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Master of Science

**Hole hopping in a disordered spin
background with iterated equations of
motion**

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Abstract

The energy gap for single charge excitation Δ in a half-filled Fermi-Hubbard model in the regime of strong interactions is studied for both a one-dimensional chain and two-dimensional squared lattice. Charge fluctuations in this regime are suppressed. Therefore, it is appropriate to use an effective model, namely the t - J model. Here, the model is used in the limit of $0 < J \ll T \ll \Delta$ to describe the movement of a hole in a disordered spin background. The energy spectrum connected to this movement provides information regarding the energy gap.

In this context, the iterated equations of motion approach represents a tool to gain insights into the dynamics of a hole and thus to resolve the energy spectrum connected to the energy gap. As in previous studies, an ansatz with a scalar product is used, which is slightly modified here. Results for the energy gap gained with this approach are compared to results from former studies using different approaches. Occurring differences are attributable to not considering spin correlations in this approach.

Kurzfassung

Im Hinblick auf die vorliegende Arbeit wird die Energie Lücke Δ für eine einzelne Ladungsanregung in einem halbgefüllten Fermi-Hubbard Modell in Bereich starker Wechselwirkung sowohl auf einer eindimensionalen Kette als auch auf einem zweidimensionalen quadratischen Gitter untersucht. Ladungsfluktuationen sind in diesem Grenzbereich stark unterdrückt, sodass es möglich ist ein effektives Modell herzuleiten, das t - J Modell. Der Grenzbereich $0 < J \ll T \ll \Delta$ soll dieses Modells in dieser Arbeit dazu dienen die Bewegung eines Loches in dem paramagnetischen halb gefüllten Zustand zu beschreiben und so Informationen über die Energie Lücke für eine einzelne Ladungsanregung zu erhalten.

Es wird eine Methode vorgestellt die es ermöglicht in Form von iterierten Bewegungsgleichungen das Energiespektrum aufzulösen und so Rückschlüsse auf die Energielücke für Ladungsanregung zu ziehen. Dafür wird ein Ansatz mit Operatorskalarprodukt verwendet, der in Vergleich zu vorigen Studien zur iterierten Bewegungsgleichungen modifiziert wird. Die resultierenden Energielücken werden mit Ergebnissen anderer Methoden verglichen. Auftretende Unterschiede werden auf die Nichtberücksichtigung von Spin Korrelationen bei diesem Ansatz zurückgeführt.

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1 Introduction

The field of physics investigating phases and phase transitions in a condensed-matter systems is a broad research area. While the variety of phases is very limited in daily life, there is a multitude of phenomena in the lower temperature range. The spectrum goes from phases which are characterized by their magnetic properties like the antiferromagnetic and ferromagnetic phase to phases determined by their electronic properties like metal, superconductor, semiconductor and Mott-Insulator or other exotic phases as the Bose-Einstein condensate only to name a few [1]. Phases characterized by different interactions and properties are of course able to overlap so there are e.g. paramagnetic Mott insulating and antiferromagnetic Mott insulating phases. All those phases despite their different behavior and form of appearance in condensed-matter physics share the property that they are built of the same building blocks electrons, protons and neutrons which then form different Atoms and Molecules. In which way those particles interact with each other in the system has an influence on the phases of the system. Due to the incredible amount of particles in a condensed-matter system, it is necessary to break down these interactions into tangible mathematical models, which still provide a sufficient description of the reality. Since in reality different phases transit into each other if parameters in the environment change, the wish to describe those transitions also in theoretical models is deeply rooted in the field of condensed-matter physics. For example superconductivity has been successfully described with the help of the BCS theory [2].

But already models considering only the bare necessary interactions can be full of physical behavior and therefore they are essential for a better physical understanding. One famous model falling into this category is the Ising model [3] which considers only spin interaction of nearest neighbors on a rigid lattice in an external magnetic field. It brought an understanding for anti- and ferromagnetic behavior. Further, it is possible in the model in two dimension to find a thermal driven phase transition of its magnetic phase. Where for a vanishing external field an analytical exact solution [4] was found, the study of other parameter regimes or higher dimensions rely on approximate approaches e.g. density matrix renormalization group [5], mean field theory [6] or Monte Carlo simulations [7]. Hence, models that at fist glance appear quite simple can become a separate field of research whose problems are anything but easy to solve. So investigating new approximate approaches in order to reach a better understanding in areas where an analytical solution is not possible is always of relevance in basic research. The results of those new approximate approaches are mostly evaluated against available analytical solutions or other establish methods and should be able to reproduce them.

This outlined procedure is part of the present work. Here, a new approach is studied in the context of a phase transition in a model also well-established in the field of condensed-matter, namely the Fermi-Hubbard model [8–10]

The Fermi-Hubbard model is capable to describe a phase transition between a Mott-insulator phase and a metal phase by considering only electrons hopping on a lattice with an on site electron-electron-interaction. Where in one dimension an exact solution of the model is possible [11], this holds not for other finite dimension. So the situation is quite similar to the Ising model and the model is study with different approximate approaches e.g. dynamic mean-field theory [12], perturbation theory [13] and variational Monte Carlo method [14]. In some borderline cases of the model deriving an effective model is also a commonly used means [15]. Regardless of the theoretical approaches, due to the progress made in the experimental physics in recent years, this first purely theoretical model can be investigated also in real systems [16, 17]. So the research on the Fermi-Hubbard model is far from complete and the application of this new approach promise new insights.

This new approach is based on the iterated equation of motion approach [18] which already was successfully applied in the context of non-equilibrium physics in the Fermi-Hubbard model [19] and large central spin models [20]. In this thesis, the iterated equation of motion approach is applied to an effective model of the Fermi-Hubbard model, the t - J model [21], to determine the motion of a hole and thus investigated the transition between the Mott-Hubbard insulating and the metal phase.

The work is structured as follows. In chapter 2 first an introduction to the Fermi-Hubbard model is given and its basic properties are discussed. After that the t - J model is introduced whereby all necessary terms in the model are discussed in detail. Then, the tool kit used in this thesis, the iterated equation of motion approach, is presented and accompanied by first considerations to connect the results of the iterated equation of motion approach with an energy spectrum. After this different approaches to determine an operator basis are discussed. In the beginning of chapter 3 the foundation is laid to apply the approach to the real problem and determine the dynamics of a hole in a disordered spin background. Here, two different cases are presented with different consequences for the applied method. Additionally, a further operator representations for this approach is discussed in more detail. Concluding the chapter 3 a form in which the results are presented is established. In chapter 4 contains all calculated results in this thesis starting with a simple model in one dimension as a testbed for this approach where the two different cases are compared to each other. Then the simple model is extended to a two-dimensional squared lattice. The approach is applied to the t - J model in both one and two dimension. In chapter 5 a summary of all obtained results within this work is given followed by an outlook.

2 Theory

2.1 Fermi-Hubbard model

This section considers the Fermi-Hubbard model, which serves as the foundation for the derivation of a t - J model in the further sections. Here an overview of the model is given and its properties are discussed. Onward all calculations are done in natural units within which $\hbar$ is set to unitary.

The Hubbard model was first independently proposed in the year 1963 by John Hubbard [8], Junjiro Kanamori [9] and Martin C. Gutzwiller [10]. It delivers a description for correlated electron systems with narrow energy bands in a solid state system and serves as an important ingredient in other topics such as high-temperature superconductors, transition metals and their oxides, polymers, heavy Fermionic materials, fullerenes and liquid Helium [22].

The model is based on the assumption that electrons face a coulomb repulsion if they are located at the very same site. Otherwise, they can move freely. Furthermore, electrons are tightly bounded at the atomic sites. So in the real space representation of the model the electron wave functions are highly localized Wannier functions [23] taking into account the periodicity of the system and form a complete set of orthogonal function. Furthermore, it is reasonable to describe the model in the second quantization where the operators $f_{l,\sigma}^\dagger$ and $f_{l,\sigma}$ either create or annihilate an electron at site l and with spin $\sigma \in \{\uparrow, \downarrow\}$. In second quantization the Hamiltonian of the model in real space reads

$$H' = H_t + H'_{\text{int}} \quad (2.1a)$$

$$H_t = -t \sum_{\langle i,j \rangle \sigma} f_{i,\sigma}^\dagger f_{j,\sigma} \quad (2.1b)$$

$$H'_{\text{int}} = U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} \quad (2.1c)$$

where $\langle i, j \rangle$ indicates that i, j are nearest neighbors to each other. Here, H_t is the kinetic part describing simple hopping processes between two nearest neighbor sites with the hopping amplitude $t > 0$ and H_{int} denotes the interaction part which considers the repulsive Coulomb interaction of electrons at the same site with the strength $U \geq 0$. Due to the Pauli exclusion principle in the Fermionic system the number operator $\hat{n}_{i,\sigma}$ is limited to the values of $\{0, 1\}$. If the number operators $\hat{n}_{i,\uparrow}$ and $\hat{n}_{i,\downarrow}$ both count an electron, two electrons occur on the same site and the system receives an energy penalty

of U . In this thesis we are dealing with a system near half-filling and thus it is convenient to make an energy shift in the Hamiltonian by the means of

$$H = H' - U \frac{N}{2} + U \frac{L}{2} . \quad (2.2)$$

with the overall number of particle N and number of sites L in the system. This leads to a Hamiltonian of the form

$$H = H_t + H_{\text{int}} \quad (2.3a)$$

$$H_t = -t \sum_{\langle i,j \rangle \sigma} f_{i,\sigma}^\dagger f_{j,\sigma} \quad (2.3b)$$

$$H_{\text{int}} = U \sum_i \left(\hat{n}_{i\uparrow} - \frac{1}{2} \right) \left(\hat{n}_{i\downarrow} - \frac{1}{2} \right) \quad (2.3c)$$

where the chemical potential is set to zero at half-filling. Furthermore, the Hamiltonian in the representation of equation (2.3) is particle-hole symmetric since in this representation empty or doubly occupied sites hold both an energy penalty of $U/4$. Here, empty sites are associated with holes in the system. Whereas a single occupied sites lower the energy by a value of $-U/4$. Apparently, removing or adding an electron in the half-filling case described by equation (2.3), so that a hole or doubly occupied site remains, requires both an energy of $U/2$. This two processes are associated with a charge excitation of the system. If we talk about the Hamiltonian of the Fermi-Hubbard model, we refer to the operator in equation (2.3). In figure 2.1 the Fermi-Hubbard model for an one-dimensional chain is illustrated.

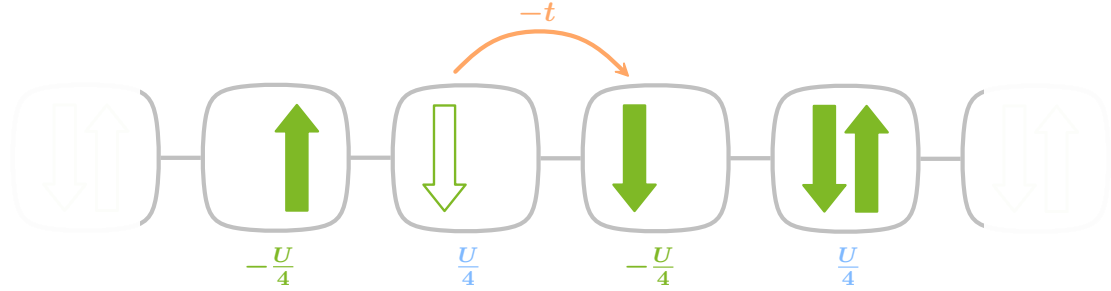


Figure 2.1: Illustration of the Fermi-Hubbard model for an one-dimensional chain. Empty or doubly occupied sites cost an energy of $\frac{U}{4}$ while single sites set free an energy of $\frac{U}{4}$. Also, hopping processes are rewarded with an energy of t .

