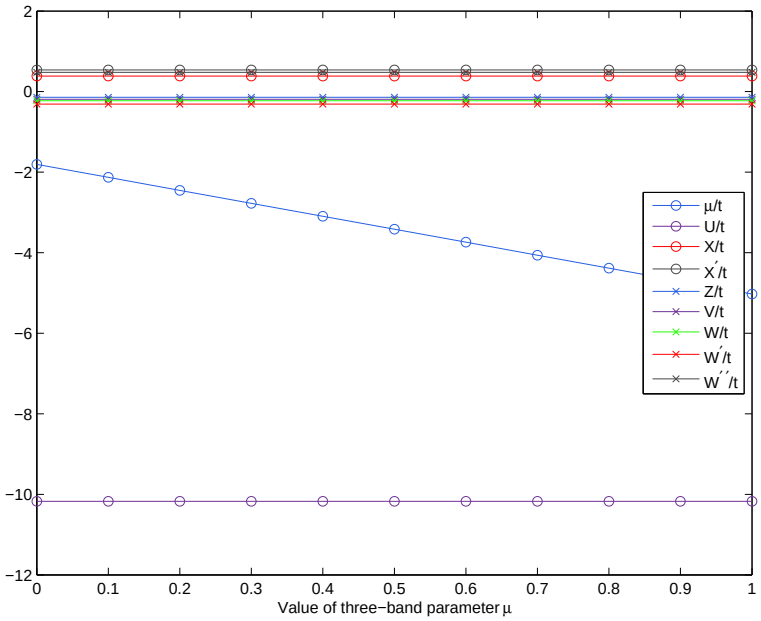

Figure 5.9: Plots of one-band parameter in units of $t = 1$, when varying the three-band chemical potential μ (Colors in electronic version)

Varying μ, the chemical potential

We fix all three-band parameters: $\epsilon_p - \epsilon_d = 3$, $t_{pd} = 1$, $t_{pp} = 0.5$, $U_{dd} = 8$, $U_{pd} = 0.5$ and $\mu = 0$. The table below gives the one-band parameters that result from varying μ_{3B}, the chemical potential in the threee-band model, between the values in the far left column. We see that adding an energy $\Delta\mu$ to the chemical potential μ_{3B} in the three-band model will result in adding the same energy $\Delta\mu$ to the one-band model chemical potential μ_{1B}, while all other one-band parameters remain unchanged. Since the association between three-band model and one-band model states preserve particle number, this was expected, and the result is a good consistency check. This is also illustrated in Figure 5.9.

μ_{3B}	μ_{1B}	U	t	X	X'	Z	V	W	W'	W''
0	0.56(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
0.3	0.86(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
0.6	1.16(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)
1	1.56(2)	3.16(0)	-0.31(1)	-0.12(0)	-0.16(7)	0.04(4)	0.05(9)	0.07(0)	0.09(6)	-0.14(9)

Chapter 6

Conclusion

We started from three-band Hubbard Hamiltonian (defined in Equation (4.1)), which is a model for fermions on a two-dimensional CuO_2 lattice of the type illustrated in Figure 4.1. Our aim was to derive an extended one-band Hubbard model that provides an effective description of the low-energy physics of the three-band model. To remove the degrees of freedom associated with the O sites on this lattice, we treated the lattice as a collection of clusters, each consisting of one Cu site and two O sites. Using a variant of the Feshbach method, we thereafter replaced each such cluster by a single site and thus obtained an extended one-band Hubbard model. Finally, we found the structure and the parameters of the latter model by matching it to the three-band model.

We found the following extended one-band Hubbard Hamiltonian for the fermions in the CuO_2 lattice, with L Cu sites:

$$\begin{aligned}\tilde{H} = &- \sum_{\langle i,j\rangle} \sum_{\sigma=\uparrow,\downarrow} (a^\dagger_{i,\sigma} a_{j,\sigma} + a^\dagger_{j,\sigma} a_{i,\sigma}) \left[t + (X + \epsilon_{ij} X')\hat{n}_{i,-\sigma} + (X - \epsilon_{ij} X')\hat{n}_{j,-\sigma}) + Z\hat{n}_{i,-\sigma}\hat{n}_{j,-\sigma}\right] - \\ &- \mu \sum_i \hat{n}_i + U \sum_i \hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow} + \\ &+ \sum_{\langle i,j\rangle} \frac{V}{2} n_i n_j + \sum_{\langle i,j\rangle} \sum_{\sigma=\uparrow,\downarrow} (W + \epsilon_{ij} W')\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}\hat{n}_{j,\sigma} + \\ &+ \sum_{\langle i,j\rangle} \sum_{\sigma=\uparrow,\downarrow} (W - \epsilon_{ij} W')\hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow}\hat{n}_{i,\sigma} + W''\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}\hat{n}_{j,\uparrow}\hat{n}_{j,\downarrow},\end{aligned} \tag{6.1}$$

where $i \in \{1, \cdots, L\}$ runs over all Cu sites, $\langle i, j\rangle$ runs over all next-neighboring pairs of Cu sites, and ϵ_{ij} is defined in Figure 5.13: $\epsilon_{ij} = 1$ if the arrow points from site i to site j, and $\epsilon_{ij} = -1$ if it points from j to i.

The values of the other parameters in (6.1) depend on the parameters of the three-band Hubbard model. We have constructed a program, using Matlab, which takes as input the parameter values of the three-band model, and gives as output the extended one-band model parameters. Throughout the derivation of the one-band model, we used as example set of three-band parameters given in [1, p. 5], which gives as result the following set of one-band model parameters: $t = -0.31(1)$,

$X = -0.12(0)$, $X' = -0.16(7)$, $Z = 0.04(4)$, $\mu = 0.56(2)$, $U = 3.16(0)$, $V = 0.05(9)$, $W = 0.07(0)$, $W' = 0.09(6)$ and $W'' = -0.14(9)$.

Finally, we tried other sets of three-band model parameters, to see how the one-band model parameters were changed. In particular, we varied each one of the three-band parameters individually, while fixing the others. The results of these tests are presented in Section 5.3.2. We found, for example, that changing the Cu-O hopping term t_{pd} in the three-band Hubbard model changes not only the hopping term parameters (t, X, X' and Z), but also the Coulomb interaction terms (U, V W W' and W''). Also, changing the on-site energies or the Coulomb interaction terms in the three-band model affects not only the interaction terms in the one-band model, but also the hopping terms. The O-O hopping term parameter t_{pp} in the three-band model, however, appears only in interaction between clusters, and consequentially it affects only the hopping terms of the extended one-band Hubbard model. Finally, changing the chemical potential μ in the three-band model changes only, and by the same amount, μ in the one-band model.

It would be interesting to study the extended one-band Hubbard model found in this thesis. In particular, it is of interest to examine the effect the smaller terms (X, X', Z, V, W, W' and W'').

References

[1] E. Arrigoni, M. Aichhorn, M. Daghofer, and W. Hanke. Phase diagram and single-particle spectrum of CuO_2 high-T_c layers: Variational cluster approach to the three-band Hubbard model. *New Journal of Physics*, 11(055066):1–13, 2009.

[2] J. Bardeen, L. N. Cooper, and J. R. Schrieffer. Theory of Superconductivity. *Physical Review Letters*, 108:1175–1204, 1957.

[3] J. Bednorz and K. Müller. Possible High T_c Superconductivity in the Ba-La-Cu-O System. *Zeitschrift für Physik B*, 64:189–193, 1986.

[4] H. Bruus and K. Flensberg. *Many-Body Quantum Theory in Condensed Matter Physics – An Introduction*. Oxford Graduate Texts, 2004.

[5] J. de Woul. A restricted Hartree-Fock study of the 2D Hubbard model. Master's thesis, Royal Institute of Technology, 2007.

[6] V. Emery. Theory of High-T_c Superconductivity in Oxides. *Physical Review Letters*, 58:2794–2797, 1987.

[7] S. Gasiorowicz. *Quantum Physics*. Wiley, third edition, 2003.

[8] C. Kittel. *Introduction to Solid State Physics*. John Wiley & Sons, eighth edition, 2005.

[9] E. Langmann. Effective one-band models for the cuprates. Unpublished paper.

[10] P.-O. Löwdin. Studies in Perturbation Theory. IV. Solution of Eigenvalue Problem by Projection Operator Formalism. *Journal of Mathematical Physics*, 3:969–971, 1962.

[11] A. McMahan, J. F. Annett, and R. M. Martin. Cuprate parameters from numerical Wannier functions. *Physical Review B*, 42:6268–6282, 1990.

[12] R. Raimondi and J. Jefferson. Effective single-band models for the high-T_c cuprates. II. Role of apical oxygen. *Physical Review B*, 53:8774–8788, 1996.

[13] Z.-A. Ren, G.-C. Che, X.-L. Dong, J. Yang, W. Lu, W. Yi, X.-L. Shen, Z.-C. Li, L.-L. Sun, F. Zhou, and Z.-X. Zhao. Superconductivity and phase diagram in iron-based arsenic-oxides $ReFeAsO_{1-\delta}$ (Re = rare-earth metal) without fluorine doping. *EPL Journal*, 83(17002):1–4, July 2008.

[14] F. C. Zhang and T. M. Rice. Effective Hamiltonian for the superconducting Cu oxides. *Physical Review B*, 37:3759–3761, 1987.

Appendix A

Notation and terminology

In this appendix we fix the notation used throughout the thesis.

When a numerical value appears (predominantly, it will be an energy expressed in eV), regardless of the number of digits given, we use a parenthesis to highlight the last significant digit. For example, we would write 3.37(3) for a numerical value in the range $3.3725 < 3.37(3) < 3.3735$.

We use the letter a for creation and annihilation operators, such that a_i annihilates, and $a_i^\dagger$ creates, a fermion in state i. We will often refer to states as sites on a lattice, and we then define the spin of the electron too, since on each site there can be one fermion with spin $\uparrow$ and one with spin $\downarrow$. In these cases, the operator that annihilates (creates) a fermion with spin σ on site i is denoted $a_{i,\sigma}^{(\dagger)}$, $\sigma \in \{\uparrow, \downarrow\}$.

We predominantly use the word *fermion*, which may refer to either an electron or a hole. If the relevant interpretation is electron or hole depends on whether the system in question is doped with holes or electrons[1].

For the particle number operator (or just number operator), we will use both the notation $\hat{N}$ (when we talk about the number operator alone) and $\hat{n}$ (when the number operator is part of a Hamiltonian operator). Without index, $\hat{n}$ (or $\hat{N}$) refers to the number operator on the global system in question (any ambiguities will be explained in the text), while $\hat{n}_{i,\sigma} = a_{i,\sigma}^\dagger a_{i,\sigma}$ refers to the number operator on site i and spin σ. We will also use the shortened notation $\hat{n}_i = \hat{n}_{i,\uparrow} + \hat{n}_{i,\downarrow}$ such that $\hat{n} = \sum_{i=1}^{L} \hat{n}_i$ for a lattice with L sites. Regardless of whether $\hat{N}$ or $\hat{n}$ is used, we use n to represent the particle number *eigenvalues*.

We define the spin operator $\hat{S}_i^z = \frac{1}{2} n_{i,\uparrow} - \frac{1}{2} n_{i,\downarrow}$ on site i, and the global spin operator $\hat{S}^z = \sum_{i=1}^{L} \hat{S}_i^z$. The eigenvalues of $\hat{S}^z$ and $\hat{S}_i^z$ will be denoted s^z and s_i^z, respectively.

We will use σ to denote the spin of a fermion, $\sigma \in \{\uparrow, \downarrow\}$. The *opposite* spin is sometimes indicated with a minus sign: $-\uparrow = \downarrow$ and $-\downarrow = \uparrow$.

Ω always denotes the empty state, i.e. $\hat{N}\Omega = 0$. In some places, Ω will have an index that indicates

[1] As described in the introduction, the cuprates consist of CuO_2 sandwiched between layers of other materials that serve to dope the CuO_2 layers with electrons or holes

in what Hilbert space that specific (empty) state belongs. In these instances, the indices will be explained in the text.

We call a *pure state* a fermion state in a system of L sites (i.e. with $2L$ accessible single-particle states, including the spin degree of freedom) a state of the following type:

$$(a^\dagger_{1,\uparrow})^{n_{1,\uparrow}}(a^\dagger_{1,\downarrow})^{n_{1,\downarrow}}(a^\dagger_{2,\uparrow})^{n_{2,\uparrow}}\cdots(a^\dagger_{L,\uparrow})^{n_{L,\uparrow}}(a^\dagger_{L,\downarrow})^{n_{L,\downarrow}}\Omega; \quad n_{i,\sigma}\in\{0,1\}\,\forall\, i,\sigma \tag{A.1}$$

The pure states in (A.1) are eigenstates to $\hat{N}$, with corresponding eigenvalue $n=\sum_{i=1}^{L} n_i$, and to $\hat{S}^z$, with eigenvalue $s^z=\frac{1}{2}\sum_i n_{i,\uparrow}-n_{i,\downarrow}$.

The *commutator* between any two operators A and B is $[A,B]=AB-BA$ and the *anticommutator* between A and B is $\{A,B\}=AB+BA$.

For the three-band Hubbard model, we use the following identifications, to clearly distinguish between annihilation (and creation) operators for Cu sites and for O sites

$$\begin{cases} d^{(\dagger)}_{i,\sigma}=a^{(\dagger)}_{i,\sigma} & \text{site } i \text{ a Cu site, annihilating (creating) an electron in the d orbit} \\ p^{(\dagger)}_{l,\sigma}=a^{(\dagger)}_{l,\sigma} & \text{site } l \text{ an O site, annihilating (creating) an electron in the p orbit,} \\ n^d_{i,\sigma}=d^\dagger_{i,\sigma}d_{i,\sigma}; \quad n^p_{l,\sigma}=p^\dagger_{i,\sigma}p_{i,\sigma} & \end{cases}$$

Apart from annihilation and creation operators, the general convention is to indicate operators with hats above them, and their matrix representations without hats. For example: A is the matrix representation (in some basis) of the operator $\hat{A}$. However H is the three-band Hamiltonian operator and $\tilde{H}$ is the Hamiltonian operator in the extended one-band Hubbard model. We make this choice, to avoid having a hat and a tilde over the same symbol.

We use brackets $[\cdots]$ for citation of references (listed in the end of the thesis). Parenthesizes $(\cdots)$ are used to refer to equations, and when referring to sections or chapters, only the number is used.

Appendix B

Mathematical details

B.1 Solution of three-band model on one cluster

In this appendix, we carry out the solution of the three-band Hubbard problem on one cluster. We give details of the analytical solution in the subspaces whose states have particle number $n = 0, n = 1$ and $n = 2$. We confirm these results by finding the same solutions numerically using Matlab. With Matlab, we also find the remaining energy eigenvalues, whose eigenstates have particle number $n = 3, 4, 5, 6$, and we present a complete list of the energies in each sector. In particular, we note that the energies associated with these higher-particle number states are considerably higher than those of the low-particle states. We use this to argue the validity of the approximation that only the four lowest-energy states will be occupied.

In the three-sites clusters there are six different states that may or may not be occupied by a fermion, taking into account spin. In matrix representation, finding the fermion energies and corresponding eigenstates in cluster i thereby amounts to finding the eigenvalues and eigenstates of a 64×64 matrix, whose elements are found by $H_{kl} = \langle P_k|H_i|P_l\rangle$, where $|P_k\rangle$ and $|P_l\rangle$ are any states in a basis that needs to be defined, and $k, l \in \{1, 2, ..., 64\}$. Furthermore, the Hamiltonian H_i in (4.2) commutes with the number operator $\hat{N}$ and the spin operator $\hat{S}^z$, and as long as we don't mix states with different particle number n or s^z in the same basis state, this allows us to construct a matrix with block-diagonal form (see Section 2.2.2 for more details), and thus solve each of these block individually.

We say that the system is in a pure state if it is in one of the following states:
$(d^\dagger_{0,\uparrow})^{n_{0,\uparrow}}(d^\dagger_{0,\downarrow})^{n_{0,\downarrow}}(p^\dagger_{+,\uparrow})^{n_{+,\uparrow}}(p^\dagger_{+,\downarrow})^{n_{+,\downarrow}}(p^\dagger_{-,\uparrow})^{n_{-,\uparrow}}(p^\dagger_{-,\downarrow})^{n_{-,\downarrow}}\Omega$, with $n_{i,\sigma} \in \{0, 1\}$. Note that we omit the index i, common to all creation operators on cluster i.

B.1.1 $\{n = 0\}$

The $n = 0$ sector is trivial, containing only one state: the empty state Ω. It is an eigenstate to H_i, with eigenvalue 0. We hence have one energy eigenvalue $E_0 = 0$, with the corresponding state $A^\dagger_{i,0}\Omega = \Omega$, where $A^\dagger_{i,0} = I$.