Contrary to higher finite dimensions the Fermi-Hubbard model in one-dimension $d = 1$ is analytically solvable via Bethe ansatz [11]. As a result of the missing analytical solution in higher finite dimension borderline cases for the model are often discussed. The Fermi-Hubbard model has two interesting borderline cases. On one side with a vanishing interaction $U = 0$ the system collapses to an effective one-particle problem and can be

solved exactly by a transformation of the kinetic part H_t into the momentum space. For a hypercubic d -dimensional lattices this results in a dispersion relation

$$\epsilon_{\mathbf{k}} = -2t \sum_{i=1}^d \cos(\mathbf{k} \mathbf{a}_i) \quad (2.4)$$

with $\mathbf{k}$ denoting the momentum vector and $\mathbf{a}_i$ representing the primitive translation vector of the used lattice. One property of interaction-free system is the bandwidth $W = 2zt$ where $z = 2d$ is the coordination number z of the underlying lattice. For half-filling this case describes a metal. Hereafter the interaction strength is expressed as a relation between U and bandwidth W in the form of W/U . The counterpart is the atomic limit $t \rightarrow 0$ where two difference energy levels are present. One is located at $-U/2$ and the other at $U/2$, which can be calculated for this case with one-electron Green function [8]. For a not vanishing hopping it can be shown with an approximation done in Ref. [24] that these two energy levels broaden into two bands, the lower (LHB) and the upper (UHB) Hubbard band. Each band has the bandwidth of W_{eff} leaving us with a spectral density $\rho(E)$ presented in a simplified manner in figure 2.2 for $U \gg W$. The UHB contains the energy spectrum of adding one electron whereas the LHB contains the spectrum of removing of an electron from the half-filled ground state and the energy difference between the energetically lowest state in the HUB and the highest in the LHB determine the gap size [22]. Due to the particle-hole symmetry in the Hamiltonian of equation (2.3) LHB and UHB are completely symmetric around zero. As shown in figure 2.2 there is an energy

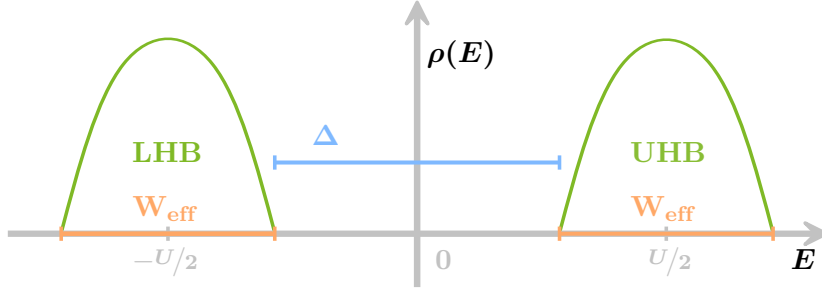


Figure 2.2: Simplified illustration of the spectral density $\rho(E)$ of the Fermi-Hubbard model in the case of $U \gg W$. With the lower LHB and the upper UHB Hubbard band have an effective bandwidth of W_{eff} and the gap for single charge excitations Δ .

gap for single charge excitation of Δ in the parameter regime of $U \gg W$. Hence, the Fermi-Hubbard model at half-filling for $U \gg W$ describes an insulator with the band gap Δ . In the case of decreasing interaction strength U the energy gap Δ separating LHB and UHB also decreases up to a point of critical interaction strength U_c where LHB and UHB finally touch and the energy gap Δ for single charge excitation vanishes. At this critical value the system undergoes a phase transition between the Mott-Hubbard insulating and metal phase. In this context, describing this transition and determining a critical interaction strength U_c is a quite difficult topic. At least in one dimension it is possible due to its integrability to generate exact results [25]. Other approaches study for example a Bethe lattice with infinite connectivity by using e.g. perturbation theory

[13] or dynamic mean-field theory [12, 26]. As mentioned in chapter 1, in this thesis a different approach to determine the critical interaction strength U_c is used by describing a hole motion in a disordered spin background.

In the limit of strong interaction $U \gg W$ doubly occupied sites and holes are highly suppressed and therefore a mapping of the Fermi-Hubbard model at half-filling in second order perturbation theory to an antiferromagnetic Heisenberg model with the coupling constant of $J = 2t^2/U$ is possible [27]. Whereas in the vicinity of half-filling it is possible to describe movements of holes and doubly occupied sites for $U \gg W$ with an effective model, the t - J model which is introduced in section 2.2. Furthermore, to realize the disordered spin background the t - J model is considered for $0 < J \ll T \ll \Delta$ with the temperature T [25].

2.2 Generalized t - J model

As mentioned in section 2.1, in the limit of strong interaction $U \gg W$ it is possible to map the Fermi-Hubbard model at half-filling to an antiferromagnetic Heisenberg model. Also, for values up to $W/U \approx 0.8$ it is justified to map the Fermi-Hubbard model to another effective model, a generalized t - J model [21]. The following section introduces the t - J model and gives an overview about the model essential for this thesis.

Starting with the Hubbard model at half-filling in the limit of strong interaction all sites each are occupied with only one electron. By reducing the interaction strength electrons are gradually allowed to move leaving some sites empty or doubly occupied. These sites are deviations from the previous one electron per site state and are referred to as a sort of charge fluctuations in the system. Here, both doubly occupied and empty sites are called double occupancies DO. In the regime of reducing the strong interaction it is possible to a certain point of the interaction strength to derive an effective Hamiltonian conserving the numbers of DOs. There are different approaches to reach an effective model which eliminates the creation of charge fluctuations in the system. One possible approach is to create an effective Hamiltonian through a degenerate perturbation theory in the scheme of [28] for the half-filled Hubbard model for $t \ll U$. Done e.g. in Ref. [29] up to the seventh order for the linear chain or in Ref. [30] for the simple cubic (sc) lattice up to the fifth order. Another approach is to use a continuous unitary transformation CUT to derive an effective Hamiltonian e.g. done in Ref. [21, 31]. Here we refer to the Hamiltonian of a generalized t - J model from the work done by A. Reischl, E. Müller-Hartmann and G. S. Uhrig [21].

Now we sketch the steps to obtain the effective model via a CUT. Within the derivation the focus lays more on the obtained effective model than the theory behind the CUT. So if a more detailed description is sought, we again refer to the studies done in Ref. [21]. Generally speaking the energy sector of different numbers of DOs are well separated for strong interaction. So through the CUT a disentanglement of the different sectors belonging to different number of DOs is achieved resulting in an effective model. By

starting to alter the representation of the normal Fermionic creator and annihilator as shown below by the means of

$$f_{i,\sigma}^\dagger = f_{i\bar{\sigma}}^\dagger \hat{n}_{i\bar{\sigma}} + f_{i\sigma}^\dagger (1 - \hat{n}_{i\bar{\sigma}}) \quad (2.5)$$

$$f_{i,\sigma} = f_{i\sigma} \hat{n}_{i\bar{\sigma}} + f_{i\bar{\sigma}} (1 - \hat{n}_{i\bar{\sigma}}) \quad (2.6)$$

it is possible to identify terms in the hopping part of the Hubbard model 2.3b depending on the effect on the count of DOs in the system. The hopping part H_0 now reads

$$H_0 = T_0 + T_{+2} + T_{-2} \quad (2.7a)$$

$$T_0 = t_0 \sum_{\langle i,j \rangle \sigma} \left[(1 - \hat{n}_{i\bar{\sigma}}) f_{i\sigma}^\dagger f_{j\sigma} (1 - \hat{n}_{j\bar{\sigma}}) + \hat{n}_{i\bar{\sigma}} f_{i\sigma}^\dagger f_{j\sigma} \hat{n}_{j\bar{\sigma}} + \text{h.c.} \right] \quad (2.7b)$$

$$T_{+2} = t_{+2} \sum_{\langle i,j \rangle \sigma} \left[\hat{n}_{i\bar{\sigma}} f_{i\sigma}^\dagger f_{j\sigma} (1 - \hat{n}_{j\bar{\sigma}}) + \hat{n}_{j\bar{\sigma}} f_{j\sigma}^\dagger f_{i\sigma} (1 - \hat{n}_{i\bar{\sigma}}) \right] \quad (2.7c)$$

$$T_{-2} = t_{-2} \sum_{\langle i,j \rangle \sigma} \left[(1 - \hat{n}_{i\bar{\sigma}}) f_{i\sigma}^\dagger f_{j\sigma} \hat{n}_{j\bar{\sigma}} + (1 - \hat{n}_{j\bar{\sigma}}) f_{j\sigma}^\dagger f_{i\sigma} \hat{n}_{i\bar{\sigma}} \right] \quad (2.7d)$$

where $\bar{\sigma} = -\sigma$ and T_i denotes terms which change the number of DOs of the system by i . The coefficients t_0, t_{-2}, t_{+2} do not differ at the beginning of the CUT from the bare hopping parameter t of the Hubbard model. Here, the transformation $-t \rightarrow t$ is performed beforehand to the Hamiltonian of equation (2.3). Due to its particle-hole symmetry on bipartite lattices, its spectrum is invariant under such transformation [32]. The figure 2.3 shows possible processes of T_0 describing only movements of a DO on the lattice while figure 2.4 illustrates process that change the number of DOs in the system.

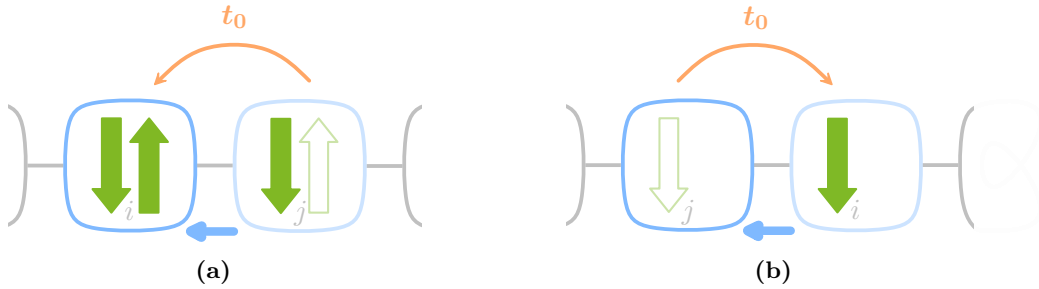


Figure 2.3: Two different process for a DO movement on the lattice. First in figure 2.3a via a doubly occupied site and second in figure 2.3b via an empty site. With the difference that in latter case electron and DO movement take place in opposite direction and in the former in the same direction.

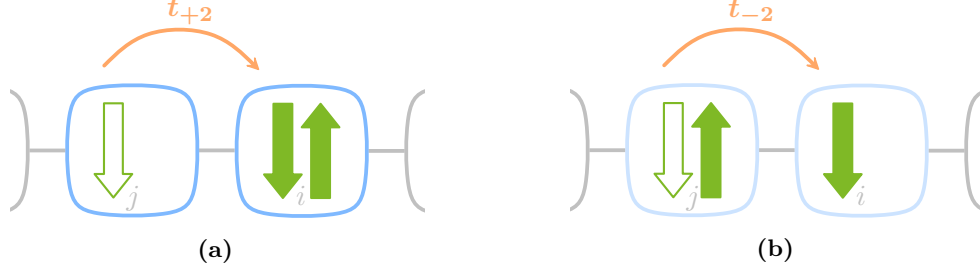


Figure 2.4: Processes that change the number of DOs in the System. In figure 2.4a the creation of two DOs is shown while figure 2.4b shows the annihilation of two DOs.

As mentioned above, we are looking for an effective model conserving the DOs. So terms like $T_{-2/2}$ should not be presented in the effective Hamiltonian. The continuous unitary transformation uses the flow equation

$$\frac{d}{dl}H(l) = [\eta(l), H(l)] \quad (2.8)$$

with the flow parameter l and the generator $\eta(l) = [\hat{D}, H(l)]$ to transform the Hamiltonian into such a model. Here, the operator

$$\hat{D} := \sum_i \left[\hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + (1 - \hat{n}_{i\uparrow}) (1 - \hat{n}_{i\downarrow}) \right] \quad (2.9)$$

counts the number of DOs in the system. Starting with $H(l=0) = H$ the effective model is obtained for $l \rightarrow \infty$. Apart from that a truncation scheme is necessary to restrict to important terms arising during the flow. Therefore, in Ref. [21] the truncation is done according to the locality of new terms referring to a two-dimensional squared lattice. The result is an effective model contains different terms describing different processes conserving the number of DOs in the system. Hopping of DOs, Spin couplings or interaction between two DOs are for example part of those processes. For this thesis terms describing the movement of one DO on a lattice are of great interest. Therefore, only spin couplings in the order of $J = t^2/U$ and hopping of one DO are terms occurring in the Hamiltonian. In the limit $0 < J \ll T \ll \Delta$ we assume that terms describing spin couplings can be neglected. In the following, all DO-hopping processes, which are necessary to describe a t - J model for a two-dimensional squared lattice according to Ref. [21], are discussed, which includes simple nearest neighbor (NN) T_0 and both simple T'_0 and spin dependent $T'_{0,s}$ next nearest neighbor (NNN) hopping on a two-dimensional squared lattice. Where for the NNN hopping a further distinction is made between diagonal T'_x and linear T''_x NNN hopping. This distinction is necessary for use of the Hamiltonian on a one-dimensional chain, since the diagonal NNN hopping does not exist in one dimension. Starting with the simple NN hopping of a DO which is equivalent to the T_0 term of equation (2.7b) with the amplitude $t_0 = t$ being equal to the hopping amplitude of the Fermi-Hubbard model. The diagonal NNN hopping has almost the same form as T_0 with the difference of

a factor -1 between the hopping of a hole and a particle DO to ensure the particle hole symmetry. So the diagonal NNN hopping reads

$$T'_0 = t' \sum_{\langle\langle i,j \rangle\rangle_{d\sigma}} \left[\left(1 - \hat{n}_{i\bar{\sigma}}\right) f_{i\sigma}^\dagger f_{j\sigma} \left(1 - \hat{n}_{j\bar{\sigma}}\right) - \hat{n}_{i\bar{\sigma}} f_{i\sigma}^\dagger f_{j\sigma} \hat{n}_{j\bar{\sigma}} + \text{h.c.} \right] \quad (2.10)$$

where $\langle\langle i,j \rangle\rangle_d$ denotes the diagonal NNN sites. Two possible processes are illustrated in the figure 2.5. The spin dependent diagonal NNN hopping reads as

$$T'_{s,0} = t'_s \sum_{\langle\langle i,k,j \rangle\rangle_{d\alpha\beta}} \left[\left(1 - \hat{n}_{i\bar{\alpha}}\right) f_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_{j\beta} \left(1 - \hat{n}_{j\bar{\beta}}\right) \cdot \mathbf{S}_k \right. \\ \left. + \hat{n}_{i\bar{\alpha}} f_{i\alpha}^\dagger \boldsymbol{\sigma}_{\alpha\beta} f_{j\beta} \hat{n}_{j\bar{\beta}} \cdot \mathbf{S}_k + \text{h.c.} \right] \quad (2.11)$$

with $\alpha, \beta \in \{\uparrow, \downarrow\}$. In the equation above $\mathbf{S}_k$ is the spin vector at site k and it is advisable to use the representation $\mathbf{S}_k = \frac{1}{2} (\sigma_k^- + \sigma_k^+, i(\sigma_k^- - \sigma_k^+), \sigma_k^z)^T$ with $\sigma_k^+ = f_{k,\uparrow}^\dagger f_{k,\downarrow}$, $\sigma_k^- = f_{k,\downarrow}^\dagger f_{k,\uparrow}$ and $\sigma_k^z = n_{k,\uparrow} - n_{k,\downarrow}$. Furthermore, $\boldsymbol{\sigma}$ denotes a vector consisting of the three Pauli matrices $(\sigma_x, \sigma_y, \sigma_z)$ where the index $\alpha\beta$ refers to the corresponding matrix element with $\uparrow=0; \downarrow=1$. As in equation (2.10) i and j are diagonal NNN and in addition k is NN of both sites which is written as $\langle\langle i,k,j \rangle\rangle_d$. For example in a two-dimensional square lattice the path connecting the sites i , k and l forms a right angle as shown in figure 2.6.

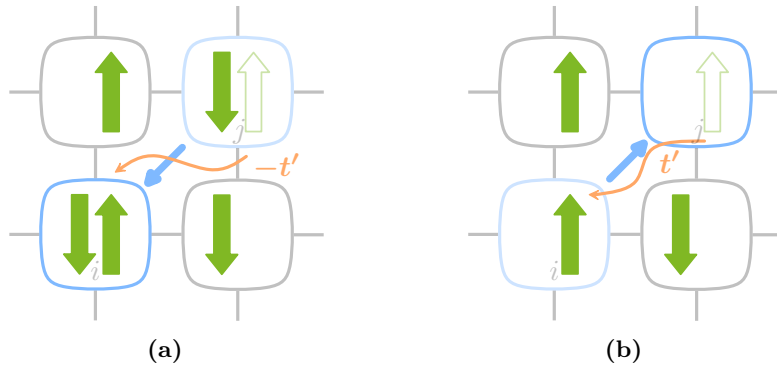


Figure 2.5: Two possible processes for a diagonal next-nearest neighbor hopping T'_0 of a DO according to (2.10) on a two-dimensional square lattice, illustrated via movements firstly of a doubly occupied site in figure 2.5a and secondly of an empty site in figure 2.5b.

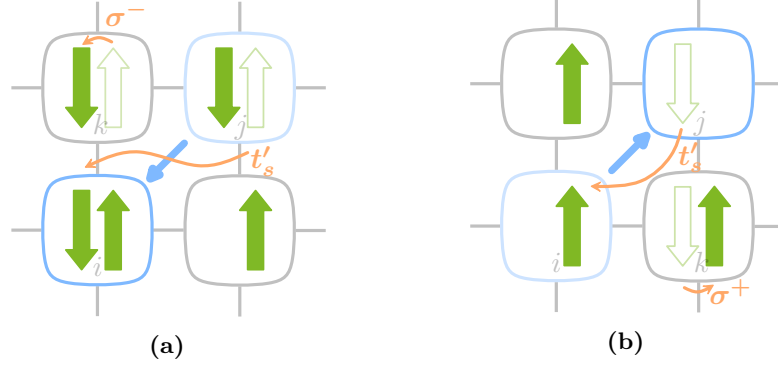


Figure 2.6: Two possible processes out of various spin dependent diagonal next-nearest neighbor hopping of a DO described by $T'_{s,0}$ in equation (2.11). In figure 2.6a the hopping of a doubly occupied site or in figure 2.6b the hopping of an empty site results in a spin flip on the site k .

Furthermore, both simple and spin-dependent linear NNN hopping has to take into consideration. The simple linear NNN hopping

$$T''_0 = t'' \sum_{\langle\langle i,j \rangle\rangle_{l\sigma}} \left[(1 - \hat{n}_{i\bar{\sigma}}) f_{i\sigma}^\dagger f_{j\sigma} (1 - \hat{n}_{j\bar{\sigma}}) - \hat{n}_{i\bar{\sigma}} f_{i\sigma}^\dagger f_{j\sigma} \hat{n}_{j\bar{\sigma}} + \text{h.c.} \right] \quad (2.12)$$

read like T'_0 with the different that $\langle\langle i,j \rangle\rangle_l$ indicates i and j are 3NN sites to each other. Possible processes of T''_0 are shown in figure 2.7. As well as the diagonal NNN hopping holds a spin-dependent part $T'_{s,0}$ the linear spin-dependent hopping $T''_{s,0}$ exists too with

$$T''_{s,0} = t''_s \sum_{\langle i,k,j \rangle_{l\alpha\beta}} \left[(1 - \hat{n}_{i\bar{\alpha}}) f_{i\alpha}^\dagger \sigma_{\alpha\beta} f_{j\beta} (1 - \hat{n}_{j\bar{\beta}}) \cdot \mathbf{S}_k + \hat{n}_{i\bar{\alpha}} f_{i\alpha}^\dagger \sigma_{\alpha\beta} f_{j\beta} \hat{n}_{j\bar{\beta}} \cdot \mathbf{S}_k + \text{h.c.} \right] . \quad (2.13)$$

It also contains the vector of Pauli matrices and the spin vector on site k which is also NN site to i and j . But now i and j are linear NNN to each other displayed by $\langle i,k,j \rangle_l$.

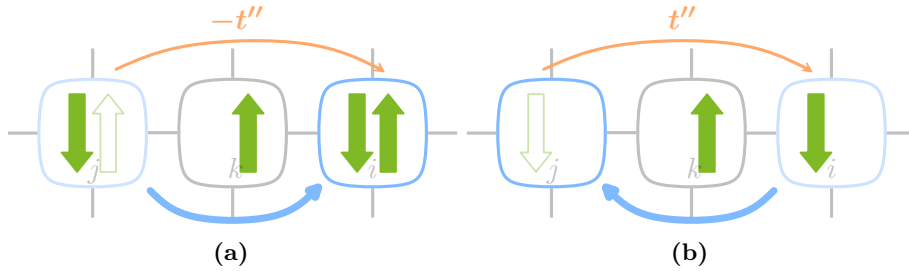


Figure 2.7: Two possible processes for a linear nearest neighbor hopping T''_0 of a DO according to equation (2.12) on a two-dimensional square lattice, illustrated via movements firstly a doubly occupied site in figure 2.7a and secondly an empty site in figure 2.7b..

Carried over to the 2D squared lattice the sites i , j and k lie all on one straight line in the lattice as shown in figure 2.8 where possible process of $T''_{s,0}$ are displayed.

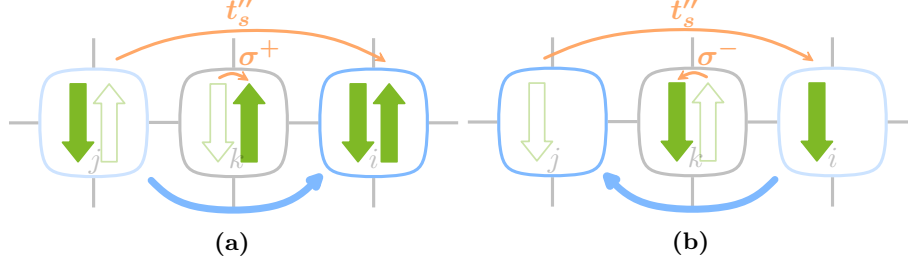


Figure 2.8: Two possible processes out of various spin dependent linear next-nearest neighbor hopping of a DO described by $T''_{s,0}$ in equation (2.13). In figure 2.8a the hopping of a doubly occupied site or in figure 2.8b the hopping of an empty site results in a spin flip on the site k .

So overall the effective Hamiltonian H_{eff} reads as

$$H_{\text{eff}} = T_0 + T'_0 + T'_{s,0} + T''_0 + T''_{s,0} + H_{\text{int}} . \quad (2.14)$$

The strength for all the different hopping amplitudes t_x^x of the various hopping terms in equations (2.10) to (2.13) is related to the simple hopping t_0 in T_0 and changes depending on the relation of W/U [21]. But as mentioned at the beginning of this section the model is only capable of describing the situation for values up to $W/U \approx 0.8$. So all in all we are able to describe the dynamics of one DO in the Hubbard model on a two-dimensional squared lattice in the parameter regime $W/U \leq 0.8$ with the in Hamiltonian described equation (2.14) of an effective t - J model.

2.3 Iterated equations of motion approach

The section 2.1 already gave a brief overview about the methods used to determine the energy gap for single charge excitation and the critical value U_c for which the gap closes. As mentioned above, an analytical solution for the Hubbard model is only possible using the Bethe ansatz in one-dimension and in infinite-dimension, where in infinite-dimension a mean field approach is used. So for finite dimensions greater than one-dimension, a semi-analytical treatment is necessary. In this section we deal with such semi-analytical approach, the iterated equation of motion approach, which will be referred to as the iEoM approach in the following. Mostly in literature, the iEoM approach is applied to calculate the time dependency of an operator $A(t)$. Nevertheless, in this thesis this approach is used to calculate a value for the energy gap for single charge excitation of the system. As the name suggests, the approach is based on an iterative scheme, where with each iteration the number of appearing equations increases steadily. For the purpose of applying the iEoM approach in this thesis this section gives an overview about the iEoM approach. The

questions how to determine the energy gap using the iEoM approach will be addressed later in section 2.4.

Since the iEoM approach dealing with time evolution a short summery of the pictures used for in quantum mechanics to describe time dependencies is given beforehand. There are three equivalent used pictures: The Schrödinger picture, Heisenberg picture and the Dirac picture [33], where the last one is only listed for the sake of completeness and finds no use in this thesis. In the Schrödinger picture the time dependency is contained in the bras $\langle\psi(t)|$ and kets $|\psi(t)\rangle$ and operators are constant in time except they have explicit time dependence. In contrast, the operators in the Heisenberg picture contain the time dependency and the states are constant in time. When A_S denotes an operator in the Schrödinger picture and A_H the corresponding in the Heisenberg picture, the transformation between these two equivalent pictures is made via

$$A_H(t) = U_S^\dagger(t, t_0) A_S U_S(t, t_0) \quad (2.15)$$

with the unitary time evolution operator $U_S(t, t_0)$. In its most general form, the time evolution operator has the following representation

$$U_S(t, t_0) = T_D \exp \left(-i \int_{t_0}^t dt' H_S(t') \right) \quad (2.16)$$

where T_D is the Dyson time ordering operator with the property

$$T_D (A(t_1)B(t_2)) = \begin{cases} A(t_1)B(t_2) & \text{if } t_1 > t_2 \\ B(t_2)A(t_1) & \text{otherwise} \end{cases} \quad (2.17)$$

and $H_S(t')$ indicates an explicit time dependence of the operator. In this thesis we do not make use of the explicit form (2.16). Despite this, the equation describing the time dependence of an operator in the Heisenberg picture is derived from equation (2.15). Leaving us with the Heisenberg equation of motion in its most general form

$$\frac{d}{dt} A_H(t) = i [H_H(t), A_H(t)] + U_S^\dagger(t, t_0) \frac{\partial}{\partial t} A_S(t) U_S(t, t_0) . \quad (2.18)$$

For a time dependence of the operator without explicit occurrence of time t in the Schrödinger picture $A_S(t) = A_S$ the Heisenberg equation of motion reduces to

$$\frac{d}{dt} A_H(t) = i [H_H(t), A_H(t)] =: i \mathcal{L}(A_H(t)) \quad (2.19)$$

whereby for future reference the Liouville superoperator $\mathcal{L}(\cdot) := [H_H(t), \cdot]$ is introduced as a shorthand notation for the commutation with the Hamiltonian $H_H(t)$ of the system. Furthermore, all operators of interest in this thesis are missing an explicit time dependence. Therefore, equation (2.19) is used as a starting point for the following calculations. In the following, all operators in the Heisenberg picture are noted as $A(t)$, where all other operator A without time dependence are operators in the Schrödinger picture.