B.1.2 $\{n = 1\}$

There are three pure states in the $\{n = 1, s^z = \frac{1}{2}\}$ sector:

$$d^\dagger_{0,\uparrow}\Omega, p^\dagger_{+,\uparrow}\Omega, p^\dagger_{-,\uparrow}\Omega,$$

and three in the $\{n = 1, s^z = -\frac{1}{2}\}$ sector:

$$d^\dagger_{0,\downarrow}\Omega, p^\dagger_{+,\downarrow}\Omega, p^\dagger_{-,\downarrow}\Omega$$

We solve sector $\{n = 1, s^z = \frac{1}{2}\}$, and thereafter note that the solution corresponds exactly to the one of $\{n = 1, s^z = -\frac{1}{2}\}$, interchanging only $\uparrow \rightarrow \downarrow$.

Instead of naively using the set of three pure states as our basis, we can construct a better basis, which will divide the 3×3 block into two smaller sub-blocks. We first note that

$$\begin{aligned} H_i d^\dagger_{0,\uparrow}\Omega &= \epsilon_d H d^\dagger_{0,\uparrow}\Omega + t_{pd}(p^\dagger_{+,\uparrow}\Omega - p^\dagger_{-,\uparrow}\Omega) \\ H_i \frac{1}{\sqrt{2}}(p^\dagger_{+,\uparrow}\Omega - p^\dagger_{-,\uparrow}\Omega) &= \frac{1}{\sqrt{2}}\epsilon_p(p^\dagger_{+,\uparrow}\Omega - p^\dagger_{-,\uparrow}\Omega) + \sqrt{2}d^\dagger_{0,\uparrow}\Omega \end{aligned}$$

Choosing the two normalized states $d^\dagger_{0,\uparrow}\Omega$ and $\frac{1}{\sqrt{2}}(p^\dagger_{+,\uparrow}\Omega - p^\dagger_{-,\uparrow}\Omega)$ in our basis will give a block-diagonal matrix: when acted upon with H_i, they only return each other, and the interaction with the rest of the matrix will be zero. Finally, we choose the third normalized basis state to be $\frac{1}{\sqrt{2}}(p^\dagger_{+,\uparrow}\Omega + p^\dagger_{-,\uparrow}\Omega)$, and we show that these states are orthogonal:

$$\begin{aligned} \langle \frac{1}{\sqrt{2}}(p^\dagger_{+,\uparrow}\Omega + p^\dagger_{-,\uparrow}\Omega) | \frac{1}{\sqrt{2}}(p^\dagger_{+,\uparrow}\Omega - p^\dagger_{-,\uparrow}\Omega)\rangle = \\ \frac{1}{2}\left(\langle p^\dagger_{+,\uparrow}\Omega | p^\dagger_{+,\uparrow}\Omega\rangle - \langle p^\dagger_{+,\uparrow}\Omega | p^\dagger_{-,\uparrow}\Omega\rangle + \langle p^\dagger_{-,\uparrow}\Omega | \langle p^\dagger_{+,\uparrow}\rangle - \langle p^\dagger_{-,\uparrow}\Omega | p^\dagger_{-,\uparrow}\Omega\rangle\right) = \\ \frac{1}{2}(1 + 0 + 0 - 1) = 0 \\ \langle d^\dagger_{0,\uparrow}\Omega | \frac{1}{\sqrt{2}}\left(p^\dagger_{+,\uparrow}\Omega + p^\dagger_{-,\uparrow}\Omega\right)\rangle = \\ \frac{1}{\sqrt{2}}\left(\langle d^\dagger_{0,\uparrow}\Omega | p^\dagger_{+,\uparrow}\Omega\rangle + \langle d^\dagger_{0,\uparrow}\Omega | p^\dagger_{-,\uparrow}\Omega\rangle\right) = \frac{1}{\sqrt{2}}(0 + 0) = 0 \\ \langle d^\dagger_{0,\uparrow}\Omega | \frac{1}{\sqrt{2}}\left(p^\dagger_{+,\uparrow}\Omega - p^\dagger_{-,\uparrow}\Omega\right)\rangle = \\ \frac{1}{\sqrt{2}}\left(\langle d^\dagger_{0,\uparrow}\Omega | p^\dagger_{+,\uparrow}\Omega\rangle - \langle d^\dagger_{0,\uparrow}\Omega | p^\dagger_{-,\uparrow}\Omega\rangle\right) = \frac{1}{\sqrt{2}}(0 - 0) = 0 \end{aligned}$$

The following thus constitutes a complete orthonormal basis in the $\{n = 1, s^z = \frac{1}{2}\}$ sector:

$$\{\psi_1 = d^\dagger_{0,\uparrow}\Omega;\ \psi_2 = \frac{1}{\sqrt{2}}\left(p^\dagger_{+,\uparrow}\Omega - p^\dagger_{-,\uparrow}\Omega\right);\ \psi_3 = \frac{1}{\sqrt{2}}\left(p^\dagger_{+,\uparrow}\Omega + p^\dagger_{-,\uparrow}\Omega\right)\} \tag{B.1}$$

We construct the elements $H_{kl}^{\{n=1,s^z=\frac{1}{2}\}} = \langle\psi_k|H_i\psi_l\rangle$ of the 3×3 Hamiltonian matrix, and get:

$$H^{\{n=1,s^z=\frac{1}{2}\}} = \begin{pmatrix} \epsilon_d & \sqrt{2}t_{pd} & 0 \\ \sqrt{2}t_{pd} & \epsilon_p & 0 \\ 0 & 0 & \epsilon_p \end{pmatrix},$$

ad find that ψ_3 is an eigenstate to H_i, with eigenvalue ϵ_p. To find the eigenvalues and eigenstates corresponding to the block $\{H^{\{n=1,s^z=\frac{1}{2}\}}\}_{1\le k,l\le 2}$, we solve the corresponding characteristic equation:

$$\begin{aligned} det\left((H^{\{n=1,s^z=\frac{1}{2}\}})_{1\le i,j\le 2} - E\times I\right) &= 0 \\ (\epsilon_d - E)(\epsilon_p - E) - 2t_{pd}^2 &= 0 \\ E^2 - E\left(\epsilon_d + \epsilon_p\right) + \epsilon_p\epsilon_d - 2t_{pd}^2 &= 0 \\ E_{1,2} = \frac{\epsilon_d + \epsilon_p}{2} &\pm \sqrt{\frac{(\epsilon_d+\epsilon_p)^2}{4} - \epsilon_d\epsilon_p + 2t_{pd}^2} \end{aligned}$$

We thus have the following energy eigenvalues in the $\{n=1, s^z=\frac{1}{2}\}$ sector:

$$\begin{aligned} E_1 &= \frac{\epsilon_d+\epsilon_p}{2} - \sqrt{\frac{(\epsilon_d+\epsilon_p)^2}{4} - \epsilon_d\epsilon_p + 2t_{pd}^2} \\ E_2 &= \frac{\epsilon_d+\epsilon_p}{2} + \sqrt{\frac{(\epsilon_d+\epsilon_p)^2}{4} - \epsilon_d\epsilon_p + 2t_{pd}^2} \\ E_3 &= \epsilon_p \end{aligned}$$

The eigenstates in the $\{H^{\{n=1,s^z=\frac{1}{2}\}}\}_{1\le k,l\le 2}$ sector are found by solving the equation:

$$\begin{pmatrix} \epsilon_d & \sqrt{2}t_{pd} \\ \sqrt{2}t_{pd} & \epsilon_p \end{pmatrix}\begin{pmatrix} C_{i,1} \\ C_{i,2} \end{pmatrix} = E_i\begin{pmatrix} C_{i,1} \\ C_{i,2} \end{pmatrix};\quad i\in\{1,2\},$$

where $C_{i,1}$ and $C_{i,2}$ are the coefficients of ψ_1 and ψ_2 respectively, in eigenstate i:
$\Psi_i = C_{i,1}\psi_1 + C_{i,2}\psi_2$. We find the following:

$$\Psi_i = C_{i,1}\left(\psi_1 + \frac{E_i - \epsilon_d}{\sqrt{2}t_{pd}}\psi_2\right)$$

We insert the assumed values of our parameters [1, p. 5] and choose the values of $C_{1,1}$ and $C_{2,1}$ such that Ψ_1 and Ψ_2 are normalized. The complete solution for the sector $\{n=1, s^z=\frac{1}{2}\}$ is:

Energy	Eigenstate
$-0.56(2)$	$-0.92(9)d^\dagger_{0,\uparrow}\Omega + 0,26(1)\left(p^\dagger_{+,\uparrow}\Omega - p^\dagger_{-,\uparrow}\Omega\right)$
$3.00(0)$	$\frac{1}{\sqrt{2}}\left(p^\dagger_{+,\uparrow}\Omega + p^\dagger_{-,\uparrow}\Omega\right)$
$3.56(2)$	$0.36(9)d^\dagger_{0,\uparrow}\Omega + 0.65(7)\left(p^\dagger_{+,\uparrow}\Omega - p^\dagger_{-,\uparrow}\Omega\right)$

Since the Hamiltonian H_i is unchanged under the interchange of $\uparrow\leftrightarrow\downarrow$ we can, choosing a basis corresponding to (B.1), just changing $\uparrow\rightarrow\downarrow$, carry out the same procedure, and find the solution of the $\{n = 1, s^z = -\frac{1}{2}\}$ sector:

Energy	Eigenstate
$-0.56(2)$	$-0.92(9)d^\dagger_{0,\downarrow}\Omega + 0,26(1)\left(p^\dagger_{+,\downarrow}\Omega - p^\dagger_{-,\downarrow}\Omega\right)$
$3.00(0)$	$\frac{1}{\sqrt{2}}\left(p^\dagger_{+,\downarrow}\Omega + p^\dagger_{-,\downarrow}\Omega\right)$
$3.56(2)$	$0.36(9)d^\dagger_{0,\downarrow}\Omega + 0.65(7)\left(p^\dagger_{+,\downarrow}\Omega - p^\dagger_{-,\downarrow}\Omega\right)$

B.1.3 $\{n = 2, s^z = 0\}$

Using the short-hand notation $|kl\rangle \equiv a^\dagger_{i,k,\uparrow}a^\dagger_{i,l,\downarrow}\Omega$[1], $k, l \in \{0, +, -\}$, the pure states in the system of cluster i are:

$|00\rangle$, $|0+\rangle$, $|0-\rangle$, $|+0\rangle$, $|++\rangle$, $|+-\rangle$, $|-0\rangle$, $|-+\rangle$, $|--\rangle$

As in the $\{n = 1\}$ sectors, we want to find a better basis than the pure states, in order to make the 9×9 matrix block-diagonal, and solve each block individually.

To find a better basis, we act with H_i on each of the pure states:

$H\|00\rangle$	$(-\epsilon_d + U_{dd})\|00\rangle$	$+t_{pd}(\|0+\rangle - \|0-\rangle + \|+0\rangle - \|-0\rangle)$
$H\|0+\rangle$	$(\epsilon_p + \epsilon_d + U_{pd})\|0+\rangle$	$+t_{pd}(\|00\rangle + \|++\rangle - \|-+\rangle$
$H\|0-\rangle$	$(\epsilon_p + \epsilon_d + U_{pd})\|0-\rangle$	$+t_{pd}(-\|00\rangle - \|--\rangle + \|+-\rangle$
$H\|+0\rangle$	$(\epsilon_p + \epsilon_d + U_{pd})\|+0\rangle$	$+t_{pd}(\|00\rangle + \|++\rangle - \|+-\rangle$
$H\|-0\rangle$	$(\epsilon_p + \epsilon_d + U_{pd})\|-0\rangle$	$+t_{pd}(-\|00\rangle - \|--\rangle + \|-+\rangle$
$H\|+-\rangle$	$-\epsilon_p\|+-\rangle$	$+t_{pd}(\|0-\rangle - \|+0\rangle$
$H\|-+\rangle$	$-\epsilon_p\|-+\rangle$	$+t_{pd}(-\|0+\rangle + \|-0\rangle$
$H\|++\rangle$	$(-\epsilon_p + U_{pp})\|++\rangle$	$+t_{pd}(\|0+\rangle + \|+0\rangle$
$H\|--\rangle$	$(-\epsilon_p + U_{pp})\|--\rangle$	$+t_{pd}(-\|0-\rangle - \|-0\rangle$

(B.2)

Guided by the results in (B.2), we choose the following basis states, labeled e_i; $i \in \{1, 2, \cdots 9\}$. This choice gives a block-diagonal matrix with four blocks. Further down, we discuss this division into blocks further, and show that it reflects the symmetries of the one-cluster Hamiltonian H_i.

[1] We use $d_{i,0,\sigma} = a_{i,0,\sigma}$ and $p_{i,\pm,\sigma} = a_{i,\pm,\sigma}$

$$
\begin{aligned}
e_1 &= \tfrac{1}{\sqrt{4}}[(|0+\rangle - |0-\rangle) - (|+0\rangle - |-0\rangle)] \\
e_2 &= |00\rangle \\
e_3 &= \tfrac{1}{\sqrt{4}}[(|0+\rangle - |0-\rangle) + (|+0\rangle - |-0\rangle)] \\
e_4 &= \tfrac{1}{\sqrt{2}}(|++\rangle + |--\rangle) \\
e_5 &= \tfrac{1}{\sqrt{2}}(|+-\rangle + |-+\rangle) \\
e_6 &= \tfrac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle) \\
e_7 &= \tfrac{1}{\sqrt{4}}[(|0+\rangle + |0-\rangle) - (|+0\rangle + |-0\rangle)] \\
e_8 &= \tfrac{1}{\sqrt{2}}(|++\rangle - |--\rangle) \\
e_9 &= \tfrac{1}{\sqrt{4}}[(|0+\rangle + |0-\rangle) + (|+0\rangle + |-0\rangle)]
\end{aligned}
\tag{B.3}
$$

The nine states e_i are normalized and mutually orthogonal, and thus span the nine-dimensional subspace that represents the $\{n = 2, s^z = 0\}$ sector of the fermion system.

The Hamiltonian matrix in the $\{n = 2, s^z = 0\}$ sector, expressed in the basis $\{e_i\}$, is:

$$
\begin{aligned}
H^{\{n=2,s^z=0\}} =& A \oplus B \oplus C \oplus D, \text{ where} \\
A =& \left(\epsilon_p + \epsilon_d + U_{pd}\right) \\
B =& \begin{pmatrix} 2\epsilon_d + U_{dd} & 2t_{pd} & 0 & 0 \\ 2t_{pd} & \epsilon_p + \epsilon_d + U_{pd} & \sqrt{2}t_{pd} & -\sqrt{2}t_{pd} \\ 0 & \sqrt{2}t_{pd} & 2\epsilon_p + U_{pp} & 0 \\ 0 & -\sqrt{2}t_{pd} & 0 & 2\epsilon_p \end{pmatrix} \\
C =& \begin{pmatrix} 2\epsilon_p & \sqrt{2}t_{pd} \\ \sqrt{2}t_{pd} & \epsilon_p + \epsilon_d + U_{pd} \end{pmatrix} \\
D =& \begin{pmatrix} 2\epsilon_p + U_{pp} & \sqrt{2}t_{pd} \\ \sqrt{2}t_{pd} & \epsilon_p + \epsilon_d + U_{pd} \end{pmatrix}
\end{aligned}
$$

In block A, we readily have one eigenstate and energy:

$$
E_1 = \epsilon_p + \epsilon_d + U_{pd};\ \frac{1}{2}\left((|0+\rangle - |0-\rangle) - (|+0\rangle - |-0\rangle)\right) \tag{B.4}
$$

In block B, the characteristic equation that we need to solve is a fourth-degree polynomial equation, which we solve numerically using Matlab. We present the results together with the solutions of the other blocks further down.

In block C, the characteristic equation gives the energies:

$$
\begin{aligned}
&(2\epsilon_p - E)(\epsilon_p + \epsilon_d + U_{pd} - E) - 2t_{pd}^2 = 0, \text{ with solutions} \\
&E_{6,7} = \frac{3\epsilon_p + \epsilon_d + U_{pd}}{2} \pm \sqrt{\frac{(3\epsilon_p + \epsilon_d + U_{pd})^2}{4} - 2\epsilon_p(\epsilon_p + \epsilon_d + U_{pd}) + 2t_{pd}^2}
\end{aligned}
$$

The characteristic equation for the block D matrix is:

$$(2\epsilon_p + U_{pp} - E)(\epsilon_p + \epsilon_d + U_{pd} - E) - 2t_{pd}^2 = 0, \text{ with solutions}$$
$$E_{8,9} = \frac{3\epsilon_p + \epsilon_d + U_{pp} + U_{pd}}{2} \pm \sqrt{\frac{(3\epsilon_p + \epsilon_d + U_{pp} + U_{pd})^2}{4} - (2\epsilon_p + U_{pp})(\epsilon_p + \epsilon_d + U_{pd}) + 2t_{pd}^2}$$

The above equations give the energy eigenvalues, and from there we find the corresponding eigenstates by solving the equations $C\Psi_i = E_i\Psi_i$ and $D\Psi_j = E_j\Psi_j$, $i \in \{6,7\}, j \in \{8,9\}$.