After this brief excursion regarding the different pictures in quantum mechanics, we now turn to the derivation of the iEoM approach. Starting with an arbitrary operator $A(t)$ in the Heisenberg picture. The operator can be written as an operator expansions

$$A(t) = \sum_i h_i(t) A_i \quad (2.20)$$

consisting of complex prefactors $h_i(t)$ which contain all time dependencies and time independent operators A_i in the Schrödinger picture taken from a certain operator basis $O = \{A_1, \dots, A_n\}$ [18]. The Heisenberg equation of motion (2.19) for the operator (2.20) reads

$$\frac{d}{dt} A(t) = i\mathcal{L}(A(t)) = i \sum_i h_i(t) \mathcal{L}(A_i) \quad (2.21)$$

where $\mathcal{L}(A_i)$ can also be written as a linear combination of other operator A_j in the given Basis O

$$\mathcal{L}(A_i) = \sum_j M_{ji} A_j . \quad (2.22)$$

Combining all previous equations (2.20) to (2.22) and considering that the time dependence is only stored in the prefactors $h_i(t)$, the following equation results

$$\sum_i \frac{d}{dt} (h_i(t)) A_i = i \sum_{ij} M_{ji} h_i(t) A_j. \quad (2.23)$$

A coefficient comparison for an operator in equation (2.23) yields

$$\frac{d}{dt} h_j(t) = i \sum_i M_{ji} h_i(t) . \quad (2.24)$$

Writing all prefactors $h_i(t)$ in a vector $\mathbf{h}(t)$ the relation in equation (2.24) is writable as a matrix vector product

$$\frac{d}{dt} \mathbf{h}(t) = i \mathbf{M} \mathbf{h}(t) . \quad (2.25)$$

The matrix $\mathbf{M}$ consists of the prefactors which arise by applying the Liouville superoperator. Thus, it will be called the Liouville matrix in the following. The equation (2.25) describes the effect of the so called Liouville matrix on the time-dependent prefactors $h_i(t)$ of the operator expansion in equation (2.20). So the time evolution of the operator $A(t)$ is obtained by solving the first order differential equation system in equation (2.25) for $\mathbf{h}(t)$. This can be done of course using either a numerical or analytical approach. In both cases necessary for the complete solution of the differential equations are initial conditions for the operator $A(t=0)$. For the starting point $t=0$ the operator $A(t)$ should be equal to the operator in the Schrödinger picture

$$A(t=0) = A . \quad (2.26)$$

Therefore, the operator A needs to be included in the operator basis O . Presuming the operator A is the first operator A_0 in the operator basis O , the first element in the vector $\mathbf{h}(t)$ is associated with the operators A_S . So the initial condition for $\mathbf{h}(t)$ reads

$$h_i(t=0) = \begin{cases} 1 & | \ i = 0 \\ 0 & | \ i \neq 0 \end{cases} . \quad (2.27)$$

With the iEoM approach we are capable to calculate the evolution in time of an operator. Hence, with this method we can study for example time dependent observables like the local occupation number or calculate time average for an operator as done in Ref. [19].

In this thesis we are not interested in the explicit time evolution of an operator but more in the energy gap of the Mott-Hubbard insulator described by the t - J model in the regime of $0 < J \ll T \ll \Delta$ as mentioned in section 2.1. Hence, we need to find parameters in the iEoM approach that provide insights into the energy values connected to the energy gap of the model. Therefore, in the next section, we consider possible approaches to the solution of the differential equations in equation (2.25) and their applications to determine the energy gap of the model.

2.4 Addressing the solution of the iterated equations of motion approach under consideration of the energy gap

As mentioned above there are two general approaches to solve the differential equation of equation (2.25). The first is a numerical solution and the other one is an analytical solution. Here the two approaches are brief summarized and it is evaluated whether they are suitable for calculating the energy gap of the system.

Numerical solution

In the numerical solution the vector $\mathbf{h}(t)$ is calculated for discrete time steps $t_n = nh$, $n \in \mathbb{N}_0$. To give an estimation for a next step $\mathbf{h}(t_n)$ the previous step t_{n-1} is taken into account. Whereby the initial vector of equation (2.27) serves as the start vector for this process. Well-known methods for this type of solutions are the Runge-Kutta methods [34]. Now the task is to rate the solution regarding its potential to give insights into the energy gap. Since the vector $\mathbf{h}(t_n)$ contains only factors h_i indicating the portion of basis operators A_i in $A(t_n)$ to a given time t_n as shown in equation (2.20), there is at first no clear connection to the energy gap. Therefore, it is not really possible to make a statement concerning the energy gap of the system unless it is possible to find an observable which is directly connected to the energy gap. Thus, this approach to the solution might not be the way to determine the energy gap. At first, we drop this approach, and we turn to an analytical one.

Analytical solution

On the other hand it is also possible to analytically solve the differential equation system in equation (2.25) by a linear transformation into the eigensystem of the Liouville matrix $\mathbf{M}$. Consider that the Liouville matrix $\mathbf{M} \in \mathbb{C}^{n \times n}$ is a diagonalizable matrix so that a linear transformation $\mathbf{Q} \in \mathbb{C}^{n \times n}$ exists which fulfills

$$\mathbf{Q}^{-1}\mathbf{M}\mathbf{Q} = \mathbf{D} \quad (2.28)$$

where the matrix $\mathbf{D} = \mathbf{Diag}(\lambda_1, \dots, \lambda_n)$ is a diagonal matrix with the eigenvalues $\lambda_i \in \mathbb{C}$ of $\mathbf{M}$. Furthermore, each eigenvalue λ_i can be associated with an eigenvector $\mathbf{v}_i \in \mathbb{C}^n$ which satisfies the eigenvalue equation

$$\mathbf{M}\mathbf{v}_i = \lambda_i\mathbf{v}_i. \quad (2.29)$$

In order to determine the eigenvalues of $\mathbf{M}$ it is necessary to compute the zeros of the characteristic polynomial

$$p(\lambda) = \det(\mathbf{M} - \lambda\mathbf{I}) = 0 \quad (2.30)$$

with the identity $\mathbf{I}$ having the same dimension $n \times n$ as $\mathbf{M}$. The zeros of the characteristic polynomial $p(\lambda)$ are the eigenvalues λ_i of $\mathbf{M}$ with the algebraic multiplicity μ which count the number of occurrence as a root of $p(\lambda)$. If the algebraic multiplicity $\mu > 1$ for some eigenvalues of $\mathbf{M}$ we say matrix $\mathbf{M}$ has degenerate eigenvalues and μ corresponding eigenvectors span the subspace of those degenerate eigenvalues. Furthermore, the eigenvectors are assumed to be normalized i.e. $\|\mathbf{v}_i\|_2 = 1$. If we now apply these considerations to the differential equation system of equation (2.25), we can analytically solve the first order differential equation system and in the end we obtain a fundamental set of solutions $\{\mathbf{y}_1(t), \dots, \mathbf{y}_n(t)\}$ with

$$\mathbf{y}_i(t) = e^{i\lambda_i t} \mathbf{v}_i. \quad (2.31)$$

Together with the initial condition in equation (2.27) the solution for $\mathbf{h}(t)$ is a superposition of the fundamental set

$$\mathbf{h}(t) = \sum_{i=1}^n \alpha_i \mathbf{y}_i(t) = \sum_{i=1}^n \alpha_i e^{i\lambda_i t} \mathbf{v}_i \quad (2.32)$$

where the coefficient set α_i ensures that the initial conditions are met.

For this approach, the possibility of gaining insights into the energy gap of the system is also being examined. In contrast to a numerical solution the analytical solution holds more information concerning the system studied. In addition to the vector $\mathbf{h}(t)$ the analytical solution delivers a set of eigenvalues $\{\lambda_i\}$ and eigenvectors $\{\mathbf{v}_i\}$ which can be interpreted in terms of their physical meaning for the system. Here, the eigenvalues are examined first. If they are made out of complex values, it leads to an exponentially diverging contribution in the time evolution of $A(t)$ which is regarded as an unphysical behavior [18, 19]. Therefore, to ensure only oscillatory contributions in $A(t)$, preventing the occurrence of complex eigenvalues λ_i of $\mathbf{M}$ is mandatory. Thus, the Liouville matrix $\mathbf{M}$ should be

either Hermitian with $\mathbf{M}^\dagger = \mathbf{M}$ or symmetric with $\mathbf{M}^T = \mathbf{M}$, since these matrices only have real eigenvalues. Furthermore, considering equation (2.22) the elements in the Liouville matrix $\mathbf{M}$ have the unit of an energy due to the fact that these coefficients occur by computing $\mathcal{L}(A)$. Consequently, the eigenvalues λ_i have the same unit. So the eigenvalues of the Liouville matrix for an operator $A(t)$ sort of unravel the energy areas in which the operator $A(t)$ seem to act on. In addition, the corresponding eigenvectors $\mathbf{v}_i$ hold information about the portion of operators included in the operator basis that are connected to the oscillation with the frequency λ_i .

Now basically the idea is to find a suitable operator $A(t)$ so that the eigenvalues of the related Liouville matrix break down the energy areas connected with the band gap of the system. Before this topic can be addressed, it is necessary to discuss a method for building an appropriated operator basis and thus ensuring a Hermitian Liouville matrix for the iEoM approach. In the next section conditions for obtaining a Hermitian Liouville matrix are considered. Then the consequences for the operator basis are also discussed.

2.5 Obtaining a Hermitian Liouville matrix

As mentioned in section 2.3 it is essential for the iterated equation of motion approach that the Liouville matrix is a Hermitian or symmetric matrix and thus has real eigenvalues. So first we need an expression for a matrix element M_{ij} . A convenient approach is to choose the operator basis O as an orthonormal operator basis with respect to a given scalar product. So the scalar product for two operators $A_i, A_j \in O$ yields

$$(A_i|A_j) = \delta_{ij}. \quad (2.33)$$

Due to this orthonormal relation and equation (2.22) it is possible to calculate the matrix element M_{ij} as the scalar product of an operator A_i with the Liouville operator $\mathcal{L}(\cdot)$ of an operator A_j

$$M_{ij} = (A_i|\mathcal{L}(A_j)). \quad (2.34)$$

Now the task is to specify the scalar product. For finite local Hilbert spaces the scalar product should be the Frobenius scalar product $(A|B)$, which was already proposed in Ref. [18] and applied in Ref. [19, 20]. The Frobenius scalar product can be interpreted as the high-temperature limit $T \rightarrow \infty$ of the thermal expectation value

$$(A|B) = \lim_{T \rightarrow \infty} \langle A^\dagger B \rangle = \lim_{T \rightarrow \infty} \text{Tr}(\rho A^\dagger B) \quad (2.35)$$

in the canonical ensemble. The density matrix operator

$$\rho = \frac{e^{-\beta H}}{\text{Tr}(e^{-\beta H})} \quad (2.36)$$

with the Hamiltonian H changes for a vanishing inverse temperature β to

$$\lim_{\beta \rightarrow 0} \rho = \mathcal{N} \mathbb{1} \quad (2.37)$$

where $\mathcal{N}$ takes care of normalization by

$$\mathcal{N} := \frac{1}{\text{Tr}(\mathbb{1})} = \frac{1}{d} \quad (2.38)$$

with the dimension d . So we are looking at a maximally disordered system where each state is equally likely with the probability of $1/d$. Thus, we obtain the Frobenius scalar product which reads

$$(A|B) = \mathcal{N} \text{Tr} \left(A^\dagger B \right) . \quad (2.39)$$

The next step is to show that with this definition of the scalar product it is possible to create a Hermitian or symmetric Liouville matrix ensuring

$$M_{ij} = M_{ji}^* . \quad (2.40)$$

Starting with the equation (2.34) for the Matrix element the proof is as follows

$$M_{ij} = \underline{(A_i | \mathcal{L}(A_j))} = \mathcal{N} \text{Tr} \left(A_i^\dagger \mathcal{L}(A_j) \right) = \mathcal{N} \text{Tr} \left(A_i^\dagger [H, A_j] \right) \quad (2.41a)$$

$$= \mathcal{N} \text{Tr} \left(A_i^\dagger (H A_j - A_j H) \right) \stackrel{*}{=} \mathcal{N} \text{Tr} \left(A_j \left(A_i^\dagger H - H A_i^\dagger \right) \right) \quad (2.41b)$$

$$= \mathcal{N} \text{Tr} \left(A_j (H A_i - A_i H)^\dagger \right) = \mathcal{N} \text{Tr} \left(A_j \mathcal{L}^\dagger(A_i) \right) \quad (2.41c)$$

$$\stackrel{*}{=} \underline{(\mathcal{L}(A_i) | A_j)} = (A_j | \mathcal{L}(A_i))^* = M_{ji}^* . \quad (2.41d)$$

The steps, denoted with $\stackrel{*}{=}$, mark where the cyclic property of the trace is used. So with the equation (2.41) we can prove that the Liouville matrix is self-adjoint $\mathbf{M} = \mathbf{M}^\dagger$. Moreover with the underlined steps of equation (2.41) and the definition

$$\left(\mathcal{L}^\dagger(A_i) | A_j \right) := \underline{(A_i | \mathcal{L}(A_j))} = \underline{(\mathcal{L}(A_i) | A_j)} \quad (2.42)$$

it follows that the Liouville operator

$$\mathcal{L} = \mathcal{L}^\dagger \quad (2.43)$$

itself is self-adjoint. Hence, it is possible to construct a Hermitian Liouville Matrix with real eigenvalues assuming an operator basis which is orthonormal with respect to the Frobenius scalar product. The next step is to build such an orthonormal operator basis.