The above solution gives the following complete set of energies and eigenstates to the $\{n = 2, s^z = 0\}$ sector. We still use the notation convention that $|kl\rangle \equiv a^\dagger_{i,k,\uparrow}a^\dagger_{i,l,\downarrow}\Omega$, and the below table gives that coefficient that multiply each of these pure states in the linear combination that constitutes respective eigenstate. The far right column tells us to which of the blocks in $H^{\{n=2,s^z=0\}}$ that each eigenstate comes from:

Energy	Eigenstate coefficients of the pure states									Block
	$\|00\rangle$	$\|0+\rangle$	$\|0-\rangle$	$\|+0\rangle$	$\|++\rangle$	$\|+-\rangle$	$\|-0\rangle$	$\|-+\rangle$	$\|--\rangle$	
2.03(7)	0.29(6)	-0.44(2)	0.44(2)	-0.44(2)	0.12(7)	-0.22(3)	0.44(2)	-0.22(3)	0.12(7)	B
2.86(3)	0	-0.45(6)	-0.45(6)	0.45(6)	0	0.29(1)	0.45(6)	-0.29(1)	0	C
3.15(8)	0	-0.48(6)	-0.48(6)	-0.48(6)	0.16(6)	0	-0.48(6)	0	-0.16(6)	D
3.5	0	0.5	-0.5	-0.5	0	0	0.5	0	0	A
6.33(4)	0.26(4)	-0.11(0)	0.11(0)	-0.11(0)	0.08(3)	0.65(9)	0.11(0)	0.65(9)	0.08(3)	B
6.63(7)	0	-0.20(5)	-0.20(5)	0.20(5)	0	-0.64(5)	0.20(5)	0.64(5)	0	C
8.49(2)	-0.80(3)	-0.09(9)	0.09(9)	-0.09(9)	0.38(9)	0.07(9)	0.09(9)	0.07(9)	0.38(9)	B
9.34(2)	0	-0.11(8)	-0.11(8)	-0.11(8)	-0.68(7)	0	-0.11(8)	0	0.68(7)	D
9.63(6)	-0.44(4)	-0.18(2)	0.18(2)	-0.18(2)	-0.57(1)	0.10(0)	0.18(2)	0.10(0)	-0.57(1)	B

It is interesting to note that the division into sub-blocks A, B, C and D reflects two symmetries of the Hamiltonian H_i on one cluster: It is possible to define two operators that commute with H_i, to which the states in (B.3) are eigenstates, and where each block is associated with a unique combination of eigenvalues. These operators are the $+ \longleftrightarrow -$ "site swap" operator $\hat{T}$ and the "spin flip" operator $\hat{F}$, both defined below:

$$\begin{aligned}
\hat{T}\hat{T}^\dagger &= \hat{T}^\dagger\hat{T} = I \\
\hat{T}p_{+,\sigma}\hat{T}^\dagger &= (-1)p_{-,\sigma} \\
\hat{T}p_{-,\sigma}\hat{T}^\dagger &= (-1)p_{+,\sigma} \\
\hat{T}d_{0,\sigma}\hat{T}^\dagger &= d_{0,\sigma} \\
\hat{T}\Omega &= \Omega
\end{aligned}$$

$$\begin{aligned}
\hat{F}\hat{F}^\dagger &= \hat{F}^\dagger\hat{F} = I \\
\hat{F}a_{k,\sigma}\hat{F}^\dagger &= a_{k,-\sigma} \\
\hat{F}\Omega &= \Omega
\end{aligned}$$

, where $-\uparrow = \downarrow$, $-\downarrow = \uparrow$, $k \in \{0,+,-\}$, $a_{\pm,\sigma} = p_{\pm,\sigma}$ and $a_{0,\sigma} = d_{0,\sigma}$ The basis states in (B.3) are eigenstates of $\hat{T}$ and $\hat{F}$, and they can be classified according the their eigenvalues associated with

these two operators: Block A: $t = 1, f = 1$; block B: $t = 1, f = -1$; block C: $t_{12} = -1, f = 1$ and block D: $t_{12} = -1, f = -1$.

I checked that $\hat{T}$ and $\hat{F}$ commute with the one cluster Hamiltonian.

B.1.4 $\{n = 2, s^z = +1/-1\}$

We will carry out the solution for the $\{n = 2, s^z = +1\}$ sector, and thereafter the solution of the $\{n = 2, s^z = -1\}$ sector.

We denote the three pure states in the $\{n = 2, s^z = +1\}$ sector as follows:

$$\begin{aligned} a^\dagger_{0,\uparrow} a^\dagger_{+,\uparrow} \Omega &\equiv |0+\rangle \\ a^\dagger_{0,\uparrow} a^\dagger_{-,\uparrow} \Omega &\equiv |0-\rangle \\ a^\dagger_{+,\uparrow} a^\dagger_{-,\uparrow} \Omega &\equiv |+-\rangle \end{aligned}$$

In analogy with the process carried out in the $\{n = 1, s^z = \frac{1}{2}\}$ and $\{n = 2, s^z = 0\}$ sectors, we act with H_i on each of the pure states to help us make a good choice of basis, that makes the matrix block-diagonal. We find:

$$\begin{aligned} H_i|0+\rangle &= (\epsilon_d + \epsilon_p + U_{pd})|0+\rangle + t_{pd}|+-\rangle \\ H_i|0-\rangle &= (\epsilon_d + \epsilon_p + U_{pd})|0-\rangle + t_{pd}|+-\rangle \\ H_i|+-\rangle &= 2\epsilon_p|+-\rangle + t_{pd}\left(|0+\rangle + |0-\rangle\right), \end{aligned}$$

such that the following choice of basis

$$\begin{aligned} e_1 &= \frac{1}{\sqrt{2}}\left(|0+\rangle - |0-\rangle\right) \\ e_2 &= \frac{1}{\sqrt{2}}\left(|0+\rangle + |0-\rangle\right) \\ e_3 &= |+-\rangle, \end{aligned}$$

will make the the matrix block-diagonal, each elements found by $H_{kl} = \langle e_k | H_i | e_l \rangle$:

$$H^{\{n=2,s^z=\frac{1}{2}\}} = \begin{pmatrix} \epsilon_d + \epsilon_p + U_{pd} & 0 & 0 \\ 0 & \epsilon_d + \epsilon_p + U_{pd} & \sqrt{2}t_{pd} \\ 0 & \sqrt{2}t_{pd} & 2\epsilon_p \end{pmatrix}$$

We conclude that e_1 is an eigenstate to $H^{\{n=2,s^z=\frac{1}{2}\}}$ with energy eigenvalue $\epsilon_d + \epsilon_p + U_{pd}$. To find the two other energies, we solve the characteristic equation:

$$
\begin{aligned}
det\begin{pmatrix}\epsilon_d+\epsilon_p+U_{pd}-E & \sqrt{2}t_{pd}\\ \sqrt{2}t_{pd} & 2\epsilon_p-E\end{pmatrix} &= 0\\
(\epsilon_d+\epsilon_p+U_{pd}-E)(2\epsilon_p-E)-2t_{pd}^2 &= 0\\
E_{2,3}=\frac{\epsilon_d+\epsilon_p+U_{pd}}{2}\pm\sqrt{\frac{(\epsilon_d+\epsilon_p+U_{pd})^2}{4}-2\epsilon_p(\epsilon_d+\epsilon_p+U_{pd})+2t_{pd}^2} &\qquad \text{(B.5)}
\end{aligned}
$$

The eigenstates in this subsector are linear combinations of e_2 and e_3, where the coefficients $C_{k,2}$ and $C_{k,3}$ before each of the basis states are determined by:

$$
\begin{pmatrix}\epsilon_d+\epsilon_p+U_{pd}-E & \sqrt{2}t_{pd}\\ \sqrt{2}t_{pd} & 2\epsilon_p-E\end{pmatrix}\begin{pmatrix}C_{k,2}\\ C_{k,3}\end{pmatrix}=E_i\begin{pmatrix}C_{k,2}\\ C_{k,3}\end{pmatrix};\quad k\in\{2,3\} \qquad \text{(B.6)}
$$

We solve (B.6), insert the parameter values into (B.5), and choose the eigenstates to be normalized. The complete solution to the $\{n=2, s^z=1\}$ sector is then:

Energy	State
2.86(2)	$-0.64(5)\left(d^\dagger_{0,\uparrow}p^\dagger_{+,\uparrow}\Omega+d^\dagger_{0,\uparrow}p^\dagger_{-,\uparrow}\Omega\right)+0.41(1)p^\dagger_{+,\uparrow}p^\dagger_{-,\uparrow}\Omega$
3.50(0)	$\frac{1}{\sqrt{2}}\left(d^\dagger_{0,\uparrow}p^\dagger_{+,\uparrow}\Omega-d^\dagger_{0,\uparrow}p^\dagger_{-,\uparrow}\Omega\right)$
6.63(7)	$0.29(1)\left(d^\dagger_{0,\uparrow}p^\dagger_{+,\uparrow}\Omega+d^\dagger_{0,\uparrow}p^\dagger_{-,\uparrow}\Omega\right)+0.91(2)p^\dagger_{+,\uparrow}p^\dagger_{-,\uparrow}\Omega$

Since H_i is unchanged upon changing the spin, we directly get the results for the $\{n=2, s^z=1\}$ sector:

Energy	State
2.86(2)	$-0.64(5)\left(d^\dagger_{0,\downarrow}p^\dagger_{+,\downarrow}\Omega+d^\dagger_{0,\downarrow}p^\dagger_{-,\downarrow}\Omega\right)+0.41(1)p^\dagger_{+,\downarrow}p^\dagger_{-,\downarrow}\Omega$
3.50(0)	$\frac{1}{\sqrt{2}}\left(d^\dagger_{0,\downarrow}p^\dagger_{+,\downarrow}\Omega-d^\dagger_{0,\downarrow}p^\dagger_{-,\downarrow}\Omega\right)$
6.63(7)	$0.29(1)\left(d^\dagger_{0,\downarrow}p^\dagger_{+,\downarrow}\Omega+d^\dagger_{0,\downarrow}p^\dagger_{-,\downarrow}\Omega\right)+0.91(2)p^\dagger_{+,\downarrow}p^\dagger_{-,\downarrow}\Omega$

B.1.5 Summary: Energies in one cluster

Having looked at details of the solution in the sectors where $n=0,1,2$, and having found the explicit expressions for the eigenstates in these sectors, we list all energy eigenvalues to the one-cluster problem, found with Matlab: [1]

[1] The Matlab code is found in Appendix C.2.1.

Quantum numbers	Energies
$n = 0$	0
$n = 1$,$s^z = \frac{1}{2}$	$-0.56(2), 3.00(0), 3.56(3)$
$n = 1$,$s^z = -\frac{1}{2}$	$-0.56(2), 3.00(0), 3.56(3)$
$n = 2$,$s^z = 0$	$2.03(7), 2.86(3), 3.15(8), 3.50(0), 6.33(4), 6.63(7), 8.49(2), 9.34(2), 9.63(6)$
$n = 2$,$s^z = 1$	$2.86(3), 3.50(0), 6.63(7)$
$n = 2$,$s^z = -1$	$2.86(3), 3.50(0), 6.63(7)$
$2 < n \leq 6$	5.92(5), 5.92(5), 6.62(8), 6.62(8), 7.00(0), 7.00(0), 7.00(0), 7.00(0), 9.26(8), 9.26(8), 9.57(9), 9.57(9), 12.00(0), 12.00(0), 12.03(7), 12.37(2), 12.37(2), 12.73(2), 12.73(2), 12.86(3), 12.86(3), 12.86(3), 13.15(8), 13.49(6), 13.49(6), 13.50(0), 13.50(0), 13.50(0), 16.33(4), 16.63(8), 16.63(8), 16.63(8), 18.49(2), 19.34(2), 19.43(8), 19.43(8), 19.63(7), 23.00(0), 23.00(0), 23.56(2), 23.56(2), 30.00(0)

We see that the four lowest-energy eigenstates are found in the sectors $\{n = 1, s^z = \frac{1}{2}\}$, $\{n = 1, s^z = -\frac{1}{2}\}$, $\{n = 0, s^z = 0\}$ and $\{n = 2, s^z = 0\}$, respectively. In Chapter 5, we will associate each of these three-band states on a cluster with a one-band model state on a site: We will argue that the three-band Hubbard model may be replaced with an extended one-band Hubbard model, where each cluster is regarded as a single lattice site, on which there can be one $\uparrow$ fermion and one $\downarrow$ fermion.

It is worth to note that we can consider ourselves lucky to find this feature in our list of energies. If we would have found, for example, that the four lowest states were all found in the $\{n = 1\}$ sector, the above explained matching between three-band and one-band states would not have been possible.

We sum up by listing the explicit expressions for the four lowest-energy eigenstates to H_i, the Hamiltonian on a cluster i. We name these states them $A^\dagger_{i,a_i}\Omega$; $a_i \in \{1, 2, 3, 4\}$, where the $A^\dagger_{i,a_i}$ are defined below. We will keep this notation convention when we make the matching to one-band states.

State	Energy
$A^\dagger_{i,1} = I$	0
$A^\dagger_{i,2} = -0.92(9)d^\dagger_{0,\uparrow} + 0.26(1)\left(p^\dagger_{+,\uparrow} - p^\dagger_{-,\uparrow}\right)$	$-0.56(2)$
$A^\dagger_{i,3} = -0.92(9)d^\dagger_{0,\downarrow} + 0.26(1)\left(p^\dagger_{+,\downarrow} - p^\dagger_{-,\downarrow}\right)$	$-0.56(2)$
$A^\dagger_{i,4} = 0.44(2)\left[d^\dagger_{0,\uparrow}\left(p^\dagger_{-,\downarrow} - p^\dagger_{+,\downarrow}\right) + \left(p^\dagger_{-,\downarrow} - p^\dagger_{+,\downarrow}\right)d^\dagger_{0,\downarrow}\right] +$ $+0.12(7)\left(p^\dagger_{+,\uparrow}p^\dagger_{+,\downarrow} + p^\dagger_{-,\uparrow}p^\dagger_{-,\downarrow}\right) -$ $-0.22(3)\left(p^\dagger_{+,\uparrow}p^\dagger_{-,\downarrow} + p^\dagger_{-,\uparrow}p^\dagger_{+,\downarrow}\right) + 0.29(6)d^\dagger_{0,\uparrow}d^\dagger_{0,\downarrow}$	$2.03(7)$

B.2 Proof of Proposition 5.2.1

Our strategy will be to consider a general model, which may represent both the three-band and the extended one-band Hubbard model. We will show that any matrix element in this general model can be written as one common sum of matrix elements on the form
$\langle \Omega A_{j,a'_j} A_{i,a'_i} | \frac{1}{T_i} H_i + \frac{1}{T_j} H_j + H_{ij} | A^\dagger_{i,a_i} A^\dagger_{j,a_j} \Omega \rangle$ (in the three-band model) or
$\langle \Omega \tilde{A}_{j,a'_j} \tilde{A}_{i,a'_i} | \frac{1}{T_i} \tilde{H}_i + \frac{1}{T_j} \tilde{H}_j + \tilde{H}_{ij} | \tilde{A}^\dagger_{i,a_i} A^\dagger_{j,a_j} \Omega \rangle$ (in the one-band model).

Having proved this, we conclude that to ensure that every matrix element $H_{n,m}$ in the three-band model is equal to its one-band correspondent $\tilde{H}_{\tilde{n},\tilde{m}}$, it is sufficient to match elements such as the ones above.

A general model

Consider L identical fermion systems, each with l sites where an $\uparrow$ spin and one $\downarrow$ spin fermion can reside, such that each system has $2l$ single-particle states that may or may not be occupied by a fermion. We agree upon an order in which we label the Hilbert spaces representing each of the L systems: $\{\mathcal{H}_1, \mathcal{H}_2, \cdots, \mathcal{H}_L\}$. We then construct the combined Hilbert space representing all fermion systems as the tensor product of the subspaces, respecting this agreed upon order:

$$\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \cdots \otimes \mathcal{H}_L \tag{B.7}$$

Each of the subspaces $\mathcal{H}_i$ is of dimension 2^{2l}. It follows from (B.7) that $\mathcal{H}$ is $(2^{2\times L\times l})$-dimensional.

Moreover, consider a complete orthonormal basis in each of the subspaces $\mathcal{H}_i$:

$$\{\omega^\dagger_{i,d_i}\Omega\}_{d_i\in\{1,2,3,\cdots,2^{2l}\}}, \tag{B.8}$$

We demand that $\omega^\dagger_{i,d_i}\Omega$ is a linear combination of pure states in $\mathcal{H}_i$, all of which have the same eigenvalue n_{d_i} of $\hat{N}_i$, such that: $\hat{N}_i\omega^\dagger_{d_i}\Omega = n_{d_i}\omega^\dagger_{d_i}\Omega$. We may now construct states $\mathbf{d}$, that form an orthonormal basis in $\mathcal{H}$:

$$\begin{aligned} |\mathbf{d}\rangle &= \omega^\dagger_{1,d_1}\omega^\dagger_{2,d_2}\cdots\omega^\dagger_{L,d_L}\Omega_L \\ \mathbf{d} &= (d_1, d_2, \cdots, d_L);\ d_i \in \{1, 2, \cdots 2^{2l}\} \end{aligned} \tag{B.9}$$

Before we prove that (B.9) is a complete orthonormal basis in $\mathcal{H}$, we introduce the notion of the *deg* operator, defined as follows:

$$deg(d_i) \equiv \begin{cases} 0, \text{ if } n_{d_i}, \text{ the particle number of } \omega^\dagger_{i,d_i}\Omega, \text{ is even} \\ 1, \text{ if } n_{d_i} \text{ is odd} \end{cases} \tag{B.10}$$

Furthermore, it follows from the orthonormality of the states $\{\omega^\dagger_{i,d_i}\Omega\}$, and from the fact that for $i \neq j$, $\omega^\dagger_{i,d_i}$ and $\omega^\dagger_{j,d_i}$ have no creation operators in common, that the following relations hold:

$$\begin{aligned}
\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j} =& (-1)^{deg(d_i)\cdot deg(d_j)}\omega^\dagger_{j,d_j}\omega^\dagger_{i,d_i}; \quad i \neq j \\
\omega_{i,d_i}\omega_{j,d_j} =& (-1)^{deg(d_i)\cdot deg(d_j)}\omega_{j,d_j}\omega_{i,d_i}; \quad i \neq j \\
\omega_{i,d_i}\omega^\dagger_{j,d_j} =& (-1)^{deg(d_i)\cdot deg(d_j)}\omega^\dagger_{j,d_j}\omega_{i,d_i}; \quad i \neq j \\
\omega_{i,d'_i}\omega^\dagger_{i,d_i} =& \delta_{d'_i,d_i} + (-1)^{deg(d'_i)deg(d_i))}\omega^\dagger_{i,d_i}\omega_{i,d'_i}
\end{aligned} \tag{B.11}$$

Using this, we now show that the states in (B.9) are normalized and mutually orthogonal:

$$\begin{aligned}
\langle \mathbf{d}'|\mathbf{d}\rangle =& \\
&= \langle \Omega\omega_{L,d'_L}\omega_{L-1,d'_{L-1}}\cdots\omega_{1,d'_1}|\omega^\dagger_{1,d_1}\omega^\dagger_{2,d_2}\cdots\omega^\dagger_{L,d_L}\Omega\rangle = \\
&= \langle \Omega\omega_{L,d'_L}\cdots\omega_{2,d'_2}|\left(\delta_{d'_1,d_1} + (-1)^{deg(d'_1)deg(d_1))}\omega^\dagger_{1,d_1}\omega_{1,d'_1}\right)\omega^\dagger_{2,d_2}\cdots\omega^\dagger_{L,d_L}\Omega_l\rangle = \\
&= \delta_{d'_1,d_1}\langle \Omega\omega_{L,d'_L}\cdots\omega_{2,d'_2}|\omega^\dagger_{2,d_2}\cdots\omega^\dagger_{L,d_L}\Omega_l\rangle + (-1)^{deg(d'_1)deg(d_1))}\langle\cdots|\cdots\underbrace{\omega_{1,d'_1}\Omega}_{=0}\rangle \\
&= \delta_{d'_1,d_1}\langle \Omega\omega_{L,d'_L}\cdots\omega_{3,d'_3}|\left(\delta_{d'_2,d_2} + (-1)^{deg(d'_2)deg(d_2))}\omega^\dagger_{2,d_2}\omega_{2,d'_2}\right)\omega^\dagger_{3,d_3}\cdots\omega^\dagger_{L,d_L}\Omega_l\rangle = \\
&\;\;\vdots \\
&= \prod_{i=1}^{L}\delta_{d'_i,d_i}\langle\Omega|\Omega\rangle = \prod_{i=1}^{L}\delta_{d'_i,d_i} = \delta_{\mathbf{d}',\mathbf{d}}
\end{aligned}$$

The states $\mathbf{d}$ are thus normalized and mutually orthogonal. Noting that there are $(2^{2l})^L = 2^{2\times L\times l}$ different such states, the same as the dimension of $\mathcal{H}$, we conclude that they constitute a complete orthonormal basis in $\mathcal{H}$.

Now, consider an operator $\hat{O}$ on $\mathcal{H}$, with the following properties:

$$\hat{O} = \sum_{i=1}^{L} \hat{O}_i + \sum_{\langle i,j \rangle} \hat{O}_{ij} + \sum_{\langle i,j \rangle} \hat{O}'_{ij}, \tag{B.12}$$

where $\langle i,j \rangle$ runs over an arbitrary number of pairs of subspaces $\mathcal{H}_i$ and $\mathcal{H}_j$, and

$\hat{O}_i$ is such that $\omega^\dagger_{i,d_i}\Omega$ is an eigenstate to $\hat{O}_i \,\forall\, d_i$, and $[\hat{O}_i, \omega_{j,d_j}] = [\hat{O}_i, \omega^\dagger_{j,d_j}] = 0 \,\forall\, i \neq j$,

$$\hat{O}_{ij} = \sum_{s=1}^{l}\sum_{s'=1}^{l}\sum_{\mathbf{m}_V} V_{(s,s'\mathbf{m}_V)} (\hat{n}_{i,s,\uparrow})^{m_{i,\uparrow}} (\hat{n}_{i,s,\downarrow})^{m_{i,\downarrow}} (\hat{n}_{j,s',\uparrow})^{m_{j,\uparrow}} (\hat{n}_{j,s',\downarrow})^{m_{j,\downarrow}},$$

where $\mathbf{m}_V$ takes on all values $\mathbf{m}_V = (m_{i,\uparrow}, m_{i\downarrow}, m_{j,\uparrow}, m_{j,\downarrow})$; $\quad m_{i,\sigma} \in \{0,1\}$,

$$\hat{O}'_{ij} = \sum_{s=1}^{l}\sum_{s'=1}^{l}\sum_{\sigma=\uparrow,\downarrow} \left(a^\dagger_{i,s,\sigma} a_{j,s',\sigma} + a^\dagger_{j,s',\sigma} a_{i,s,\sigma}\right) \left[\sum_{\mathbf{m}_T} T_{(s,s',\mathbf{m}_T)} (\hat{n}_{i,s,-\sigma})^{m_{i,-\sigma}} (\hat{n}_{j,s',-\sigma})^{m_{j,-\sigma}}\right],$$

where $\mathbf{m}_T$ takes on all values $\mathbf{m}_T = (m_{i,-\sigma}, m_{i,-\sigma})$; $\quad m_{j,-\sigma} \in \{0,1\}$,

and $V_{(s,s'\mathbf{m}_V)}$ and $T_{(s,s',\mathbf{m}_T)}$ are complex numbers. It follows from the anti-commutator relations for creation and annihilation operators that

$$\begin{aligned} [\omega^\dagger_{k,d_k}, \hat{n}_{i,s,\sigma}] = 0 \quad \forall\, k \neq i; \quad \forall\, d_k, s, \sigma, \text{ and} \\ [\omega^\dagger_{k,d_k}, a^\dagger_{i,s,\sigma} a_{i,s,\sigma}] = 0 \quad \forall\, k \neq i, j; \quad \forall\, d_k, s, s'\sigma \end{aligned} \tag{B.13}$$

We now consider any element of O, the matrix representation of $\hat{O}$ in the basis $|\mathbf{d}\rangle$:

$$\begin{aligned} O_{\mathbf{d}',\mathbf{d}} = \langle \mathbf{d}'|\hat{O}|\mathbf{d}\rangle &= \sum_{i=1}^{L} \langle \mathbf{d}'|\hat{O}_i|\mathbf{d}\rangle + \sum_{\langle i,j \rangle} \langle \mathbf{d}'|\hat{O}_{ij}|\mathbf{d}\rangle + \sum_{\langle i,j \rangle} \langle \mathbf{d}'|\hat{O}'_{ij}|\mathbf{d}\rangle = \\ &= \sum_{\langle i,j \rangle} \left(\frac{1}{T_i} \langle \mathbf{d}'|\hat{O}_i|\mathbf{d}\rangle + \frac{1}{T_j} \langle \mathbf{d}'|\hat{O}_j|\mathbf{d}\rangle + \langle \mathbf{d}'|\hat{O}_{ij}|\mathbf{d}\rangle + \langle \mathbf{d}'|\hat{O}'_{ij}|\mathbf{d}\rangle \right), \end{aligned} \tag{B.14}$$

where T_i is the number of $\langle i,j \rangle$ pairs in the original sum $\sum_{\langle i,j \rangle}$ in (B.12), of which $\mathcal{H}_i$ is part. This factor is needed when we change to a common sum.

We study each of the terms in (B.14) individually[1]:

[1] We assume, without loss of generality, that $i < j$

$$\begin{aligned}
\langle \mathbf{d}'|\hat{O}_i|\mathbf{d}\rangle &= \langle \Omega\omega_{L,d'_L}\cdots\omega_{i,d'_i}\cdots\omega_{1,d'_1}|\hat{O}_i|\omega^\dagger_{1,d_1}\cdots\omega^\dagger_{i,d_i}\cdots\omega^\dagger_{L,d_L}\Omega\rangle = \\
&= \{ \text{ use that } [\hat{O}_i,\omega_{j,d_j}]=0\,\forall\, i\neq j \text{ and (B.11) to move operators} \\
&\quad \omega_{k,d'_k} \text{ where } k\neq i \text{ to the right } \} = \\
&= \left(\prod_{k=1}^{i-1}\delta_{d'_k,d_k}\right)\langle \Omega\omega_{L,d'_L}\cdots\omega_{i,d'_i}|\hat{O}_i|\omega^\dagger_{i,d_i}\cdots\omega^\dagger_{L,d_L}\Omega\rangle = \\
&= \left(\prod_{k=1}^{i-1}\delta_{d'_k,d_k}\right)(-1)^{\left[deg(d'_i)+deg(d_i)\right]\sum_{k=i+1}^{L}deg(d_k)}\left(\prod_{k=i+1}^{L}\delta_{d'_k,d_k}\right)\langle \Omega\omega_{i,d'_i}|\hat{O}_i|\omega^\dagger_{i,d_i}\Omega\rangle = \\
&= \{ \text{ Due to that } \omega^\dagger_{i,d_i}\Omega \text{ is an eigenstate to } \hat{O}_i, \\
&\quad \text{the above may be nonzero only if } d'_i=d_i. \text{ We can thus set } deg(d'_i)=deg(d_i)\} = \\
&= \left(\prod_{k\neq i}\delta_{d'_k,d_k}\right)\underbrace{(-1)^{2deg(d_i)\sum_{k=i+1}^{L}deg(d_k)}}_{=1}\langle \Omega\omega_{i,d'_i}|\hat{O}_i|\omega^\dagger_{i,d_i}\Omega\rangle = \\
&= \left(\prod_{k\neq i}\delta_{d'_k,d_k}\right)\langle \Omega\omega_{i,d'_i}|\hat{O}_i|\omega^\dagger_{i,d_i}\Omega\rangle
\end{aligned} \tag{B.15}$$

$$\begin{aligned}
\langle \mathbf{d}'|\hat{O}_{ij}|\mathbf{d}\rangle &= \langle \Omega\omega_{L,d'_L}\cdots\omega_{j,d'_j}\cdots\omega_{i,d'_i}\cdots\omega_{1,d'_1}|\hat{O}_{ij}|\omega^\dagger_{1,d_1}\cdots\omega^\dagger_{i,d_i}\cdots\omega^\dagger_{j,d_j}\cdots\omega^\dagger_{L,d_L}\Omega\rangle = \\
&= \{ \text{ use (B.13) and (B.11), and move operators} \\
&\quad \omega_{k,d'_k} \text{ where } k\neq i \text{ to the right } \} = \\
&= \left(\prod_{k\neq i,j}\delta_{d'_k,d_k}\right)\times(-1)^{\left[deg(d'_i)+deg(d_i)\right]\sum_{k=i+1}^{L}deg(d_k)}\times \\
&\quad \times(-1)^{\left[deg(d'_j)+deg(d'_i)+deg(d_i)+deg(d_j)\right]\sum_{k=j+1}^{L}deg(d_k)}\times \\
&\quad \times\langle \Omega\omega_{j,d'_j}\omega_{i,d'_i}|\hat{O}_{ij}|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle = \\
&= \{\text{Due to the structure of } \hat{O}_{ij}, \text{ described in (B.12), } \omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega \text{ is an} \\
&\quad \text{eigenstates to } \hat{O}_{ij}, \\
&\quad \text{and the above may be nonzero only if } d'_i=d_i \text{ and } d'_j=d_j \\
&\quad . \text{ We can thus set } deg(d'_i)=deg(d_i) \text{ and } deg(d'_j)=deg(d_j)\} = \\
&= \left(\prod_{k\neq i,j}\delta_{d'_k,d_k}\right)\underbrace{(-1)^{2deg(d_i)\sum_{k=i+1}^{j-1}deg(d_k)}}_{=1}\times\underbrace{(-1)^{2(deg(d_i)+deg(d_j))\sum_{k=j+1}^{L}deg(d_k)}}_{=1}\times \\
&\quad \times\langle \Omega\omega_{j,d'_j}\omega_{i,d'_i}|\hat{O}_{ij}|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle = \\
&= \left(\prod_{k\neq i,j}\delta_{d'_k,d_k}\right)\langle \Omega\omega_{j,d'_j}\omega_{i,d'_i}|O_{ij}|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle
\end{aligned} \tag{B.16}$$

$$\begin{aligned}\langle \mathbf{d}'|\hat{O}'_{ij}|\mathbf{d}\rangle &= \langle \Omega\omega_{L,d'_L}\cdots\omega_{j,d'_j}\cdots\omega_{i,d'_i}\cdots\omega_{1,d'_1}|\hat{O}'_{ij}|\omega^\dagger_{1,d_1}\cdots\omega^\dagger_{i,d_i}\cdots\omega^\dagger_{j,d_j}\cdots\omega^\dagger_{L,d_L}\Omega\rangle = \\ &= \{\text{ Use (B.13) and (B.11) and move operators} \\ &\quad \omega_{k,d'_k} \text{ where } k\neq i,j \text{ to the right }\} = \\ &= \left(\prod_{k\neq i,j}\delta_{d'_k,d_k}\right)\times(-1)^{\left[deg(d'_i)+deg(d_i)\right]\sum_{k=i+1}^{j-1}deg(d_k)}\times \\ &\quad \times(-1)^{\left[deg(d'_j)+deg(d'_i)+deg(d_i)+deg(d_j)\right]\sum_{k=j+1}^{L}deg(d_k)}\times \\ &\quad \times\langle\Omega\omega_{j,d'_j}\omega_{i,d'_i}|\hat{O}'_{ij}|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle = \end{aligned} \tag{B.17}$$

The situation for the $deg(d_i)$ factors in (B.17) is more delicate than in (B.15) and (B.16). To examine the case where $\langle\Omega\omega_{j,d'_j}\omega_{i,d'_i}|\hat{O}'_{ij}|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle$ is non-zero, we first note that the factor $\left[\sum_{\mathbf{m}_T}T_{(s,s',\mathbf{m}_T)}(\hat{n}_{i,s,-\sigma})^{m_{i,-\sigma}}(\hat{n}_{j,s',-\sigma})^{m_{j,-\sigma}}\right]$ has $\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega$ as eigenstate. Thus, the action of this $[\cdots]$ factor does not change n_{d_i} or n_{d_j}. Furthermore, acting with $a^\dagger_{i,s,\sigma}a_{j,s',\sigma}$ (or $a^\dagger_{j,s',\sigma}a_{i,s,\sigma}$) on $\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega$ will result in that $n_{i,s,\sigma}\to n_{i,s,\sigma}+1$ and $n_{j,s',\sigma}\to n_{j,s',\sigma}-1$ (or $n_{i,s,\sigma}\to n_{i,s,\sigma}-1$ and $n_{j,s',\sigma}\to n_{j,s',\sigma}+1$), and all other $n_{i,s'',\sigma'}=n_{j,s'',\sigma'}=0;\quad s''\neq s,s';\ \sigma'\neq\sigma$.