2.6 Approaches to determine the operator basis

Now that we are aware of the demands on an operator basis discussed in section 2.5 which leads to a Hermitian Liouville Matrix with real eigenvalues, we take a closer look how to build an orthonormal operator basis meeting this demands. Therefore, we visit different approaches to determine an operator basis $\{A_i\}$ done by former studies concerning an iterated equation of motion approach.

Starting with the so called m -loop approach used in e.g. [35–37]. Basically the idea is to use the Liouville superoperator $\mathcal{L}(\cdot)$ to generate new operators which then are added to the operator basis. The operator basis after each loop m will be denoted with O_m . As a starting point to determine the operator basis O_m for $A(t)$ the operator A_0 is used corresponding to the operator $A(t)$ in the Schrödinger picture. The operator A_0 is inevitably a part of the operator basis, because without it the initial condition $A(t=0) = h_0(t=0)A_0$ mentioned in the section 2.3 cannot be fulfilled. So we start the calculation with the operator basis O_0 only containing $\{A_0\}$. By calculating the Liouville superoperator for all operators in the operator basis $k_m \geq 0$ new operators rise. Therefore, the operator expansion reads

$$\xrightarrow{\mathcal{L}(O_0)} A(t) = \sum_{i=0}^{k_1} h_i(t) A_i \quad (2.44)$$

after the first loop. In the m -loop approach it is necessary to effectively apply the Liouville superoperator $m+1$ times to the operator basis. But operators rising in the last loop for the first time are neglected and only the projection of each onto the operators already contained in the operator basis is kept to achieve a closed differential equation system for the prefactors $h_i(t)$. In general the number of operators in the basis for a m -loop is $f = 1 + \sum_{i=1}^m k_i$ and so the final operator expansion for $A(t)$ results in

$$A(t) = \sum_{i=0}^{f-1} h_i(t) A_i \quad (2.45)$$

with the operator basis $O_m = \{A_0, \dots, A_{f-1}\}$. To obtain the solution for the time dependent coefficient vector $\mathbf{h}(t) = (h_0(t), h_1(t), \dots, h_{f-1}(t))^T$ in this approach it is necessary to determine the matrix elements M_{ij} via a coefficient comparison.

In contrast to the previous considerations about the Frobenius scalar product, the Liouville matrix here is not necessarily a Hermitian matrix. One problem lies in the assignment of new operators after an application of $\mathcal{L}(\cdot)$. This happens since second quantization operators can be written in various forms. Therefore, to emphasize the problem that arise with the m -loop approach, let us consider that e.g. the operator $d_{i,\downarrow}^\dagger$ creating a doubly occupied site at the position i in second quantization is already part of O_m . Furthermore, with the anticommutator for Fermions the operator $d_{i,\downarrow}^\dagger$ can be written as

$$d_{0,\downarrow}^\dagger = f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger f_{i,\uparrow} = f_{i,\downarrow}^\dagger - f_{i,\downarrow}^\dagger f_{i,\uparrow} f_{i,\uparrow}^\dagger. \quad (2.46)$$

So let the right-hand side of equation (2.46) appear after an application of $\mathcal{L}(\cdot)$ in the $m+1$ -loop the assignment to two new operators would be incorrect, because the operator on the left-hand side is already contained in the operator basis. So this assignment would result in a non-Hermitian Liouville matrix. Of course in this example it is not so difficult to distinguish between old and new operators, but for operators containing more monomials this can become a nontrivial task. Furthermore, it is assumed that an arbitrary operator A_i of the operator basis have a form of

$$\tilde{A}_i = \prod_j^n F_{\alpha_j} \quad (2.47)$$

$$A_i = a_i \tilde{A}_i \quad (2.48)$$

with $F_{\alpha_j} \in \{f_{\alpha_j}^\dagger, f_{\alpha_j}\}$ denoting creator or annihilator for a Fermion with a full set of quantum numbers α_j . Altogether an operator A_i consists of a product of n Fermionic operators and a prefactor where the choice of the prefactor a_i is not defined by the m -loop approach. But this choice has a major influence on the appearance of the Liouville matrix e.g. whether the matrix is Hermitian [38]. Basically the m -loop approach without any modification is in general not convenient to determine the operator basis suited for our purpose.

Another idea is to build an orthonormal operator basis beforehand with respect to the Frobenius scalar product described in section 2.5. There, the operators can have a slightly different form as in equation (2.48), where the factors F_{α_j} are now not only creators or annihilators, but instead F_{α_j} are a superposition of them. For example an operator A_i can have the following form

$$A_i = a_i \tilde{A}_i = a_i \left(f_{\alpha_j}^\dagger f_{\alpha_j} - \frac{1}{2} \right) \left(f_{\alpha_k}^\dagger + f_{\alpha_k} \right) \dots \quad (2.49)$$

Now the prefactors a_i are determined by requiring orthonormality so that

$$(A_i | A_j) = a_i a_j^* (\tilde{A} | \tilde{A}) = \delta_{ij} \quad (2.50)$$

is orthonormal. This approach ensures a Hermitian Liouville matrix as shown in equation (2.41). With this approach it is possible to select operators by means of their importance for the time evolution for different parameter regimes. This approach is used e.g. in Ref. [19] by dividing the Liouville operator $\mathcal{L}$ of the Hubbard model into a hopping $\mathcal{L}_0(\cdot) = [H_t, A]$ and an interaction part $\mathcal{L}_{\text{int}}(\cdot) = [H_{\text{int}}, A]$. For a dominating interaction part new operators are determined through $\mathcal{L}_{\text{int}}(\cdot)$ and vice versa for the kinetic hopping part with $\mathcal{L}_0(\cdot)$. To ensure the operators' orthonormality a Gram-Schmidt processes is used before adding them to the operator basis. During the Gram-Schmidt processes, many scalar products are calculated with operators in the form as in equation (2.49). To calculate a scalar product of two arbitrary operators A, B composed of Fermionic operators $\{f_{\alpha_j}^\dagger, f_{\alpha_j}\}$ by the means of

$$(A | B) = \mathcal{N} \text{Tr} \left(A^\dagger B \right) \quad (2.51)$$

many traces of a product of Fermionic operators must be calculated. For beforehand constructed general operators this can be a non-trivial task and is discussed in detail in Ref. [38].

Here, we try to combine these two approaches. So the operator basis is not constructed beforehand, but instead build with a m -loop approach. Since all operators should be orthonormal concerning the Frobenius norm, we thus avoid the problem of ambiguity of the operators. Of course a Gram-Schmidt processes can be used to ensure orthonormality of the new operators to all former operators in the operator basis. But this involves calculations of many elaborate traces especially for high loops. Therefore, this is not a feasible option. To avoid this problem new operator rising in the m -loop approach need to be orthonormal by construction. The aim of the following paragraphs is now to define an operator form to solve this issue.

We start again with scalar product of two operators A and B , but now we presume that they act on separable Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. Therefore, the trace over the complete Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ in the Frobenius norm can be split up according to

$$(A|B) = \mathcal{N}_{\mathcal{H}} \text{Tr}_{\mathcal{H}} \left(A^\dagger B \right) = \mathcal{N}_{\mathcal{H}_A} \text{Tr}_{\mathcal{H}_A} \left(A^\dagger \right) \mathcal{N}_{\mathcal{H}_B} \text{Tr}_{\mathcal{H}_B} \left(B \right) \quad (2.52)$$

where $\text{Tr}_{\mathcal{H}_x}(\cdot)$ refers to the trace over $\mathcal{H}_x$ with the related inverse dimension $\mathcal{N}_{\mathcal{H}_x}$. As a result of dealing with operators consisting of Fermionic operators acting only on a certain site, each operator has a finite and well separable Hilbert space. Hence, it is possible to split the trace into calculations of a scalar product as in equation (2.52) every time. This allows us to make a statement about the required shape of the operators in the operator basis to fulfill the orthonormal condition in equation (2.33).

First we assume that it is possible to find local operators $\hat{\sigma}_n^j$ consisting of a linear combination of Fermionic operators $\{f_{\alpha_j}^\dagger, f_{\alpha_j}\}$ which act all on the same local Hilbert space $\mathcal{H}_d^L$ for a single site j with the dimension d and satisfy the relations

$$(\hat{\sigma}_n^j | \hat{\sigma}_m^j) = \frac{1}{d} \text{Tr}_{\mathcal{H}_d^L} \left((\hat{\sigma}_n^j)^\dagger \hat{\sigma}_m^j \right) = \delta_{nm} \quad (2.53)$$

$$(\mathbb{1}_j | \hat{\sigma}_m^j) = 0 . \quad (2.54)$$

Here $\mathbb{1}_j$ marks the identity for the local Hilbert space $\mathcal{H}_d^L$ of the site j . Hence, the set of these local operators $\{\mathbb{1}_j, \hat{\sigma}_1^j, \dots, \hat{\sigma}_n^j\}$ builds an orthonormal operator basis for the site j we can combine these type of operators for all different sites which yield advantageous operators of the form

$$A_i = \prod_j^n \hat{\mathcal{R}}_j^{A_i} \quad (2.55)$$

where $\hat{\mathcal{R}}_j^{A_i} \in \{\mathbb{1}_j, \hat{\sigma}_1^j, \dots, \hat{\sigma}_n^j\}$ denotes an orthonormal operators for a site j and with the product going over all sites n of the system. So looking one more time on a scalar

product of two operators A and B which possessing now the form of equation (2.55). Therefore, the scalar product reads

$$(A|B) = \mathcal{N} \text{Tr}_{\mathcal{H}} \left(\left(\prod_j^n \hat{\mathcal{R}}_j^A \right)^\dagger \prod_i^n \hat{\mathcal{R}}_i^B \right) \stackrel{(2.52)}{=} \prod_i^n \frac{1}{d} \text{Tr}_{\mathcal{H}_d^L} \left(\left(\hat{\mathcal{R}}_i^A \right)^\dagger \hat{\mathcal{R}}_i^B \right) \quad (2.56)$$

$$\stackrel{(2.53)}{=} \begin{cases} 1 & \text{if } \hat{\mathcal{R}}_i^A = \hat{\mathcal{R}}_i^B \quad \forall i \\ 0 & \text{otherwise} \end{cases} \quad (2.57)$$

where in the first step the trace is divided into the product of all traces over the local Hilbert spaces of each site according to (2.52) and finally the orthonormality relation between two local operators of (2.53) is used. Apparently the scalar product of two operators which are constructed as in equation (2.55) results in either one if all their factors of one site operators $\hat{\mathcal{R}}_i^X$ are identical thus the operators itself are exact the same or zero if already two factors on a site i differ from each other. So the advantage of these operators is that they fulfill the orthonormal relation in equation (2.33) by construction. Henceforth, only factors $\hat{\mathcal{R}}_j^A$ in the product of equation (2.55) which are different from the identity $\mathbb{1}$ on a site are written down. Basically an operator acting on three different sites i, j and k would be noted as

$$A_i = \hat{\mathcal{R}}_i^A \hat{\mathcal{R}}_j^A \hat{\mathcal{R}}_k^A . \quad (2.58)$$

Referring back to the m -loop approach we now have a well-defined operator form and therefore avoid the possible mistakes in the assigning of the operators after a loop since resulting operators have a form like in equation (2.58). Furthermore, by calculating the Liouville superoperator for each operator in the set $\{\hat{o}_1^j, \dots, \hat{o}_n^j\}$ the Liouville operator of an arbitrary operator in the form of equation (2.58) can be calculated easily like the following example shows with the operator of equation (2.58)

$$\mathcal{L}(A_i) = \left[\hat{o}_m^i \hat{o}_n^j \hat{o}_o^k, H \right] = \left[\hat{o}_m^i, H \right] \hat{o}_n^j \hat{o}_o^k + \hat{o}_m^i \left[\hat{o}_n^j, H \right] \hat{o}_o^k + \hat{o}_m^i \hat{o}_n^j \left[\hat{o}_o^k, H \right] \quad (2.59)$$

$$= \mathcal{L}(\hat{o}_m^i) \hat{o}_n^j \hat{o}_o^k + \hat{o}_m^i \mathcal{L}(\hat{o}_n^j) \hat{o}_o^k + \hat{o}_m^i \hat{o}_n^j \mathcal{L}(\hat{o}_o^k) . \quad (2.60)$$