To have a non-zero result for $\langle\Omega\omega_{j,d'_j}\omega_{i,d'_i}|\hat{O}'_{ij}|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle$, it is thus necessary that $deg(d'_i)+deg(d'_j)=deg(d_i)+deg(d_j)$, and additionally that $deg(d'_i)=deg(d_i)\pm1$, with $+$ for the $a^\dagger_{i,s,\sigma}a_{j,s',\sigma}$ term and $-$ for the $a^\dagger_{j,s',\sigma}a_{i,s,\sigma}$ term. This allows us to make the following, in the case where $\langle\Omega\omega_{j,d'_j}\omega_{i,d'_i}|\hat{O}'_{ij}|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle\neq0$:

$$\begin{aligned}deg(d'_i)+deg(d'_j)+deg(d_i)+deg(d_j) &= 2\left(deg(d_i)+deg(d_j)\right), \text{ an even number, and} \\ deg(d'_i)+deg(d_i) &= 2deg(d_i)\pm1, \text{ an odd number}\end{aligned}$$

Using this, we may now rewrite (B.17):

$$\langle \mathbf{d}'|\hat{O}'_{ij}|\mathbf{d}\rangle = \left(\prod_{k\neq i,j}\delta_{d'_k,d_k}\right)\times(-1)^{\sum_{k=i+1}^{j-1}deg(d_k)}\langle\Omega\omega_{j,d'_j}\omega_{i,d'_i}|\hat{O}'_{ij}|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle \tag{B.18}$$

Finally, we note that terms such as in (B.15) can be modified

$$\begin{aligned}\langle \mathbf{d}'|\hat{O}_i|\mathbf{d}\rangle &= \left(\prod_{k\neq i}\delta_{d'_k,d_k}\right)\langle\Omega\omega_{i,d'_i}|\hat{O}_i|\omega^\dagger_{i,d_i}\Omega\rangle = \\ &= \left(\prod_{k\neq i,j}\delta_{d'_k,d_k}\right)\langle\Omega\omega_{j,d'_j}\omega_{i,d'_i}|\hat{O}_i|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle, \text{ for an arbitrary } j>i\end{aligned} \tag{B.19}$$

Using the results (B.15)-(B.19), we can now write the last sum in (B.14) as

$$\langle \mathbf{d}'|\hat{O}|\mathbf{d}\rangle = \\ = \sum_{\langle ij\rangle}\left(\prod_{k\neq i,j}\delta_{d'_k,d_k}\right)\langle\Omega\omega_{j,d'_j}\omega_{i,d'_i}|\frac{1}{T_i}\hat{O}_i+\frac{1}{T_j}\hat{O}_j+\hat{O}_{ij}+(-1)^{\sum_{k=i+1}^{j-1}deg(d_k)}\hat{O}'_{ij}|\omega^\dagger_{i,d_i}\omega^\dagger_{j,d_j}\Omega\rangle \quad \text{(B.20)}$$

Any matrix element can thus be expressed as a sum of terms in each of which the non-trivial arguments are matrix elements obtained when considering only two two subspaces $\mathcal{H}_i$ and $\mathcal{H}_j$.

We will now show that the three-band and the extended one-band Hubbard models both are special cases of the above described model.

The three-band Hubbard model as a special case

The three-band Hubbard model on the whole CuO_2 lattice is a special case of the general model described in Equations (B.7), (B.8) and (B.12). We see this if we do the following identifications:

- $l = 3$. There are three sites in each cluster.
- The Hilbert space representing the fermion states on the whole lattice is a tensor product of the Hilbert spaces representing the state in each cluster.
- $\{A^\dagger_{i,a_i}\Omega\}_{a_i\in\{1,2,\cdots,64\}}$ is a complete orthonormal basis in $\mathcal{H}_i$, and fulfills the condition that every state $A^\dagger_{i,a_i}\Omega$ is a linear combination of pure states, all of which with the same particle number n_{a_i}
- Each one-cluster operator H_i has the property that $H_iA^\dagger_{i,a_i}\Omega = E_iA^\dagger_{i,a_i}\Omega$, and that $[H_i, A^\dagger_{j,a_j}] = 0\,\forall\, i\neq j$, and is thus an operator of type $\hat{O}_i$ in (B.12).

The Hamiltonian H_{ij}, coupling a given pair $\langle i,j\rangle$ of clusters, contains interaction (U_{pd}) terms and hopping (t_{pd} and t_{pp}) terms. This operator H_{ij} is an operator of type $\hat{O}_{ij}+\hat{O}'_{ij}$ in (B.12):

- We obtain H_{ij} for a type A/D of cluster pair $\langle i,j\rangle$, with the labeling convention in Figure B.1, with the following values of the parameters $V_{s,s',\mathbf{m}_V}$ and $T_{(s,s',\mathbf{m}_T)}$ in (B.12):[1]
  $V_{(-,0,[1,0,1,0])} = V_{(-,0,[1,0,0,1])} = V_{(-,0,[0,1,1,0])} = V_{(-,0,[0,1,0,1])} = U_{pd}$,
  $T_{(-,0,[0,0])} = t_{pd}$, $T_{(-,-,[0,0])} = t_{pp}$, $T_{(-,+,[0,0])} = -t_{pp}$, and $V_{s,s',\mathbf{m}_V} = T_{(s,s',\mathbf{m}_T)} = 0$ for all other combinations of s,s', $\mathbf{m}_V$ and $\mathbf{m}_T$.
- We obtain H_{ij} for a type B/C of cluster pair $\langle i,j\rangle$, with the labeling convention in Figure B.1, with the following values of if the parameters $V_{s,s',\mathbf{m}_V}$ and $T_{(s,s',\mathbf{m}_T)}$ in (B.12):
  $V_{(+,0,[1,0,1,0])} = V_{(+,0,[1,0,0,1])} = V_{(+,0,[0,1,1,0])} = V_{(+,0,[0,1,0,1])} = U_{pd}$,
  $T_{(+,0,[0,0])} = -t_{pd}$, $T_{(+,+,[0,0])} = t_{pp}$, $T_{(+,-,[0,0])} = -t_{pp}$, and $V_{s,s',\mathbf{m}_V} = T_{(s,s',\mathbf{m}_T)} = 0$ for all other combinations of s,s', $\mathbf{m}_V$ and $\mathbf{m}_T$.

[1] Since we label the sites in a three-band model cluster as 0, + and −, we have $s, s' \in \{0,+,-\}$

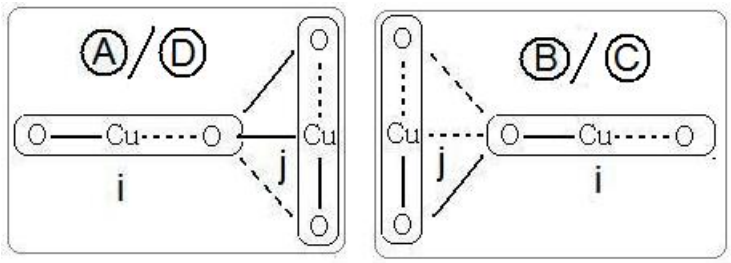

Figure B.1: Illustration of the four types of cluster pair combinations. In this figure, we have used that types A and D of cluster combinations are equivalent, as are types B and C. The labeling convention for i and j, for both types of cluster pairs is shown. Full lines represent $\alpha^{pd} = 1$ or $\alpha^{pp} = 1$, and dashed lines represent $\alpha^{pd} = -1$ or $\alpha^{pp} = -1$, α^{pd} being the Cu-O hopping sign and $\alpha^{pp} = 1$ the O-O hopping sign.

- If the labeling i and j is chosen oppositely from as is done in Figure B.1, the identifications of $V_{(s,s',\mathbf{m}_V)}$ and $T_{(s,s',\mathbf{m}_T)}$ will differ from the above, in both the case of A/D and B/C cluster pairs. The process however remains the same, and we omit the explicit expressions for these cases.

The extended one-band Hubbard model as a special case

- $l = 1$. Each subspace is one site.

- The Hilbert space representing the fermion states on the whole lattice is a tensor product of the Hilbert spaces representing the states on each site.

- $\{\tilde{A}^\dagger_{i,a_i}\Omega\}_{a_i\in\{1,2,3,4\}}$ is a complete orthonormal basis in $\mathcal{H}_i$, and fulfills the condition that every state $\tilde{A}^\dagger_{i,a_i}\Omega$ is a linear combination of pure states, all of which with the same particle number n_{a_i}.

- Each operator $\tilde{H}_i = -\mu\hat{n}_i + U\hat{n}_{i,\uparrow}\hat{n}_{i,\downarrow}$ fulfills that $\tilde{A}^\dagger_{i,a_i}\Omega$ is an eigenstate to $\tilde{H}_i$, and that $[\tilde{H}_i, \tilde{A}^\dagger_{j,a_j}] = 0\,\forall\, j \neq i$. $\tilde{H}$ is thus of type $\hat{O}_i$.

- In the ansatz for an extended one-band Hamiltonian in Equation (5.9), the part $\tilde{H}_{ij}$ is an operator of the type $\hat{O}_{ij}+\hat{O}'_{ij}$. This is seen by assigning the following values to the parameters $V_{s,s',\mathbf{m}_V}$ and $T_{(s,s',\mathbf{m}_T)}$ in (B.12):[2] $V_{[1,0,1,0]} = V_{[1,0,0,1]} = V_{[0,1,1,0]} = V_{[0,1,0,1]} = \frac{V}{2}$, $V_{[1,1,1,0]} = V_{[1,1,0,1]} = W + \epsilon_{ij}W'$, $V_{[1,0,1,1]} = V_{[0,1,1,1]} = W - \epsilon_{ij}W'$, $V_{1,1,1,1} = W''$, $T_{[0,0]} = -t$, $T_{[1,0]} = -(X + \epsilon_{ij}X')$, $T_{[0,1]} = -(X - \epsilon_{ij}X')$ and $T_{[1,1]} = -Z$

[2]Since, in the one-band model case, $l = 1$, i.e. there is only one site in each subspace $\mathcal{H}_i$, the indexes s and s' do not vary in the operator $\hat{O}_{ij} + \hat{O}'_{ij}$, and are omitted.

Concluding the proof

We have now shown that in a certain class of models, defined in Equations (B.7), (B.8) and (B.12), any element in O, the matrix representation of an operator $\hat{O}$, in a basis $\{\omega^\dagger_{i,d_i}\Omega\}$, can be written as the sum in (B.20). Furthermore, we have shown that the three-band Hubbard model, with the basis $\{A^\dagger_{i,a_i}\Omega\}_{a_i\in\{1,2,\cdots,64\}}$, and the one-band Hubbard model, with the basis $\{\tilde{A}^\dagger_{i,a_i}\Omega\}_{a_i\in\{1,2,3,4\}}$, are special cases of this general model.

Now, let $|\mathbf{a}\rangle = \prod_{i=1}^{L} A^\dagger_{i,a_i}\Omega$, $a_i \in \{1,2,3,4\}$, and $|\tilde{\mathbf{a}}\rangle = \prod_{i=1}^{L} \tilde{A}^\dagger_{i,a_i}\Omega$, $a_i \in \{1,2,3,4\}$. Then for any three-band model matrix element $H_{\mathbf{a}',\mathbf{a}}$ and corresponding one-band matrix element $\tilde{H}_{\tilde{\mathbf{a}}',\tilde{\mathbf{a}}}$:

$$
\begin{aligned}
&H_{\mathbf{a}',\mathbf{a}} = \\
&= \sum_{\langle i,j\rangle} \left(\prod_{k\neq i,j} \delta_{a'_k,a_k} \right) \langle \Omega A_{j,a'_j} A_{i,a'_i} | \frac{1}{T_i} H_i + \frac{1}{T_j} H_j + H_{ij} + (-1)^{\sum_{k=i+1}^{j-1} deg(a_k)} H'_{ij} | A^\dagger_{i,a_i} A^\dagger_{j,a_j} \Omega \rangle, \text{ and}
\end{aligned} \tag{B.21}
$$

$$
\begin{aligned}
&\tilde{H}_{\tilde{\mathbf{a}}',\tilde{\mathbf{a}}} = \\
&= \sum_{\langle i,j\rangle} \left(\prod_{k\neq i,j} \delta_{a'_k,a_k} \right) \langle \Omega \tilde{A}_{j,a'_j} \tilde{A}_{i,a'_i} | \frac{1}{T_i} \tilde{H}_i + \frac{1}{T_j} \tilde{H}_j + \tilde{H}_{ij} + (-1)^{\sum_{k=i+1}^{j-1} deg(a_k)} \tilde{H}'_{ij} | \tilde{A}^\dagger_{i,a_i} \tilde{A}^\dagger_{j,a_j} \Omega \rangle
\end{aligned} \tag{B.22}
$$

Lastly, we note that due to the fact that any state $A^\dagger_{i,a_i} A^\dagger_{j,a_j}\Omega$ ($\tilde{A}^\dagger_{i,a_i} \tilde{A}^\dagger_{j,a_j}\Omega$) is an eigenstate to H_i ($\tilde{H}_i$), H_j ($\tilde{H}_j$) and H_{ij} ($\tilde{H}_{ij}$), the contributions of these operators can be non-zero only in diagonal terms, i.e. terms where $a'_i = a_i$ and $a'_j = a_j$. H'_{ij} and $\tilde{H}'_{ij}$, on the contrary, will give non-zero contribution only to off-diagonal terms with $a'_i \neq a_i$ and $a'_j \neq a_j$. Therefore, when we set (B.21)=(B.22) to find the one-band Hamiltonian $\tilde{H}$, the factor$(-1)^{\sum_{k=i+1}^{j-1} deg(a_k)}$ will appear only in off-diagonal matrix elements, and then it will cancel out. Therefore, we can conclude that to ensure that each three-band model matrix element $H_{\mathbf{a}',\mathbf{a}}$ is equal to the corresponding one-band element $\tilde{H}_{\tilde{\mathbf{a}}',\tilde{\mathbf{a}}}$, it is sufficient to match elements such as

$$
\begin{aligned}
\langle \Omega A_{j,a'_j} A_{i,a'_i} | \frac{1}{T_i} H_i + \frac{1}{T_j} H_j + H_{ij} + H'_{ij} | A^\dagger_{i,a_i} A^\dagger_{j,a_j} \Omega \rangle = \\
= \langle \Omega \tilde{A}_{j,a'_j} \tilde{A}_{i,a'_i} | \frac{1}{T_i} \tilde{H}_i + \frac{1}{T_j} \tilde{H}_j + \tilde{H}_{ij} + \tilde{H}'_{ij} | \tilde{A}^\dagger_{i,a_i} \tilde{A}^\dagger_{j,a_j} \Omega \rangle,
\end{aligned}
$$

which finalizes the proof of Proposition 5.2.1.

Appendix C

Matlab codes

C.1 The Hubbard model – a simple example

C.1.1 Energies in the two-sites case

The following Matlab code uses the analytical solution of the Hubbard model, defined and solved in Section 3.1. In the code, we keep the hopping amplitude parameter t fixed at 1 eV, and vary the interaction parameter U such that $U/t \in \{0, 1, \cdots, 8\}$. The program plots the eigenvalues in each of these instances. This plot is shown in Figure 3.2

```
clear, close all
clc

E = [];
t=1; % Fixing t = 1 eV
for n=0:8
    U = n*t; % Varying U
    I = []; Es = [];
    %We insert the solution obtained analytically. The vector Ei below
    %contains the energies of the eigenstates with n=i.
    E0 = 0;
    E1 = [-t -t t t];
    E2 = [0 U/2-sqrt(4*t^2+U^2/4) U/2+sqrt(4*t^2+U^2/4) U 0 0];
    E3 = [U-t U-t U+t U+t];
    E4 = 2*U;
    Ev = [E0 E1 E2 E3 E4 n]';
    E = [E Ev];
end

% The j:th column of E now contains the energies as obtained with the j:th
% input value of U.

X = [0 1 1 1 1 2 2 2 2 2 2 3 3 3 3 4']; %Used as x-axis.

for m=1:length(E(1,:))
    % Below, plotting energy values from lowest to highest, with section.
    Ratio = num2str(E(end,m));
```

```
    Titeln = strcat('U/t =',Ratio); %Plot title
    subplot(3,3,m)
    plot(X, E(1:end-1,m), 'o')
    title(Titeln)
    hold on, grid on
    if m == length(E(1,:)) %Making a PDF on the last loop.
        print('-dpdf',['Figure_Twositesenergies' num2str(m)])
    end
end
```

C.1.2 Energies in the L-sites case

The following code solves the Hubbard model Hamiltonian in Section 3.2 on L sites located in a ring (a link in the case where L=2). In addition, it tells us the time spent by the program to find the solution.

```
clear all
close all
clc
profile on

%Solving the Hubbard model problem on a ring of m sites (link, when m=2).

l = 2; %Number of sites
m = 2*l; %Number of accessible one-particle states, including spin
t = 1; %Strength of the hopping term
U = 3; %Strength of the interaction term

% For one state, containing zero or one particles
o = [0;1]; %We let this represent an empty one-particle state
c = [0 1;0 0]; %Creation operator
a = [0 0;1 0]; %Annihilation operator
I = eye(2);
Im = [1 0;0 -1]; % Ensuring CAR relations

%For the system of m one-particle states, creating the empty state:

G= [1];
for i=1:m
    G = kron(G,o); %Tensor product of all states empty
end

%Making one creation and one annihilation operator for each state
C =[];
A =[];
tic
for i = 1:m %Number of sites, including spin
    Ci = 1;
    Ai = 1;
    for j=1:(i-1)
        Ci = kron(Ci,Im);
        Ai = kron(Ai,Im) ;
    end
    Ci = kron(Ci,c);
```

```
    Ai = kron(Ai,a);
    for j=(i+1):m
        Ci = kron(Ci,I);
        Ai = kron(Ai,I);
    end
    A = cat(3,A,Ai);
    C = cat(3,C,Ci);
end

buildingoperatorstime=toc;

% Z will contain m [2^m,2^m]-matrices that will multiply the ground
% state, to obtain the basis.

Z = [];
Z(:,:,1:m) = C; % In the {n=1} sector, there are m=6 possible states.

k=(1:m)'; %used to keep track of where to add next operator
n=[0;ones(length(k),1)];% Will identify each sector with specific n.
s=[0;zeros(length(k),1)]; % Will identify each subsector specific s^z

for i=2:length(k)+1
    s(i)= 0.5*(-1)^(mod(i,2)); %setting spin: + for odd, - for even.
end

tic
for i=2:m %Each loop is a sector with a certain n
    Ztemp = [];
    ktemp=[];
    stemp=[];
    for j=1:length(k) % There are k elements in previous sector
        for h=k(j)+1:m % To add the correct number of operators
            T = Z(:,:,end-length(k)+j)*C(:,:,h); %Creating...
            Ztemp = cat(3,Ztemp,T); %...and saving the operator.
            ktemp = [ktemp;h]; % Adding to the counter
            n=[n;i]; % Save the particle number
            spin = 0.5*(-1)^(mod(h,2)+1); % Identifying the spin of C(:,:,h)
            stemp=[stemp;s(end-length(k)+j)+spin]; % Adding spin
        end
    end
    Z = cat(3,Z,Ztemp); %Saving away the operators in this sector.
    k = ktemp; %Saving the counter, to next loop
    s = [s; stemp]; %Saving the spin
end
buildingbasistime=toc;

% Z has dimension [64,64,63]. It has sixty three 64x64 matrices

B=zeros(2^m,2^m); % Each of B:s column vectors will be a basis state
B(:,1) = G; % Ground state in column 1

for i=1:2^m-1
    B(:,i+1)=Z(:,:,i)*G; % Column 2-64 are created.
end

% We have our basis B, in which we now will express the [64,64] Hamiltonian
```

```
% matrix H:

H = spalloc(2^m,2^m,2^m); % Pre-allocating a 2^m x 2^m matrix

tic

% Pre-allocate arrays to fasten

qw=2^m;
dt=spalloc(qw*(m-2),qw*(m-2),qw^2*(m-2));
du=spalloc(qw*m/2,qw*m/2,qw^2*m/2);

% Create 2D matrices with square matrices on the diagonal

for i=1:m-2
    dt((i-1)*qw+1:i*qw,(i-1)*qw+1:i*qw) =...
        C(:,:,i)*A(:,:,i+2) + C(:,:,i+2)*A(:,:,i);
end
for i=1:2:m
    du((ceil(i/2)-1)*qw+1:ceil(i/2)*qw,(ceil(i/2)-1)*qw+1:ceil(i/2)*qw)=...
        C(:,:,i)*A(:,:,i)*C(:,:,i+1)*A(:,:,i+1);
end

% Used to obtain i=L <--> i=1 hopping:
Mcorrup = C(:,:,1)*A(:,:,m-1) + C(:,:,m-1)*A(:,:,1);
Mcorrdown = C(:,:,2)*A(:,:,m) + C(:,:,m)*A(:,:,2);

% Looping to create the 2^m * 2^m Hamiltonian matrix:

for p=1:2^m
    for q=1:2^m
        if n(q)==n(p) && s(q)==s(p) % If we're in the same sector
            Htcorrup=0; Htcorrdown=0;

            %The hopping term
            bpp=kron(eye(m-2),B(:,p)');
            bqq=kron(eye(m-2),B(:,q));
            Kt=bpp*dt*bqq;

            %The interaction term
            bpp=kron(eye(m/2),B(:,p)');
            bqq=kron(eye(m/2),B(:,q));
            Ht=t*sum(sum(Kt));
            Ku=bpp*du*bqq;
            Hu=U*sum(sum(Ku));

            %Correcting for the last term, hopping site l <--> site 1:
            Htcorrup = Htcorrup + t* B(1:end,p)' * Mcorrup * B(1:end,q);
            Htcorrdown = Htcorrdown + t* B(1:end,p)' *...
                Mcorrdown * B(1:end,q);

            if m == 4 % Making sure we don't double count in case l=2
                Htcorrup = 0;
                Htcorrdown = 0;
            end
            % The full H(p,q) matrix element:
```

```
151             H(p,q) = H(p,q) + Ht + Htcorrup + Htcorrdown + Hu;
152         end
153     end
154     disp(strcat(num2str(p),' / ',num2str(2^m)));
155 end
156 hamiltoniantime=toc;
157
158 tic
159
160 E = eig(H); % Diagonalising the Hamiltonian matrix.
161
162 eigenvaluetime=toc;
163 times=[l buildingoperatorstime...
164     buildingbasistime hamiltoniantime eigenvaluetime];
165 totaltime = l+buildingoperatorstime +...
166     buildingbasistime+hamiltoniantime+eigenvaluetime;
167
168 disp('    l         oper      basis     hamil     eigen')
169 disp(times)
170 disp('Total time')
171 disp(totaltime)
```

C.2 Three-band to one-band model

C.2.1 Solving one cluster

The following Matlab code solves the three-band Hubbard model on one-cluster. On rows 12-19, we specify the three-band parameters. We get the eigenvalues as diagonal entries in the 64×64 matrix E, and the eigenvectors as columns in the 64×64 matrix V. It is worth mentioning that the program uses the 64 pure states as basis, in the following order:

$$
\begin{aligned}
&\Omega; \\
&p^\dagger_{+,\uparrow}\Omega, p^\dagger_{+,\downarrow}\Omega, d^\dagger_{0,\uparrow}\Omega, d^\dagger_{0,\downarrow}\Omega, p^\dagger_{-,\uparrow}\Omega, p^\dagger_{-,\downarrow}\Omega; \\
&p^\dagger_{+,\uparrow}p^\dagger_{+,\downarrow}\Omega, p^\dagger_{+,\uparrow}d^\dagger_{0,\uparrow}\Omega, \cdots, p^\dagger_{+,\uparrow}p^\dagger_{-,\downarrow}\Omega, p^\dagger_{+,\downarrow}d^\dagger_{0,\uparrow}\Omega, \cdots, p^\dagger_{-,\uparrow}p^\dagger_{-,\downarrow}\Omega; \\
&p^\dagger_{+,\uparrow}p^\dagger_{+,\downarrow}d^\dagger_{0,\uparrow}\Omega, p^\dagger_{+,\uparrow}p^\dagger_{+,\downarrow}d^\dagger_{0,\downarrow}\Omega, \cdots, d^\dagger_{0,\downarrow}p^\dagger_{-,\uparrow}p^\dagger_{-,\downarrow}\Omega \\
&p^\dagger_{+,\uparrow}p^\dagger_{+,\downarrow}d^\dagger_{0,\uparrow}d^\dagger_{0,\downarrow}\Omega, \cdots, d^\dagger_{0,\uparrow}d^\dagger_{0,\downarrow}p^\dagger_{-,\uparrow}p^\dagger_{-,\downarrow}\Omega; \\
&p^\dagger_{+,\uparrow}p^\dagger_{+,\downarrow}d^\dagger_{0,\uparrow}d^\dagger_{0,\downarrow}p^\dagger_{-,\uparrow}\Omega, \cdots, p^\dagger_{+,\downarrow}d^\dagger_{0,\uparrow}d^\dagger_{0,\downarrow}p^\dagger_{-,\uparrow}p^\dagger_{-,\downarrow}\Omega \\
&p^\dagger_{+,\uparrow}p^\dagger_{+,\downarrow}d^\dagger_{0,\uparrow}d^\dagger_{0,\downarrow}p^\dagger_{-,\uparrow}p^\dagger_{-,\downarrow}\Omega
\end{aligned}
\tag{C.1}
$$

```
1 clear all
2 close all
3 clc
4
5 format long
6
```

```
l = 3 ; %Number of sites in one cluster
m = 2*l; %Number of accessible fermion states, including spin

% Parameters of the Three band Hubbard model:

Ed = 0; %Onsite potential on Cu site
Ep = 3; %Onsite potentiel on O site
Tpd = 1; %Hopping amplitude Cu <--> O
Tpp = 0.5; %Hopping amplitude O <--> O
Udd= 8; %Interaction between fermions both residing on a Cu site
Upd= 0.5; %Interaction between fermions on neighbouring Cu-O pairs
Upp= 3; %Interaction between fermions both residing on an O site
Chem = 0; %Chemical Potential

% Elements to represent the fermion system on each accesible state:
o = [0;1]; %Representing an empty one-particle state
c = [0 1;0 0]; %Creation operator. c*o = [1;0], the occupied state
a = [0 0;1 0]; %Annihilation operator, a*o = 0
I = eye(2);
Im = [1 0;0 -1]; % Ensuring CAR relations

%For n one-particle states, creating the ground state, a [2^m,1] vector:

G = 1;
for i=1:m
    G = kron(G,o); % kron(A,B) does tensor product between A and B
end

% Making one creation and one annihilation operator for each accessible
% one-particle state:

tic

C =[];
A =[];

for i = 1:m
    Ci = 1;
    Ai = 1;
    for j=1:(i-1)
        Ci = kron(Ci,Im);
        Ai = kron(Ai,Im);
    end
    Ci = kron(Ci,c);
    Ai = kron(Ai,a);
    for j=(i+1):m
        Ci = kron(Ci,I);
        Ai = kron(Ai,I);
    end
    A = cat(3,A,Ai); %Saving annihilation operators in a 3D array
    C = cat(3,C,Ci); %...and likewise with the creation operators
end

buildingoperatorstime = toc;

% The 6 creation and 6 annihilation operators are now stored in
```

```
% these two [2^6,2^6,6] arrays. We use these to define our basis:

tic

% Z will contain the [2^6,2^6]-matrices that will multiply the ground
% state, to obtain the basis.

Z = [];

Z(:,:,1:m) = C; % In the {n=1} sector, there are m=6 possible states.

k=(1:m)'; % Used to keep track of where to add next operator
n=[0;ones(length(k),1)]; % Will identify each sector with specific n.
s=[0;zeros(length(k),1)]; % Will identify each subsector specific s^z

for i=2:length(k)+1
    s(i)= 0.5*(-1)^(mod(i,2)); %setting spin: + for odd, - for even.
end

for i=2:m %Each loop is a sector with a certain n
    Ztemp = [];
    ktemp=[];
    stemp=[];
    for j=1:length(k) % There are k elements in the previous sector
        for h=k(j)+1:m % To add the correct number of operators
            T = Z(:,:,end-length(k)+j)*C(:,:,h); % Creating...
            Ztemp = cat(3,Ztemp,T); % ...and saving the operator.
            ktemp = [ktemp;h]; % Adding to the counter
            n=[n;i]; % Save the particle number
            spin = 0.5*(-1)^(mod(h,2)+1); % Identifying the spin of C(:,:,h)
            stemp=[stemp;s(end-length(k)+j)+spin]; % Adding spin
        end
    end
    Z = cat(3,Z,Ztemp); % Saving the operators in this sector.
    k = ktemp; % Saving the counter, to next loop
    s = [s; stemp]; % Saving the spin
end

% Z has dimension [64,64,63]. It has sixty three 64x64 matrices

B=zeros(2^m,2^m); % Each of B:s column vectors will be a basis state
B(:,1) = G; % Ground state in column 1

for i=1:2^m-1
    B(:,i+1)=Z(:,:,i)*G; % Column 2-64 are created.
end

buildingbasistime = toc;

% We have our basis B, in which we now will express the [64,64] Hamiltonian
% matrix H:

tic

H = zeros(length(B(1,:)),length(B(1,:))); % Pre-allocating space
Ox = [1 2 5 6]; % We label the sites in the cluster as follows:
```

```
Cu = [3 4]; % [O_upspin O_down Cu_up Cu_down O_up O_down] = [1 2 3 4 5 6]

Hopsigns = [1 1 -1 -1]; % Signs of the hopping term differ

for p=1:length(B(1,:))
    for q=1:length(B(1,:)) % H(p,q) = <B(:,p)|H|B(:,q)>

        Ht=0; % Set to zero at the beginning of each loop
        Hu=0;

        for i=1:m-2 % Hopping energy for Cu <--> O hopping
            Ht = Ht + Tpd * Hopsigns(i) * B(1:end,p)' *...
                ( C(:,:,i)*A(:,:,i+2) + C(:,:,i+2)*A(:,:,i) )...
                * B(1:end,q);
        end

        for i=1:length(Ox) % Onsite energy on Oxygen
            Hu = Hu + Ep * B(1:end,p)' *...
                C(:,:,Ox(i))*A(:,:,Ox(i)) * B(1:end,q);
        end
        for i=1:length(Cu) % Onsite energy on Copper
            Hu = Hu + Ed * B(1:end,p)' *...
                C(:,:,Cu(i))*A(:,:,Cu(i)) * B(1:end,q);
        end

        for i=1:4:5 % Interaction energy on the Oxygen sites
            Hu = Hu + Upp * B(1:end,p)' *...
                C(:,:,i)*A(:,:,i)*C(:,:,i+1)*A(:,:,i+1) * B(1:end,q);
        end
        for i=3 % Interaction energy on the Copper sites
            Hu = Hu + Udd * B(1:end,p)' *...
                C(:,:,i)*A(:,:,i)*C(:,:,i+1)*A(:,:,i+1) * B(1:end,q);
        end

        for i=1:length(Ox) % Interaction term between <O,Cu> sites
            for j=1:length(Cu)
                Hu = Hu + Upd * B(1:end,p)' *...
                    C(:,:,Ox(i))*A(:,:,Ox(i)) *...
                    C(:,:,Cu(j))*A(:,:,Cu(j)) * B(1:end,q);
            end
        end

        if p == q
            Hu = Hu -Chem*n(p); % Add Chemical potential
        end

        H(p,q) = H(p,q) + Ht + Hu; %This is the full H(p,q) term.
    end
end

buildinghamiltoniantime = toc;

tic
[V,E]=eig(H); % Solving the one cluster problem

solvingeigenequationtime = toc;
```

```
175
176 % E is diagonal. E(i,i) is the i:th eigenvalues of H. The i:th column of V,
177 % V(:,i), is the i:th eigenstate of H.
```

C.2.2 Matching three-band to one-band model

The code in Appendix C.2.1 solved the one-cluster problem. It gives a diagonal matrix E, where E(i,i) is the i:th eigenvalue, and a matrix V, whose i:th column represents the i:th eigenstate. The following code is added to the above , uses its results, and combines the states and energies to find numerical values to the elements[1] $\langle\Omega A_{j,a_j} A_{i,a_i}|\frac{1}{T_i}H_i + \frac{1}{T_j}H_j + H_{ij}|A^\dagger_{i,a_i}A^\dagger_{j,a_j}\Omega\rangle$; $\quad a_i \in \{1,2,3,4\}$ of the 16×16 three-band Hamiltonian matrix on two clusters.

Note that in the solution of the one-cluster problem, there is a degree of freedom in choosing the eigenstates: Consider $A^\dagger_{i,a_i}\Omega$, a normalized eigenstate to the one-cluster Hamiltonian H_i. Then $\bar{A}^\dagger_{i,a_i}\Omega = e^{i\theta}A^\dagger_{i,a_i}\Omega$; $\quad \theta\in\mathbb{R}$ is also a normalized eigenstate with the same eigenvalue. It turns out that Matlab chooses, when running the same piece of code, $\theta = 0$ sometimes and $\theta = \pi$ sometimes, in a seemingly arbitrary manner. Moreover, the lowest energy is two fold degenerate (corresponding to eigenstates $A^\dagger_2\Omega$ and $A^\dagger_3\Omega$), and Matlab will interchangably order these two eigenstates as $\cdots, A^\dagger_2\Omega, A^\dagger_3\Omega, \cdots$, and as $\cdots, A^\dagger_3\Omega, A^\dagger_2\Omega, \cdots$, as it seems arbitrarily.

For the above reasons, rows 1-41 in the first code below ensure that Matlab has defined the same four eigenvectors (taking the phase factor into account) in the same order as in our convention: $\{A^\dagger_1\Omega, A^\dagger_2\Omega, A^\dagger_3\Omega, A^\dagger_4\Omega\}$. After that, the code combines one-cluster states into two-cluster states.