So the Liouville superoperator breaks down by applying a commutator identity into many Liouville superoperators of local operators. Although the procedure is fairly straightforward, an annotation must be made. In the case that a Liouville superoperator $\mathcal{L}(\cdot)$ yields local operators on other sites which are already present in the whole operator, they need to be simplified. For example let $\mathcal{L}(\hat{o}_m^i)$ has a part with an operator acting on the site k

$$\mathcal{L}(\hat{o}_m^i) = a \hat{o}_n^i \hat{o}_m^k + \dots \quad (2.61)$$

with an arbitrary prefactor a . Consequently, the underlined term of equation (2.60) has two operators acting on the same site k

$$\mathcal{L}(\hat{o}_m^i) \hat{o}_n^j \hat{o}_o^k = a \hat{o}_n^i \hat{o}_m^k \hat{o}_n^j \hat{o}_o^k + \dots . \quad (2.62)$$

Since these operators, when acting on different sites and thus acting on different subspace of the Hilbert space, (anti-)commute with each other pending on whether their properties are Fermionic or Bosonic. As a result, the operator of equation (2.62) can be written so that the two local operators acting on the same site are side by side, possibly resulting in a change in the overall sign of the operator

$$a\hat{o}_n^i \hat{o}_m^k \hat{o}_n^j \hat{o}_o^k = (-)a\hat{o}_n^i \hat{o}_n^j \hat{o}_m^k \hat{o}_o^k . \quad (2.63)$$

Furthermore, products of two local operators acting on the same site can be written as a superposition of the orthonormal operator basis for a single site $\{\mathbb{1}_k, \hat{o}_1^k, \dots, \hat{o}_n^k\}$

$$\hat{o}_m^k \hat{o}_o^k = b_0 \mathbb{1}_k + \sum_x b_x \hat{o}_x^k \quad (2.64)$$

with arbitrary prefactor b_x . So after inserting equation (2.64) into equation (2.63) only the sum of operators in form of equation (2.55) remains which all fulfill the relation of equation (2.57). Therefore, the Liouville superoperator $\mathcal{L}(\cdot)$ of the operator A_i possesses the following form

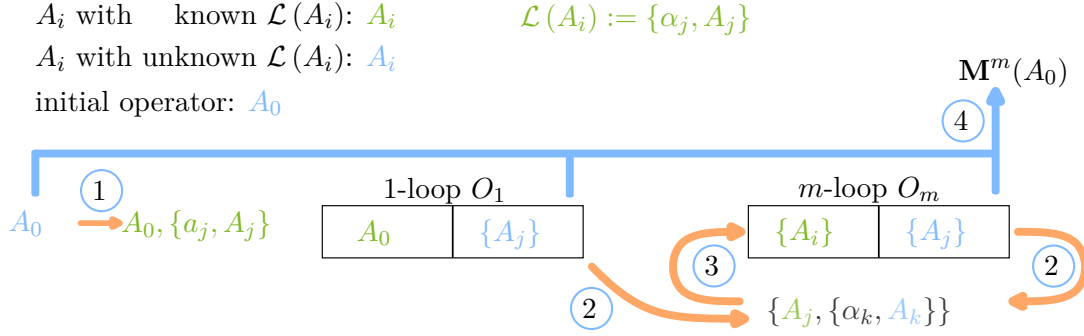
$$\mathcal{L}(A_i) = \underbrace{(-)ab_0}_{\alpha_j} \underbrace{\hat{o}_n^i \hat{o}_n^j}_{A_j} + \sum_x \underbrace{(-)b_x a}_{\alpha_j} \underbrace{\hat{o}_n^i \hat{o}_n^j \hat{o}_x^k}_{A_j} + \dots = \sum_j \alpha_j A_j . \quad (2.65)$$

where all factor which occur during all steps (2.62)-(2.64) are merged into one prefactor α_j for the new operator A_j . Referring back to equation (2.34), it is obvious that the prefactors α_j corresponds to the matrix elements

$$M_{ji} = (A_j | \mathcal{L}(A_i)) = \alpha_j \quad (2.66)$$

of the Liouville matrix. Another important aspect in order to ensure the correct sign of the matrix elements is to order all local operators of an entire operator A_i towards a certain rule e.g. in one dimension in ascending order corresponding to the sites.

In summary, to calculate the Liouville superoperator $\mathcal{L}(\cdot)$ of an operator A_i these steps are followed. First, insert for each local operator $\hat{o}_n^i$ in A_i the corresponding precalculated $\mathcal{L}(\hat{o}_n^i)$ as shown in equation (2.62). Then sort in the new operators all local operators towards the predefined rule, bearing in mind that those commutations can lead to a change in the sign. After that, if two local operators act on the same site, they are simplified with the predefined rules as in equation (2.64). The result is a sum of operator A_j with prefactors α_j . In the m -loop approach the operators then are added to the operator basis if they occur the first time. Now that we have discussed all the steps to determine an orthonormal operator basis for the iterated equation of motion approach in this thesis, figure 2.9 shows concludingly a scheme of the m -loop approach with unambiguous and orthonormal operators A_i to calculate a Hermitian Liouville matrix $\mathbf{M}^m$ of the m -th loop.



- ① calculate $\mathcal{L}(.)$ for initial operator A_0 in OB set new operators with $\mathcal{L}(.)$
- ② calculate for each $\{A_j\}$ in OB $\mathcal{L}(.)$ and so generate new operators A_k
- ③ Add new operators $\{A_k\}$ to $\{A_j\}$ in OB if $A_k \notin \text{OB}$ and add $\{A_j\}$ to $\{A_i\}$
- ④ calculate for each $\{A_j\}$ in OB $\mathcal{L}(.)$ and build Liouville matrix with all α_i

Figure 2.9: Scheme of the operator basis expansion as it is done in the m -loop approach with the unambiguous and orthonormal operators A_i . It is possible to determine the operator basis O_m together with the corresponding Liouville matrix $\mathbf{M}^m$ in the m -th loop for the iEoM approach by following the simple steps 1-4. Whereby steps 2-3 are repeated until the desired number of loops m is reached.

3 Methods

With this chapter all tools will be provided to use the m -loop approach displayed in figure 2.9 to determine an orthonormal operator basis O_m for the iEoM approach and build the corresponding Liouville matrix $\mathbf{M}^m$ for an operator $A(t)$ and finally determine the energy gap for single charge excitation of the given Hamiltonian in equation (2.14). By combining all aspects of the former chapter, the first aspect we have to address is the choice of the operator $A(t)$ providing insides in the energy gap for single charge excitation of the system at half-filling. Then we have to tackle the choice of the local operators $\hat{o}_n^i$ so that they form an orthonormal set on a local i relative to the Frobenius scalar product. Furthermore, two different implementations of the Frobenius scalar product are discussed which lead to two different sets of local operators and some restrictions regarding the Liouville operator. Moreover, one of the implementations has an advantage so that the algorithm discussed at the end of section 2.6 used to determine new operators can be adjusted. Then another representation, the momentum space representation, for the operators A_i is introduced which yields certain advantages over the real space representation used so far. At that point the Lanczos algorithm is presented as a method to study extreme eigenvalues of large matrices. Since large Liouville matrices are unavoidable for whichever operator representation in higher loops, this method is very valuable for this thesis. Closing this chapter, a detailed procedure for calculating the energy gap is given and a specific form is defined in which the results are presented in the next chapter.

3.1 Considerations for the initial operator

So we are looking for an operator that can be assigned to resolve a specified energy area of the given system. For the considered system at half-filling as described in section 2.1 the energy gap Δ for single charge excitation is the desirable parameter to be determined. Hence, we are interested in the distance between LHB and UHB as shown in figure 2.2. With the iEoM approach providing a method to resolve the energy range of an operator $A(t)$ if a Hermitian Liouville matrix is used, it appears convenient to consider the time evolution of an operator inducing a single charge excitation for this purpose. Here at first only an excitation as a result of removing one electron from the half-filled case is treated. The operator for such a process is for example $h_{i\sigma}^\dagger = f_{i\sigma}(1 - \hat{n}_{i\bar{\sigma}})$ which creates a single charge excitation in the form of a hole by removing an electron with spin σ on a single occupied site i . This process correspond to an excitation in the lower Hubbard band. Of course, an operator $d_{i\sigma}^\dagger = f_{i\sigma}^\dagger \hat{n}_{i\bar{\sigma}}$ creating a doubly occupied site by adding an electron with spin σ on a single occupied site i can be chosen instead of creator of a hole.

This process describes an excitation in the upper Hubbard band. Due to particle-hole symmetry it is sufficient to treat only one type of single charge excitation.

The spin σ has no influence, because the system does not prefer certain spin orientations. Thus, for $h_{i\sigma}^\dagger(t)$ the spectrum of eigenvalues $\Lambda(\lambda_i) = \{\lambda_{\min}, \dots, \lambda_{\max}\}$ for the corresponding Liouville matrix lie in the range of the energy spectrum of the LHB, so the idea. Therefore, the energy gap Δ in this picture is $\Delta = \lambda_{\min}(\text{LHB}) + \lambda_{\min}(\text{UHB}) = 2\lambda_{\min}(\text{LHB})$ due to the particle-hole symmetry.

A distinction regarding the size of the used operator basis O in the iEoM approach must be made. Since in iEoM approach, the Liouville matrix for $h_{i\sigma}^\dagger(t)$ is only determined for an operator basis O_m which is built with the m -loops approach, the result is only an approximation for $h_{i\sigma}^\dagger(t)$ and higher m leads to an improved accuracy. As a result, the lowest eigenvalue $\lambda_{\min}^m$ also depends on m and so only yields an estimation for the energy gap Δ^m of the system. Due to the fact that the spectrum of the eigenvalues $\Lambda(\lambda_i^m)$ lays always inside the band and the lowest eigenvalues $\lambda_{\min}^m$ only approaches the real bound of the band with each loop m , $2\lambda_{\min}^m$ serves as an upper bound for the true energy gap Δ and we expect a behavior as shown in figure 3.1 for increasing m .

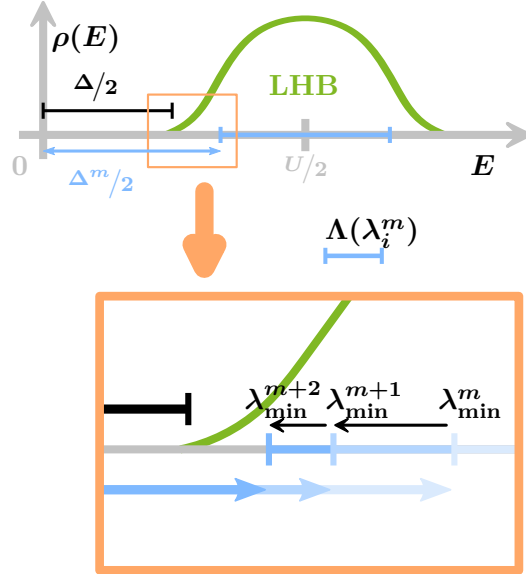


Figure 3.1: Scheme of the behavior of the spectrum of the eigenvalues $\Lambda(\lambda_i^m)$ for the Liouville matrix in an iEoM m -loop approach. Where the initial operator $h_{i\sigma}^\dagger$ induces a single charge excitation in the lower Hubbard Band LHB in form of a hole. The calculated energy gap for charge excitation Δ^m approaches for increasing m the true energy gap Δ as an upper bound. In the language of one-particle green's function as shown in figure 2.2 processes in the LHB are of course mirrored along the vertical axis [39].

3.2 The local basis choices for iterated equation of motion approach

So now that the initial operator in form of a creator of a hole $h_{i\sigma}^\dagger$ is selected we can turn to the issue of choosing a local orthonormal operator basis. Thereby the choice of the local Hilbert spaces $\mathcal{H}_d^L$ with the dimension d has an impact on the local operator basis so its choice is crucial. One option is to choose a four-dimensional local Hilbert space $\mathcal{H}_4^L$ without any restrictions to the spin configurations so that all four states for a single site $|\rangle, |\uparrow\rangle, |\downarrow\rangle$ and $|\uparrow\downarrow\rangle$ are allowed as done in previous works where a fermionic systems is examined with the iEoM approach [19]. Here it should be noted that with this choice of the local Hilbert space, it is not possible to incorporate the half-filling state of the whole system into the iEoM approach. The proof for a Hermitian Liouville matrix of equation (2.41) is not possible if states are weighted according to a density matrix ρ . As a result, all four states are equally weighted in the local Hilbert space, which is an argument against this specific choice. Nevertheless, the $\mathcal{H}_4^L$ case is considered here. Another option is a two-dimensional local Hilbert space $\mathcal{H}_2^L$ with respect to the strict half filling. Then the only allowed spin configurations are $|\uparrow\rangle$ and $|\downarrow\rangle$ in the $\mathcal{H}_2^L$ case. In the following the two possible choices are examined towards their influence on the local orthonormal operator basis starting with the four-dimensional local Hilbert space $\mathcal{H}_4^L$.

Four-dimensional local Hilbert space $\mathcal{H}_4^L$

Since the local Hilbert space consists of four different states with the spin configurations $|\rangle, |\uparrow\rangle, |\downarrow\rangle, |\uparrow\downarrow\rangle$ we need sixteen local operators $\hat{o}_n^i$ to describe all possible changes of the local states. The table 3.1 contains the first ansatz for the operator basis. Since the operator are neither orthogonal nor normalized, they are referred as $\tilde{o}_n^i$ and chosen such that the transition element is $\langle \cdot | \tilde{o}_n^i | \cdot \rangle = 1$.

Table 3.1: All local operators $\tilde{o}_n^i$ which have an transition element $\langle \cdot | \tilde{o}_n^i | \cdot \rangle = 1$ are listed. For the $\mathcal{H}_4^L$ case these operators form an operators basis for a single site i . Whereas the orthonormality of the operators $\tilde{o}_n^i$ with respect to the Frobenius scalar product is not guaranteed at first. Operators that violate the required orthogonality are marked in red.

	$ \rangle$	$ \uparrow\rangle$	$ \downarrow\rangle$	$ \uparrow\downarrow\rangle$
$\langle $	$\mathbb{1}$	$f_{i,\uparrow}$	$f_{i,\downarrow}$	$f_{i,\downarrow}f_{i,\uparrow}$
$\langle \uparrow $	$f_{i,\uparrow}^\dagger$	$\hat{n}_{i,\uparrow}$	$\sigma_i^+ = f_{i,\uparrow}^\dagger f_{i,\downarrow}$	$d_{i,\downarrow} = f_{i,\downarrow} f_{i,\uparrow}^\dagger f_{i,\uparrow}$
$\langle \downarrow $	$f_{i,\downarrow}^\dagger$	$\sigma_i^- = f_{i,\downarrow}^\dagger f_{i,\uparrow}$	$\hat{n}_{i,\downarrow}$	$d_{i,\downarrow} = f_{i,\downarrow} f_{i,\uparrow}^\dagger f_{i,\uparrow}$
$\langle \uparrow\downarrow $	$f_{\downarrow}^\dagger f_{\uparrow}^\dagger$	$d_{\downarrow}^\dagger = f_{\downarrow}^\dagger f_{\uparrow}^\dagger f_{\uparrow}$	$d_{i,\uparrow}^\dagger = f_{i,\uparrow}^\dagger f_{i,\downarrow}^\dagger f_{i,\downarrow}$	$\hat{n}_{i,\downarrow} \hat{n}_{i,\uparrow}$

Some local operators in table 3.1 marked in red not meet the orthogonality conditions of equation (2.53) for the local orthonormal operator basis. Furthermore, all operators of table 3.1 except $\mathbb{1}$ are not normalized and most important the initial operator $h_{i\sigma}^\dagger$ is not yet part of the local operator basis, but this happens naturally in the process by satisfying the demands on a local orthonormal operator basis. Here are two examples for operators

of table 3.1 violate both orthogonality and normality. This is corrected in the following leaving only local operators $\hat{o}_n^i$ that are completely orthonormal.

$$\text{operator: } \hat{n}_{i,\uparrow} \quad \text{orthogonality: } (\mathbb{1}|\hat{n}_{i,\uparrow}) = \frac{1}{4} \text{Tr}_{\mathcal{H}_4^L}(\hat{n}_{i,\uparrow}) = \frac{1}{2} \neq 0 \quad (3.1a)$$

$$\hat{n}_{i,\uparrow} \Rightarrow \hat{n}_{i,\uparrow} - \frac{1}{2} \quad (3.1b)$$

$$\text{normality: } (\hat{n}_{i,\uparrow} - \frac{1}{2}|\hat{n}_{i,\uparrow} - \frac{1}{2}) = \frac{1}{4} \neq 1 \quad (3.1c)$$

$$\Rightarrow \hat{o}_n^i = 2 \left(\hat{n}_{i,\uparrow} - \frac{1}{2} \right) \quad (3.1d)$$

$$\text{operator: } f_{i,\uparrow}^\dagger \quad \text{orthogonality: } (f_{i,\uparrow}^\dagger|d_{i,\uparrow}^\dagger) \stackrel{(2.6)}{=} (d_{i,\uparrow}^\dagger + h_{i,\uparrow}^\dagger|d_{i,\uparrow}^\dagger) \neq 0 \quad (3.2a)$$

$$f_{i,\uparrow}^\dagger \Rightarrow f_{i,\uparrow}^\dagger - d_{i,\uparrow}^\dagger = h_{i,\uparrow}^\dagger \quad (3.2b)$$

$$\text{normality: } (h_{i,\uparrow}^\dagger|h_{i,\uparrow}^\dagger) = \frac{1}{4} \neq 1 \quad (3.2c)$$

$$\Rightarrow \hat{o}_n^i = 2h_{i,\uparrow}^\dagger \quad (3.2d)$$

After checking, the orthonormality for all operators of table 3.1, the local orthonormal operator basis reads as in table 3.2. To improve readability, the operators are used here in the non-normalized form! Of course, the normalization factor N of a non-normalized local operator $\hat{o}_n^i$ can be simply determined by means of

$$N = \sqrt{\frac{1}{(\hat{o}_n^i|\hat{o}_n^i)}} = \sqrt{\frac{d}{\text{Tr}_{\mathcal{H}_d^L}((\hat{o}_n^i)^\dagger \hat{o}_n^i)}}. \quad (3.3)$$

Table 3.2: All local operators $\hat{o}_n^i$ which in the $\mathcal{H}_4^L$ case form an orthonormal operators basis with respect to the Frobenius scalar product for a single site i . For readability reasons, the operators $\hat{o}_n^i$ are presented without their normalization factor and is determined by equation (3.3).

$\mathbb{1}$	$n_i^u = \left(n_{i,\downarrow} - \frac{1}{2}\right) \left(n_{i,\uparrow} - \frac{1}{2}\right)$	$\sigma_i^+ = f_{i,\uparrow}^\dagger f_{i,\downarrow}$	$f_{i,\downarrow} f_{i,\uparrow}$
$\tilde{n}_{i,\downarrow} = \left(n_{i,\downarrow} - \frac{1}{2}\right)$	$\tilde{n}_{i,\uparrow} = \left(n_{i,\uparrow} - \frac{1}{2}\right)$	$\sigma_i^- = f_{i,\downarrow}^\dagger f_{i,\uparrow}$	$f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger$
$d_{i,\downarrow}^\dagger = f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger f_{i,\uparrow}$	$d_{i,\uparrow}^\dagger = f_{i,\uparrow}^\dagger f_{i,\downarrow}^\dagger f_{i,\downarrow}$	$h_{i,\downarrow}^\dagger = f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger f_{i,\uparrow}$	$h_{i,\uparrow}^\dagger = f_{i,\uparrow}^\dagger f_{i,\downarrow}^\dagger f_{i,\downarrow}$
$d_{i,\downarrow} = f_{i,\downarrow} f_{i,\uparrow} f_{i,\uparrow}^\dagger$	$d_{i,\uparrow} = f_{i,\uparrow} f_{i,\downarrow} f_{i,\downarrow}^\dagger$	$h_{i,\downarrow} = f_{i,\downarrow} f_{i,\uparrow} f_{i,\uparrow}^\dagger$	$h_{i,\uparrow} = f_{i,\uparrow} f_{i,\downarrow} f_{i,\downarrow}^\dagger$

Now we only need to calculate the Liouville operator for all local operators $\hat{o}_n^i$ in table 3.2 and determine the result of the product if two local operators of table 3.2 act on the same site. Only an example for operator $h_{i,\uparrow}^\dagger$ will be shown here and the other results are listed in the appendix A. Furthermore in the example the Hamiltonian for the Liouville operator

consists only of the simple DO NN-hopping T_0 (2.7b) on a one-dimensional chain and the interaction part H_{int} (2.3c). Again the normalization factor N is omitted.

$$\text{Liouville operator: } \mathcal{L}(h_{i,\uparrow}^\dagger) = [T_0, h_{i,\uparrow}^\dagger] + [H_{\text{int}}, h_{i,\uparrow}^\dagger] \quad (3.4a)$$

$$[H_{\text{int}}, h_{i,\uparrow}^\dagger] = \frac{U}{2} h_{i,\uparrow}^\dagger \quad (3.4b)$$

$$[T_0, h_{i,\downarrow}^\dagger] = t_0 \left(-\underline{f_{i,\downarrow} f_{i,\uparrow}} d_{i\pm 1,\downarrow}^\dagger - \sigma_i^- h_{i\pm 1,\uparrow}^\dagger + \tilde{n}_{i,\downarrow} h_{i\pm 1,\uparrow}^\dagger - \frac{1}{2} h_{i\pm 1,\uparrow}^\dagger \right) \quad (3.4c)$$

simplification rules:

$$h_{i,\uparrow}^\dagger h_{i,\uparrow} = n_i^u - \frac{1}{2} \left(n_{i,\uparrow} - \frac{1}{2} \right) - \frac{1}{2} \left(n_{i,\downarrow} - \frac{1}{2} \right) + \frac{1}{4} \quad h_{i,\uparrow}^\dagger d_{i,\downarrow} = -f_{i,\downarrow} f_{i,\uparrow} \quad (3.5a)$$

$$h_{i,\uparrow}^\dagger \left(n_{i,\uparrow} - \frac{1}{2} \right) = \frac{1}{2} h_{i,\uparrow}^\dagger \quad h_{i,\uparrow}^\dagger n_i^u = -\frac{1}{4} h_{i,\uparrow}^\dagger \quad (3.5b)$$

$$h_{i,\uparrow}^\dagger \tilde{n}_{i,\downarrow} = -\frac{1}{2} h_{i,\uparrow}^\dagger \quad h_{i,\uparrow}^\dagger \sigma_i^+ = h_{i,\downarrow}^\dagger \quad (3.5c)$$

Combining all these aspects we are able to calculate the Liouville matrix with the m -loop approach described in section 2.6 and furthermore determine its eigenvalues. Now that we are capable of building the Liouville matrix for the local operator basis in the $\mathcal{H}_4^L$ case we turn towards the local orthonormal operator basis for the $\mathcal{H}_2^L$ case.

Two-dimensional local Hilbert space $\mathcal{H}_2^L$

To identify the operators which are part of the orthonormal operator basis for the two-dimensional local Hilbert space $\mathcal{H}_2^L$, we resort to the already orthonormal local operators $\hat{o}_n^i$ of the $\mathcal{H}_4^L$ case from table 3.2. Therefore the local operators of table 3.2 are categorized in different groups $\mathcal{Q}_{xy}^i$ where x and y denote the number of DOs after and before application of the operator on a site i . There are four different groups since on a local site there can be either one or zero DOs. In table 3.3 the operators are listed in their respective group, though some operators appear due to their ambiguity in more than one group simultaneously. It is necessary for each local operator in the two-dimensional Hilbert space that a clear classification in these different group exists. This is because only operators belonging to the groups $\mathcal{Q}_{00}^i$ and $\mathcal{Q}_{10}^i$ have an effect on half-filling whereas operators in $\mathcal{Q}_{0,1}^i$ and $\mathcal{Q}_{1,1}^i$ vanish for half-filling. Of course, the identity is an exception regarding this classification. So the operators $n_i^u, \tilde{n}_{i,\uparrow}, \tilde{n}_{i,\downarrow}$ have a part in $\mathcal{Q}_{00}^i$ as well as in $\mathcal{Q}_{11}^i$. We are only interested in the $\mathcal{Q}_{00}^i$ part. For n_i^u it is quite obvious that

$$n_i^u = \begin{cases} \frac{1}{4} \mathbb{1} & \text{if } n_i^u \in \mathcal{Q}_{11}^i \\ -\frac{1}{4} \mathbb{1} & \text{if } n_i^u \in \mathcal{Q}_{00}^i \end{cases} \quad (3.6)$$

Table 3.3: The local operators $\hat{o}_n^i$ from the $\mathcal{H}_4^L$ case, sorted into four different groups $\mathcal{Q}_{xy}^i$, where x indicates the number of DOs after and y before application. Due to ambiguity, some operators appear in more than one group.