Cluster combination type A and D

The below code treats the cluster combination type A (and D which is equivalent to A, see Figure 4.4) with the i and j labelling convention described in Figure 5.2.

```
1  % 1: Ensuring that the degenerate {n=1,s=1/2} and {n=1,s=-1/2} eigenstates
2  % are ordered as in our convention:
3
4  if abs(V(4,1)) < 0.000001 % If this is zero, the order is wrong
5      V(:,[1,2]) = V(:,[2,1]);
6  end
7
8  % 2: Now we know the order is according to convention. Ensuring phase:
9
10 % If any eigenvector is not real, abort:
11 if isreal(V(1,3)) == 0 || isreal(V(4,1)) == 0 || ...
12         isreal(V(5,2)) == 0 || isreal(V(17,4)) == 0
13     disp('Error, complex eigenvalue')
14     exit
15 end
16
17 % 3: Now we know vectors are real. Ensuring sign convention:
```

[1] H_{ij} being the part of the three-band Hamiltonian H, that couple clusters i and j, consisting of terms with coefficients t_{pd}, t_{pp} and U_{pd}

```
18
19 if V(1,3) < 0 % n=0 (should be = 1)
20     V(:,3) = -V(:,3);
21 end
22 if V(4,1) > 0 % n=1, s^z = 1/2 (should be negative)
23     V(:,1) = -V(:,1);
24 end
25 if V(5,2) > 0 % n=1, s^z = -1/2 (should be negative)
26     V(:,2) = -V(:,2);
27 end
28 if V(17,4) < 0 % n=2, s^z = 0 (should be positive)
29     V(:,4) = -V(:,4);
30 end
31
32 % 4: Finally, we order the four states with lowest energy
33 % according to n and s^z: {0,0},{1,1/2},{1,-1/2},{2,0}
34
35 RV = V(:,1:4);
36 Es = E(1:4,1:4);
37
38 RV(:,[1,3])=RV(:,[3,1]);
39 Es([1,3],[1,3])=Es([3,1],[3,1]);
40 RV(:,[2,3])=RV(:,[3,2]);
41 Es([2,3],[2,3])=Es([3,2],[3,2]);
42
43 % What we need are the operators A1, A2, A3 and A4, and not the states that
44 % result from acting with these operators on the ground state. I.e., in the
45 % equation A(i)*G = S(i) we search the operator A(i) and not the state S(i).
46 % Therefore, we need to do this:
47
48 AS = zeros(64,64,4); %We'll put our four operators here
49
50 AS(:,:,1) =eye(64); %The first is the identity operator.
51
52 for i = 2:4
53     ASi = zeros(64,64);
54     for j = 1:63
55         ASi = ASi + RV(j+1,i)*Z(:,:,j);
56     end
57     AS(:,:,i) = ASi;
58 end
59
60 % States in the two cluster system are represented by tensor products of
61 % one-cluster states. We label the two clusters (cluster i and cluster
62 % j) and define an order convention i<j. Using the below 64x64
63 % matrix (Imtwo)^{particle number of state j}, we ensure that CAR relations
64 % are respected.
65
66 Imtwo = sparse(kron(kron(kron(Im,Im),Im),kron(kron(Im,Im),Im)));
67 Itwo = sparse(eye(64));
68
69 Gtwo = sparse(kron(G,G)); %Empty two-cluster state
70
71 Number = [0 1 1 2]'; %Denoting the particle number of each state
72 Spin = [0 0.5 -0.5 0]'; % Denoting the spin of each state
73
```

```
% Creating the two-cluster states:

Rtwo = sparse(2^m*2^m,4*4); % Pre-allocate space
Etwo = zeros(4*4,1);

% n=0, s=0
Rtwo(:,1) = kron(AS(:,:,1),Itwo)*kron(Imtwo^(Number(1)),AS(:,:,1))*Gtwo;
Etwo(1) = Es(1,1) + Es(1,1);

% n=1,s=0.5
Rtwo(:,2) = kron(AS(:,:,2),Itwo)*kron(Imtwo^(Number(1)),AS(:,:,1))*Gtwo;
Etwo(2) = Es(2,2) + Es(1,1);

Rtwo(:,3) = kron(AS(:,:,1),Itwo)*kron(Imtwo^(Number(2)),AS(:,:,2))*Gtwo;
Etwo(3) = Es(1,1) + Es(2,2);

% n=1,s=-0.5
Rtwo(:,4) = kron(AS(:,:,3),Itwo)*kron(Imtwo^(Number(1)),AS(:,:,1))*Gtwo;
Etwo(4) = Es(3,3) + Es(1,1);

Rtwo(:,5) = kron(AS(:,:,1),Itwo)*kron(Imtwo^(Number(3)),AS(:,:,3))*Gtwo;
Etwo(5) = Es(1,1) + Es(3,3);

% n=2,s=1
Rtwo(:,6) = kron(AS(:,:,2),Itwo)*kron(Imtwo^(Number(2)),AS(:,:,2))*Gtwo;
Etwo(6) = Es(2,2) + Es(2,2);

% n=2, s=0
Rtwo(:,7) = kron(AS(:,:,4),Itwo)*kron(Imtwo^(Number(1)),AS(:,:,1))*Gtwo;
Etwo(7) = Es(4,4) + Es(1:1);

Rtwo(:,8) = kron(AS(:,:,2),Itwo)*kron(Imtwo^(Number(3)),AS(:,:,3))*Gtwo;
Etwo(8) = Es(2,2) + Es(3,3);

Rtwo(:,9) = kron(AS(:,:,3),Itwo)*kron(Imtwo^(Number(2)),AS(:,:,2))*Gtwo;
Etwo(9) = Es(3,3) + Es(2,2);

Rtwo(:,10) = kron(AS(:,:,1),Itwo)*kron(Imtwo^(Number(4)),AS(:,:,4))*Gtwo;
Etwo(10) = Es(1,1) + Es(4,4);

% n=2, s=-1
Rtwo(:,11) = kron(AS(:,:,3),Itwo)*kron(Imtwo^(Number(3)),AS(:,:,3))*Gtwo;
Etwo(11) = Es(3,3) + Es(3,3);

% n=3, s=0.5
Rtwo(:,12) = kron(AS(:,:,4),Itwo)*kron(Imtwo^(Number(2)),AS(:,:,2))*Gtwo;
Etwo(12) = Es(4,4) + Es(2,2);

Rtwo(:,13) = kron(AS(:,:,2),Itwo)*kron(Imtwo^(Number(4)),AS(:,:,4))*Gtwo;
Etwo(13) = Es(2,2) + Es(4,4);

% n=3, s=-0.5
Rtwo(:,14) = kron(AS(:,:,4),Itwo)*kron(Imtwo^(Number(3)),AS(:,:,3))*Gtwo;
Etwo(14) = Es(4,4) + Es(3,3);

Rtwo(:,15) = kron(AS(:,:,3),Itwo)*kron(Imtwo^(Number(4)),AS(:,:,4))*Gtwo;
```

```
Etwo(15) = Es(3,3) + Es(4,4);

% n=4, s=0
Rtwo(:,16) = kron(AS(:,:,4),Itwo)*kron(Imtwo^(Number(4)),AS(:,:,4))*Gtwo;
Etwo(16) = Es(4,4) + Es(4,4);

%Rtwo now constains 16 states, each represented by a 4096-column
%vector.

%Now, create our creation operators acting on the two-cluster states. C
%and A are (64,64,6)-arrays for one cluster. We need to manufacture
%corresponding (4096,4096,12)-arrays for the two-cluster situation.
%Following the same rules as we did when creating the C and A arrays, and
%using the associativity of the tensor product:

tic

%Pre-allocating memory. The operators will be placed one next to the other
%in two {4096 x 12*4096}-matrices.(there are 12 A-operators and 12
%C-operators)

Atwo=sparse(2^12,12*2^12);
Ctwo=sparse(2^12,12*2^12);

% Creating and saving the operators:

for i=1:6
    Atwo(:,(i-1)*2^12+1:i*2^12)=kron(sparse(A(:,:,i)),eye(2^6));
    Ctwo(:,(i-1)*2^12+1:i*2^12)=kron(sparse(C(:,:,i)),eye(2^6));
    Atwo(:,(6+i-1)*2^12+1:(6+i)*2^12)=kron(Imtwo,sparse(A(:,:,i)));
    Ctwo(:,(6+i-1)*2^12+1:(6+i)*2^12)=kron(Imtwo,sparse(C(:,:,i)));
end

creatingtwoclusteroperatorstime=toc;

Htwo = zeros(16,16);

e_pd = + 1; %The sign factor for Tpd hopping
e_plus = - 1; %One of the sign factors for Tpp hopping
e_minus = + 1; %THe other sign factor for Tpp hopping

tic

Ti = 4; %The number of <ij> pairs in which i and j take part.

% We create H|Rtwo(l)> first, and then multiply <Rtwo(k)| from the left
% Numbers are such that {i,k} = k and {j,k} = k+6; k = 1,2,...,6

for l = 1:16

    Hop75 = Atwo(:,(7-1)*2^12+1:7*2^12)*Rtwo(:,l);
    Hop75 = Ctwo(:,(5-1)*2^12+1:5*2^12)*Hop75; % 7->5 Tpp hopping term
    Hop57 = Atwo(:,(5-1)*2^12+1:5*2^12)*Rtwo(:,l);
    Hop57 = Ctwo(:,(7-1)*2^12+1:7*2^12)*Hop57;  % 5->7 Tpp hopping term

    Hop86 = Atwo(:,(8-1)*2^12+1:8*2^12)*Rtwo(:,l);
```

```
    Hop86 = Ctwo(:,(6-1)*2^12+1:6*2^12)*Hop86; % 8->6 Tpp hopping term
    Hop68 = Atwo(:,(6-1)*2^12+1:6*2^12)*Rtwo(:,l);
    Hop68 = Ctwo(:,(8-1)*2^12+1:8*2^12)*Hop68; % 6->8 Tpp hopping

    Hop115 = Atwo(:,(11-1)*2^12+1:11*2^12)*Rtwo(:,l);
    Hop115 = Ctwo(:,(5-1)*2^12+1:5*2^12)*Hop115; % 11->5 Tpp hopping
    Hop511 = Atwo(:,(5-1)*2^12+1:5*2^12)*Rtwo(:,l);
    Hop511 = Ctwo(:,(11-1)*2^12+1:11*2^12)*Hop511;  % 5->11 Tpp hopping

    Hop126 = Atwo(:,(12-1)*2^12+1:12*2^12)*Rtwo(:,l);
    Hop126 = Ctwo(:,(6-1)*2^12+1:6*2^12)*Hop126; % 12->6 Tpp hopping
    Hop612 = Atwo(:,(6-1)*2^12+1:6*2^12)*Rtwo(:,l);
    Hop612 = Ctwo(:,(12-1)*2^12+1:12*2^12)*Hop612; % 6->12 Tpp hopping

    Hop95 = Atwo(:,(9-1)*2^12+1:9*2^12)*Rtwo(:,l);
    Hop95 = Ctwo(:,(5-1)*2^12+1:5*2^12)*Hop95; % 9->5 Tpd hopping
    Hop59 = Atwo(:,(5-1)*2^12+1:5*2^12)*Rtwo(:,l);
    Hop59 = Ctwo(:,(9-1)*2^12+1:9*2^12)*Hop59; % 5->9 Tpd hopping

    Hop106 = Atwo(:,(10-1)*2^12+1:10*2^12)*Rtwo(:,l);
    Hop106 = Ctwo(:,(6-1)*2^12+1:6*2^12)*Hop106; % 10->6 Tpd hopping
    Hop610 = Atwo(:,(6-1)*2^12+1:6*2^12)*Rtwo(:,l);
    Hop610 = Ctwo(:,(10-1)*2^12+1:10*2^12)*Hop610; % 6->10 Tpd hopping

    Inter59 = Atwo(:,(5-1)*2^12+1:5*2^12)*Rtwo(:,l);
    Inter59 = Ctwo(:,(5-1)*2^12+1:5*2^12)*Inter59;
    Inter59 = Atwo(:,(9-1)*2^12+1:9*2^12)*Inter59;
    Inter59 = Ctwo(:,(9-1)*2^12+1:9*2^12)*Inter59; %Upd 5-9(up-up))

    Inter510 = Atwo(:,(5-1)*2^12+1:5*2^12)*Rtwo(:,l);
    Inter510 = Ctwo(:,(5-1)*2^12+1:5*2^12)*Inter510;
    Inter510 = Atwo(:,(10-1)*2^12+1:10*2^12)*Inter510;
    Inter510 = Ctwo(:,(10-1)*2^12+1:10*2^12)*Inter510; %Upd 5-10 (up-down)

    Inter69 = Atwo(:,(6-1)*2^12+1:6*2^12)*Rtwo(:,l);
    Inter69 = Ctwo(:,(6-1)*2^12+1:6*2^12)*Inter69;
    Inter69 = Atwo(:,(9-1)*2^12+1:9*2^12)*Inter69;
    Inter69 = Ctwo(:,(9-1)*2^12+1:9*2^12)*Inter69; %Upd 6-9 (down-up)

    Inter610 = Atwo(:,(6-1)*2^12+1:6*2^12)*Rtwo(:,l);
    Inter610 = Ctwo(:,(6-1)*2^12+1:6*2^12)*Inter610;
    Inter610 = Atwo(:,(10-1)*2^12+1:10*2^12)*Inter610;
    Inter610 = Ctwo(:,(10-1)*2^12+1:10*2^12)*Inter610; %Upd 6-10(down-down)

    for k = 1:16

        % Add the onsite energy of each of the two clusters:
        if k == l
            Htwo(k,l) = Htwo(k,l) + (1/Ti)*Etwo(k); % Note: T_i = T_j = 4
        end

        % Hopping and interaction::
        Htwo(k,l) = Htwo(k,l) + Rtwo(:,k)' *...
            (e_plus*Tpp*(Hop57+Hop75+Hop68+Hop86) +...
            e_minus*Tpp*(Hop115+Hop511+Hop126+Hop612) +...
            e_pd*Tpd*(Hop95+Hop59+Hop106+Hop610) +...
```

```
            Upd*(Inter59 + Inter510 + Inter69 + Inter610));
    end
end

creatingtwoclustermatrixelementstime=toc;

%Below we calculate the one-band parameter values:

%Mu, chemical potential:
P1 = - Ti*Htwo(2,2);

% U, interaction on one specific site
P4 = Ti*Htwo(7,7) + 2*P1;

% t, the hopping amplitude
P2 = - Htwo(2,3);
% X, additional hopping term: n_i + n_j
P5 = (Htwo(7,9)+Htwo(9,10))/2-P2;
% X', additional hopping term: n_i - n_j
P6 = (Htwo(7,9)-Htwo(9,10))/2;
%Z, additional hopping parameter: n_i*n_j
P9 = Htwo(12,13)-P2-2*P5;


% V, interaction between neighbouring sites:
P3 = 2*Htwo(6,6)+4*P1/Ti;
% W, additional interaction parameter: n_i + n_j
P7 = (Htwo(12,12)+Htwo(13,13))/2+(3*P1-P4)/Ti-P3;
% W', additional interaction parameter: n_i - n_j
P8 = (Htwo(12,12)-Htwo(13,13))/2;
%W'', addtnl interact. param n_i*n_j:
P10 = Htwo(16,16)+(4*P1-2*P4)/Ti-2*P3-4*P7;

% The total time for the program to run:
```

Cluster combination type A and D – reversed labeling

To do the matching on a cluster combination of type A/D, but with the opposite labeling convention compared to Figure 5.2, $i \to j$ and $j \to i$, the below code replaces rows 167-244 in the above code:

```
e_pd = + 1; %The sign factor for Tpd hopping
e_plus = - 1; %One of the sign factors for Tpp hopping
e_minus = + 1; %THe other sign factor for Tpp hopping

tic

Ti = 4; %The number of <ij> pairs in which i and j take part.

%Adding all the terms for each of the 16*16 elements.
for l = 1:16

    Hop11_1 = Atwo(:,(11-1)*2^12+1:11*2^12)*Rtwo(:,l);
    Hop11_1 = Ctwo(:,(1-1)*2^12+1:1*2^12)*Hop11_1; %11->1 Tpp hopping term
    Hop1_11 = Atwo(:,(1-1)*2^12+1:1*2^12)*Rtwo(:,l);
```

```
    Hop1_11 = Ctwo(:,(11-1)*2^12+1:11*2^12)*Hop1_11;  %1->11 Tpp hopping term

    Hop12_2 = Atwo(:,(12-1)*2^12+1:12*2^12)*Rtwo(:,l);
    Hop12_2 = Ctwo(:,(2-1)*2^12+1:2*2^12)*Hop12_2; %12->2 Tpp hopping term
    Hop2_12 = Atwo(:,(2-1)*2^12+1:2*2^12)*Rtwo(:,l);
    Hop2_12 = Ctwo(:,(12-1)*2^12+1:12*2^12)*Hop2_12;  %2->12 Tpp hopping

    Hop11_3 = Atwo(:,(11-1)*2^12+1:11*2^12)*Rtwo(:,l);
    Hop11_3 = Ctwo(:,(3-1)*2^12+1:3*2^12)*Hop11_3; %11->3 Tpd hopping
    Hop3_11 = Atwo(:,(3-1)*2^12+1:3*2^12)*Rtwo(:,l);
    Hop3_11 = Ctwo(:,(11-1)*2^12+1:11*2^12)*Hop3_11;  %3->11 Tpd hopping

    Hop12_4 = Atwo(:,(12-1)*2^12+1:12*2^12)*Rtwo(:,l);
    Hop12_4 = Ctwo(:,(4-1)*2^12+1:4*2^12)*Hop12_4; %12->4 Tpd hopping
    Hop4_12 = Atwo(:,(4-1)*2^12+1:4*2^12)*Rtwo(:,l);
    Hop4_12 = Ctwo(:,(12-1)*2^12+1:12*2^12)*Hop4_12;  %4->12 Tpd hopping

    Hop11_5 = Atwo(:,(11-1)*2^12+1:11*2^12)*Rtwo(:,l);
    Hop11_5 = Ctwo(:,(5-1)*2^12+1:5*2^12)*Hop11_5; %11->5 hopping. (Tpp)
    Hop5_11 = Atwo(:,(5-1)*2^12+1:5*2^12)*Rtwo(:,l);
    Hop5_11 = Ctwo(:,(11-1)*2^12+1:11*2^12)*Hop5_11; %5->11 hopping. (Tpp)

    Hop12_6 = Atwo(:,(12-1)*2^12+1:12*2^12)*Rtwo(:,l);
    Hop12_6 = Ctwo(:,(6-1)*2^12+1:6*2^12)*Hop12_6; %12->6 hopping. (Tpp)
    Hop6_12 = Atwo(:,(6-1)*2^12+1:6*2^12)*Rtwo(:,l);
    Hop6_12 = Ctwo(:,(12-1)*2^12+1:12*2^12)*Hop6_12; %6->12 hopping. (Tpp)

    Inter11_3 = Atwo(:,(11-1)*2^12+1:11*2^12)*Rtwo(:,l);
    Inter11_3 = Ctwo(:,(11-1)*2^12+1:11*2^12)*Inter11_3;
    Inter11_3 = Atwo(:,(3-1)*2^12+1:3*2^12)*Inter11_3;
    Inter11_3 = Ctwo(:,(3-1)*2^12+1:3*2^12)*Inter11_3; %Upd 11-3 (up-up)

    Inter11_4 = Atwo(:,(11-1)*2^12+1:11*2^12)*Rtwo(:,l);
    Inter11_4 = Ctwo(:,(11-1)*2^12+1:11*2^12)*Inter11_4;
    Inter11_4 = Atwo(:,(4-1)*2^12+1:4*2^12)*Inter11_4;
    Inter11_4 = Ctwo(:,(4-1)*2^12+1:4*2^12)*Inter11_4; %Upd 11-4 (up-down)

    Inter12_3 = Atwo(:,(12-1)*2^12+1:12*2^12)*Rtwo(:,l);
    Inter12_3 = Ctwo(:,(12-1)*2^12+1:12*2^12)*Inter12_3;
    Inter12_3 = Atwo(:,(3-1)*2^12+1:3*2^12)*Inter12_3;
    Inter12_3 = Ctwo(:,(3-1)*2^12+1:3*2^12)*Inter12_3; %Upd 12-3 (down-up)

    Inter12_4 = Atwo(:,(12-1)*2^12+1:12*2^12)*Rtwo(:,l);
    Inter12_4 = Ctwo(:,(12-1)*2^12+1:12*2^12)*Inter12_4;
    Inter12_4 = Atwo(:,(4-1)*2^12+1:4*2^12)*Inter12_4;
    Inter12_4 = Ctwo(:,(4-1)*2^12+1:4*2^12)*Inter12_4; %Upd 12-4 (down-up)

    for k = 1:16

        % Add the onsite energy of each of the two clusters:
        if k == l
            Htwo(k,l) = Htwo(k,l) + (1/Ti)*Etwo(k); %Note: T_i = T_j = 4
        end

        % The interaction between clusters:
        Htwo(k,l) = Htwo(k,l) + Rtwo(:,k)' *...
```

```
            (e_plus*Tpp*(Hop11_1+Hop1_11+Hop12_2+Hop2_12) +...
            e_minus*Tpp*(Hop11_5+Hop5_11+Hop12_6+Hop6_12) +...
            e_pd*Tpd*(Hop11_3+Hop3_11+Hop12_4+Hop4_12) +...
            Upd*(Inter11_3 + Inter11_4 + Inter12_3 + Inter12_4));
    end
end
```

Cluster combination type B and C

To instead do the matching on a cluster combination of type B (and C, which is equivalent to B, see Figure 4.4), with the i and j labelling convention described in Figure 5.2, the following code replaces row 167-244 in the first code:

```
e_pd = - 1; %The sign factor for Tpd hopping
e_plus = + 1; %One of the sign factors for Tpp hopping
e_minus = - 1; %The other sign factor for Tpp hopping

tic

Ti = 4; %The number of <ij> pairs in which i and j take part.

for l = 1:16

    Hop71 = Atwo(:,(7-1)*2^12+1:7*2^12)*Rtwo(:,l);
    Hop71 = Ctwo(:,(1-1)*2^12+1:1*2^12)*Hop71; %7->1 Tpp hopping term
    Hop17 = Atwo(:,(1-1)*2^12+1:1*2^12)*Rtwo(:,l);
    Hop17 = Ctwo(:,(7-1)*2^12+1:7*2^12)*Hop17;  %1->7 Tpp hopping term

    Hop82 = Atwo(:,(8-1)*2^12+1:8*2^12)*Rtwo(:,l);
    Hop82 = Ctwo(:,(2-1)*2^12+1:2*2^12)*Hop82; %8->2 Tpp hopping term
    Hop28 = Atwo(:,(2-1)*2^12+1:2*2^12)*Rtwo(:,l);
    Hop28 = Ctwo(:,(8-1)*2^12+1:8*2^12)*Hop28;  %2->8 Tpp hopping

    Hop11_1 = Atwo(:,(11-1)*2^12+1:11*2^12)*Rtwo(:,l);
    Hop11_1 = Ctwo(:,(1-1)*2^12+1:1*2^12)*Hop11_1; %11->1 Tpp hopping
    Hop1_11 = Atwo(:,(1-1)*2^12+1:1*2^12)*Rtwo(:,l);
    Hop1_11 = Ctwo(:,(11-1)*2^12+1:11*2^12)*Hop1_11;  %1->11 Tpp hopping

    Hop122 = Atwo(:,(12-1)*2^12+1:12*2^12)*Rtwo(:,l);
    Hop122 = Ctwo(:,(2-1)*2^12+1:2*2^12)*Hop122; %12->2 Tpp hopping
    Hop212 = Atwo(:,(2-1)*2^12+1:2*2^12)*Rtwo(:,l);
    Hop212 = Ctwo(:,(12-1)*2^12+1:12*2^12)*Hop212;  %2->12 Tpp hopping

    Hop91 = Atwo(:,(9-1)*2^12+1:9*2^12)*Rtwo(:,l);
    Hop91 = Ctwo(:,(1-1)*2^12+1:1*2^12)*Hop91; %9->1 hopping. (Tpd)
    Hop19 = Atwo(:,(1-1)*2^12+1:1*2^12)*Rtwo(:,l);
    Hop19 = Ctwo(:,(9-1)*2^12+1:9*2^12)*Hop19; %1->9 hopping. (Tpd)

    Hop102 = Atwo(:,(10-1)*2^12+1:10*2^12)*Rtwo(:,l);
    Hop102 = Ctwo(:,(2-1)*2^12+1:2*2^12)*Hop102; %10->2 hopping. (Tpd)
    Hop210 = Atwo(:,(2-1)*2^12+1:2*2^12)*Rtwo(:,l);
    Hop210 = Ctwo(:,(10-1)*2^12+1:10*2^12)*Hop210; %2->10 hopping. (Tpd)

    Inter19 = Atwo(:,(1-1)*2^12+1:1*2^12)*Rtwo(:,l);
```

```
    Inter19 = Ctwo(:,(1-1)*2^12+1:1*2^12)*Inter19;
    Inter19 = Atwo(:,(9-1)*2^12+1:9*2^12)*Inter19;
    Inter19 = Ctwo(:,(9-1)*2^12+1:9*2^12)*Inter19; %Upd 1-9 (up-up)

    Inter110 = Atwo(:,(1-1)*2^12+1:1*2^12)*Rtwo(:,l);
    Inter110 = Ctwo(:,(1-1)*2^12+1:1*2^12)*Inter110;
    Inter110 = Atwo(:,(10-1)*2^12+1:10*2^12)*Inter110;
    Inter110 = Ctwo(:,(10-1)*2^12+1:10*2^12)*Inter110; %Upd 1-10 (up-down)

    Inter29 = Atwo(:,(2-1)*2^12+1:2*2^12)*Rtwo(:,l);
    Inter29 = Ctwo(:,(2-1)*2^12+1:2*2^12)*Inter29;
    Inter29 = Atwo(:,(9-1)*2^12+1:9*2^12)*Inter29;
    Inter29 = Ctwo(:,(9-1)*2^12+1:9*2^12)*Inter29; %Upd 2-9 (down-up)

    Inter210 = Atwo(:,(2-1)*2^12+1:2*2^12)*Rtwo(:,l);
    Inter210 = Ctwo(:,(2-1)*2^12+1:2*2^12)*Inter210;
    Inter210 = Atwo(:,(10-1)*2^12+1:10*2^12)*Inter210;
    Inter210 = Ctwo(:,(10-1)*2^12+1:10*2^12)*Inter210; %Upd 2-10 (down-down)

    for k = 1:16

        % Add the onsite energy of each of the two clusters:
        if k == l
            Htwo(k,l) = Htwo(k,l) + (1/Ti)*Etwo(k); %Note: T_i = T_j = 4
        end

        % The interaction between clusters:
        Htwo(k,l) = Htwo(k,l) + Rtwo(:,k)' *...
            (e_plus*Tpp*(Hop17+Hop71+Hop28+Hop82) +...
            e_minus*Tpp*(Hop11_1+Hop1_11+Hop122+Hop212) +...
            e_pd*Tpd*(Hop91+Hop19+Hop102+Hop210) +...
            Upd*(Inter19 + Inter110 + Inter29 + Inter210));
    end
end
```

Cluster combination type B and C – reversed labeling

To do the matching on a cluster combination of type B/C, but with the opposite labeling convention compared to Figure 5.2, $i \to j$ and $j \to i$, the below code replaces rows 167-244 in the above code:

```
e_pd = - 1; %The sign factor for Tpd hopping
e_plus = + 1; %One of the sign factors for Tpp hopping
e_minus = - 1; %The other sign factor for Tpp hopping

tic

Ti = 4; %The number of <ij> pairs in which i and j take part.

for l = 1:16

    Hop7_1 = Atwo(:,(7-1)*2^12+1:7*2^12)*Rtwo(:,l);
    Hop7_1 = Ctwo(:,(1-1)*2^12+1:1*2^12)*Hop7_1; %7->1 Tpp hopping term
    Hop1_7 = Atwo(:,(1-1)*2^12+1:1*2^12)*Rtwo(:,l);
    Hop1_7 = Ctwo(:,(7-1)*2^12+1:7*2^12)*Hop1_7;  %1->7 Tpp hopping term
```

```
15
16      Hop8_2 = Atwo(:,(8-1)*2^12+1:8*2^12)*Rtwo(:,l);
17      Hop8_2 = Ctwo(:,(2-1)*2^12+1:2*2^12)*Hop8_2; %8->2 Tpp hopping term
18      Hop2_8 = Atwo(:,(2-1)*2^12+1:2*2^12)*Rtwo(:,l);
19      Hop2_8 = Ctwo(:,(8-1)*2^12+1:8*2^12)*Hop2_8;  %2->8 Tpp hopping
20
21      Hop7_3 = Atwo(:,(7-1)*2^12+1:7*2^12)*Rtwo(:,l);
22      Hop7_3 = Ctwo(:,(3-1)*2^12+1:3*2^12)*Hop7_3; %7->3 Tpd hopping
23      Hop3_7 = Atwo(:,(3-1)*2^12+1:3*2^12)*Rtwo(:,l);
24      Hop3_7 = Ctwo(:,(7-1)*2^12+1:7*2^12)*Hop3_7;  %3->7 Tpd hopping
25
26      Hop8_4 = Atwo(:,(8-1)*2^12+1:8*2^12)*Rtwo(:,l);
27      Hop8_4 = Ctwo(:,(4-1)*2^12+1:4*2^12)*Hop8_4; %8->4 Tpd hopping
28      Hop4_8 = Atwo(:,(4-1)*2^12+1:4*2^12)*Rtwo(:,l);
29      Hop4_8 = Ctwo(:,(8-1)*2^12+1:8*2^12)*Hop4_8;  %4->8 Tpd hopping
30
31      Hop7_5 = Atwo(:,(7-1)*2^12+1:7*2^12)*Rtwo(:,l);
32      Hop7_5 = Ctwo(:,(5-1)*2^12+1:5*2^12)*Hop7_5; %7->5 hopping. (Tpp)
33      Hop5_7 = Atwo(:,(5-1)*2^12+1:5*2^12)*Rtwo(:,l);
34      Hop5_7 = Ctwo(:,(7-1)*2^12+1:7*2^12)*Hop5_7; %7->5 hopping. (Tpp)
35
36      Hop8_6 = Atwo(:,(8-1)*2^12+1:8*2^12)*Rtwo(:,l);
37      Hop8_6 = Ctwo(:,(6-1)*2^12+1:6*2^12)*Hop8_6; %8->6 hopping. (Tpp)
38      Hop6_8 = Atwo(:,(6-1)*2^12+1:6*2^12)*Rtwo(:,l);
39      Hop6_8 = Ctwo(:,(8-1)*2^12+1:8*2^12)*Hop6_8; %6->8 hopping. (Tpp)
40
41      Inter7_3 = Atwo(:,(7-1)*2^12+1:7*2^12)*Rtwo(:,l);
42      Inter7_3 = Ctwo(:,(7-1)*2^12+1:7*2^12)*Inter7_3;
43      Inter7_3 = Atwo(:,(3-1)*2^12+1:3*2^12)*Inter7_3;
44      Inter7_3 = Ctwo(:,(3-1)*2^12+1:3*2^12)*Inter7_3; %Upd 7-3 (up-up)
45
46      Inter7_4 = Atwo(:,(7-1)*2^12+1:7*2^12)*Rtwo(:,l);
47      Inter7_4 = Ctwo(:,(7-1)*2^12+1:7*2^12)*Inter7_4;
48      Inter7_4 = Atwo(:,(4-1)*2^12+1:4*2^12)*Inter7_4;
49      Inter7_4 = Ctwo(:,(4-1)*2^12+1:4*2^12)*Inter7_4; %Upd 7-4 (up-down)
50
51      Inter8_3 = Atwo(:,(8-1)*2^12+1:8*2^12)*Rtwo(:,l);
52      Inter8_3 = Ctwo(:,(8-1)*2^12+1:8*2^12)*Inter8_3;
53      Inter8_3 = Atwo(:,(3-1)*2^12+1:3*2^12)*Inter8_3;
54      Inter8_3 = Ctwo(:,(3-1)*2^12+1:3*2^12)*Inter8_3; %Upd 8-3 (up-up)
55
56      Inter8_4 = Atwo(:,(8-1)*2^12+1:8*2^12)*Rtwo(:,l);
57      Inter8_4 = Ctwo(:,(8-1)*2^12+1:8*2^12)*Inter8_4;
58      Inter8_4 = Atwo(:,(4-1)*2^12+1:4*2^12)*Inter8_4;
59      Inter8_4 = Ctwo(:,(4-1)*2^12+1:4*2^12)*Inter8_4; %Upd 8-4 (up-up)
60
61      for k = 1:16
62
63          % Add the onsite energy of each of the two clusters:
64          if k == l
65              Htwo(k,l) = Htwo(k,l) + (1/Ti)*Etwo(k); %Note: T_i = T_j = 4
66          end
67
68          % The interaction between clusters:
69          Htwo(k,l) = Htwo(k,l) + Rtwo(:,k)' *...
70              (e_plus*Tpp*(Hop1_7+Hop7_1+Hop2_8+Hop8_2) +...
```

```
71              e_minus*Tpp*(Hop7_5+Hop5_7+Hop8_6+Hop6_8) +...
72              e_pd*Tpd*(Hop7_3+Hop3_7+Hop8_4+Hop4_8) +...
73              Upd*(Inter7_3 + Inter7_4 + Inter8_3 + Inter8_4));
74      end
75  end
```