$\mathcal{Q}_{00}^i$:	$\mathbb{1}$	n_i^u	$\tilde{n}_{i,\uparrow}$	$\tilde{n}_{i,\downarrow}$	σ_i^+	σ_i^-
$\mathcal{Q}_{10}^i$:	$d_{i,\downarrow}^\dagger$	$h_{i,\downarrow}^\dagger$	$d_{i,\uparrow}^\dagger$	$h_{i,\uparrow}^\dagger$		
$\mathcal{Q}_{01}^i$:	$d_{i,\downarrow}$	$d_{i,\uparrow}$	$h_{i,\downarrow}$	$h_{i,\uparrow}$		
$\mathcal{Q}_{11}^i$:	$\mathbb{1}$	n_i^u	$\tilde{n}_{i,\uparrow}$	$\tilde{n}_{i,\downarrow}$	$f_{i,\downarrow}f_{i,\uparrow}$	$f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger$

since this is the operator in the interaction part of the Hamiltonian in equation (2.3). For the other two operator $\tilde{n}_{i,\uparrow}$ and $\tilde{n}_{i,\downarrow}$ we express them as a linear combination of two new operators

$$\bar{n}_i = n_{i,\uparrow} + n_{i,\downarrow} - \mathbb{1} \quad \sigma_i^z = n_{i,\uparrow} - n_{i,\downarrow} \quad (3.7)$$

where $\bar{n}_i$ measures the deviation towards half-filling and σ_i^z measures the spin orientation regarding the axis of quantization. With these operators the old operators read

$$\tilde{n}_{i,\uparrow} = \frac{1}{2} (\bar{n}_i + \sigma_i^z) \quad \tilde{n}_{i,\downarrow} = \frac{1}{2} (\bar{n}_i - \sigma_i^z) . \quad (3.8)$$

The new operators have the advantage that they can be uniquely assigned to a group. The operator $\bar{n}_i$ only gives a non-zero result when applied to a site i with a DO and is therefore a part of $\mathcal{Q}_{11}^i$. For the operator σ^z the opposite is true and so $\sigma^z \in \mathcal{Q}_{00}^i$. As a result the operator basis for the two-dimensional local Hilbert space is listed in table 3.4 where the normalization factor N is left out to increase the readability. The normalization factor can be calculated again via equation (3.3). Whereby the Frobenius norm is for the two dimension Hilbert space. For example in equation (3.9b) the normalization factor of $h_\downarrow$ changes compared to the previously for the $\mathcal{H}_4^L$ case in equation (3.2d) calculated factor.

$$\text{operator: } h_{i,\uparrow}^\dagger \quad \text{normality: } (h_\downarrow^\dagger | h_\downarrow^\dagger) = \frac{1}{2} \neq 1 \quad (3.9a)$$

$$\Rightarrow \tilde{f}_i = \sqrt{2} h_\downarrow^\dagger \quad (3.9b)$$

Furthermore, the two-dimensional local Hilbert space has also some restrictions regarding

Table 3.4: All local operators $\hat{o}_n^i$ which in the $\mathcal{H}_2^L$ case form an orthonormal operators basis with respect to the Frobenius scalar product for a single site i . Normalization is omitted here.

$\mathbb{1}$	σ^z	σ^+	σ^-
$d_\downarrow^\dagger$	$h_\downarrow^\dagger$	$d_\uparrow^\dagger$	$h_\uparrow^\dagger$

the Liouville operators and simplification rules of operators in the new orthonormal operator basis. Operators in the operator base for the iEoM approach which partly consist of local operators in the groups $\mathcal{Q}_{11}^i$ or $\mathcal{Q}_{01}^i$ have a Frobenius norm with itself equals zero

and therefore for those operators every matrix element is $M_{ij} = 0$. For example let us consider an operator $A = h_{i,\uparrow}^\dagger \sigma_j^+ \bar{n}_k$. When the Frobenius norm with itself is calculated

$$(A|A) = \mathcal{N} \text{Tr} \left(\left(h_{i,\uparrow}^\dagger \sigma_j^+ \bar{n}_k \right)^\dagger d_{i,\uparrow}^\dagger \sigma_j^+ \bar{n}_k \right) = \mathcal{N} \text{Tr} \left(\bar{n}_k \sigma_j^- h_{i,\uparrow} h_{i,\uparrow}^\dagger \sigma_j^+ \bar{n}_k \right) \quad (3.10)$$

$$\stackrel{(2.52)}{=} \frac{1}{8} \text{Tr}_{\mathcal{H}_2^L} \left(h_{i,\uparrow} h_{i,\uparrow}^\dagger \right) \text{Tr}_{\mathcal{H}_2^L} \left(\sigma_j^- \sigma_j^+ \right) \underline{\text{Tr}_{\mathcal{H}_2^L} \left(\bar{n}_k \bar{n}_k \right)} = 0 \quad (3.11)$$

the result is zero. The reason is the underlined trace with the operator $\bar{n}_k \in \mathcal{Q}_{11}^i$ since $\bar{n}_k$ applied on a half-filled state is always zero as examined before. Consequently, operators in $\mathcal{Q}_{11}^i$ and $\mathcal{Q}_{01}^i$ cannot be a part of the operator basis for the iEoM approach. So far in the used m -loop approach only the Liouville operator is responsible for new operators. But now with condition above, parts of the Liouville operators of some local operators need to be neglected. For example $\mathcal{L} \left(d_{i,\downarrow}^\dagger \right)$ in equation (3.4c) the underlined operator $f_{i,\downarrow} f_{i,\uparrow}$ is part of $\mathcal{Q}_{1,1}^i$ and therefore the new operators $f_{i,\downarrow} f_{i,\uparrow} h_{i\pm 1,\uparrow}^\dagger$ have no effect when using the two-dimensional local Hilbert space. Furthermore, all Liouville operators in appendix A produce for operators that are not part of the group $\mathcal{Q}_{1,0}^i$ new operators terms with partly local operators belonging to prohibited groups. Of course, these new operators also cannot be a part of the operator basis. In contrast, make the same statement about operators that rise from these neglected operators in the next loop is not possible without further consideration. Since in the first place, with all simplification rules in mind, it is not clear why a Liouville operator for a forbidden operator cannot produce allowed operator terms. Therefore, we start the considerations with an operator Q partly consisting of local operators which are part of $\mathcal{Q}_{11}^i$ or $\mathcal{Q}_{01}^i$. Furthermore, we introduce the state of half-filling $|\text{HF}\rangle$ where each site in the system is only occupied with one electron in the state spin up or spin down. Applying the operator Q on $|\text{HF}\rangle$ in the Schrödinger picture the result

$$Q |\text{HF}\rangle = 0 \quad (3.12)$$

is trivial. The next step is to apply the Liouville operator to the state of half-filling

$$\mathcal{L}(Q) |\text{HF}\rangle = [H, Q] |\text{HF}\rangle = HQ - QH |\text{HF}\rangle = 0 \quad (3.13)$$

where equation (3.12) and the fact that the Hamiltonian only contributions, if at least one DO is in the system, are used to show that also the Liouville operator is equal to zero when applied to $|\text{HF}\rangle$. Consequently, all operators partly consisting of local operators that occur during a loop can be taken form the operator basis for an iEoM approach that uses a Frobenius norm assuming a two-dimensional local Hilbert space. This fact allows some modifications to the calculation of new operators for the operator basis as well as the representation of those operators.

3.3 Modifications to operator representation for the two-dimensional local Hilbert space

Here we propose a new representation of the operators and show how that simplifies the process of a loop to determine new basis operators compared to the four-dimensional local Hilbert space in the iEoM approach. As already indicated, the operators for the two-dimensional local Hilbert space consist only of local operators from the introduced groups $\mathcal{Q}_{10}^i$ and $\mathcal{Q}_{00}^i$. The group $\mathcal{Q}_{10}^i$ consists of all operators creating a DO on a site $d_{\downarrow}^{\dagger}$, $d_{\uparrow}^{\dagger}$, $h_{\downarrow}^{\dagger}$ and $h_{\uparrow}^{\dagger}$ and for the group $\mathcal{Q}_{00}^i$ these are spin operators on a site σ^z , σ^- , σ^+ and the unitary $\mathbb{1}$.

The Liouville operators applied to operators from the group $\mathcal{Q}_{00}^i$ do not have a contribution since they produce only operators partly consisting of local operators from the prohibited groups $\mathcal{Q}_{11}^i$ or $\mathcal{Q}_{01}^i$ therefore it follows that

$$\mathcal{L}(\mathcal{Q}_{0,0}^i) = 0. \quad (3.14)$$

With this observation we can completely neglect terms where the Liouville operator is applied to a local operator $\mathcal{L}(\hat{o}_n^i)$ with $\hat{o}_n^i \in \mathcal{Q}_{0,0}^i$ when calculating the Liouville operator as described in section 2.6. Here, a short example for an operator $A = \mathcal{Q}_{10}^i \mathcal{Q}_{00}^j \mathcal{Q}_{00}^k$ is given

$$\mathcal{L}(A) = \mathcal{L}(\mathcal{Q}_{10}^i \mathcal{Q}_{00}^j \mathcal{Q}_{00}^k) \quad (3.15)$$

$$\stackrel{(2.60)}{=} \mathcal{L}(\mathcal{Q}_{10}^i) \mathcal{Q}_{00}^j \mathcal{Q}_{00}^k + \underbrace{\mathcal{Q}_{10}^i \mathcal{L}(\mathcal{Q}_{00}^j) \mathcal{Q}_{00}^k}_{=0} + \underbrace{\mathcal{Q}_{10}^i \mathcal{Q}_{00}^j \mathcal{L}(\mathcal{Q}_{00}^k)}_{=0} \quad (3.16)$$

$$\stackrel{(3.14)}{=} \mathcal{L}(\mathcal{Q}_{10}^i) \mathcal{Q}_{00}^j \mathcal{Q}_{00}^k. \quad (3.17)$$

So only Liouville operators which belong to the local operators of the group $\mathcal{Q}_{10}^i$ are of importance. All those Liouville operators shown explicit in appendix A have a certain pattern, which is that an $\mathcal{Q}_{10}^i$ operator hops to another site leaving an operator $\mathcal{Q}_{00}^i$ on initial site and depending on the Hamiltonian also on the sites on a path connecting initial and final site. So a Liouville operators of $\mathcal{Q}_{10}^i$ can have the following form

$$\mathcal{L}(\mathcal{Q}_{10}^i) = \dots \mathcal{Q}_{10}^{i+1} \mathcal{Q}_{00}^i + \mathcal{Q}_{10}^{i+2} \mathcal{Q}_{00}^{i+1} \mathcal{Q}_{00}^i \dots \quad (3.18)$$

After a loop two operators can be still acting on the same site. In contrast to the case in which we consider a four-dimensional local Hilbert space it is not necessary to keep track of the sign if these two operators are commutated in such a way that they stand side by side as in equation (2.63). This results from the fact that all operators of the group $\mathcal{Q}_{00}^i$ at different sites commute with each other due to their bosonic properties and there is only one operator of the group $\mathcal{Q}_{10}^i$ which has fermionic properties. So the only necessary commutation rules are

$$\left[\mathcal{Q}_{00}^i, \mathcal{Q}_{00}^j \right] \stackrel{i \neq j}{=} 0 \quad \left[\mathcal{Q}_{10}^i, \mathcal{Q}_{00}^j \right] \stackrel{i \neq j}{=} 0. \quad (3.19)$$

Furthermore for two operators acting on the same site the idea for simplification rules is the same as in equation (2.64). The simplification rules vary between the different local Hilbert spaces. Again for the two-dimensional local Hilbert space simplification rules only between operators of $\mathcal{Q}_{00}^i$ and $\mathcal{Q}_{10}^i$ are of interest. In general simplifying an operator of $\mathcal{Q}_{10}^i$ with operator of $\mathcal{Q}_{00}^i$ results in either an operator $\mathcal{Q}_{10}^i$ or the term vanishing completely. While the result between two operators $\mathcal{Q}_{00}^i$ acting on the same site is either again part of $\mathcal{Q}_{00}^i$ or vanishes.

Combining all these results both for the Liouville operator and the simplification rules in the two-dimensional local Hilbert space we can record that the operators in the iEoM approach consist of one operator from $\mathcal{Q}_{10}^i$ and a series of $\mathcal{Q}_{0,0}^i$ operators. Provided, of course, that the starting operator is from the group $\mathcal{Q}_{10}^i$. So an arbitrary operator A for the two-dimensional local Hilbert space looks like

$$A = \mathcal{Q}_{10}^k \prod_{i=0}^n \mathcal{Q}_{00}^i \quad | \quad k \neq i \quad (3.20)$$

where the number of $\mathcal{Q}_{00}^i$ operators n has an upper limit in the amount of loops done. Since all operators commute with each other we place the $\mathcal{Q}_{01}^i$ operator up front so it becomes the head operator of the queue of $\mathcal{Q}_{00}^i$ operators.

Now a loop in this new setting consists only of applying the Liouville operator on the head operator and then simplify all operators acting on the same site instead of doing this for all local operators in the entire operator. This decreases the amount of new operators rising in a new loop significantly and therefore also the dimension of the Liouville matrix to be diagonalized for the system. All necessary Liouville operators and simplification rules are listed in appendix B. In the next section another approach is presented to reduce the amount of operators independent of the local Hilbert space used.

3.4 Momentum space representation of the operators

In this section we present another representation for the operators used in the iEoM approach. In the previous chapters every operator is in its real space representation where operators used are a cluster of local operators located relative to the vector $\mathbf{l}$ on the lattice to which to the initial operator, the creator of a DO, is applied. Now due to the translation invariance of the system, the operators can be modified with the aid of the Fourier transform so that they act in the momentum space and have the following form

$$A_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{\mathbf{l}} A_{\mathbf{l}} e^{i\mathbf{k}\mathbf{l}} \quad (3.21)$$

where $\mathbf{k}$ is a momentum vector in the first Brillouin zone and N is the number of unit cells in the crystal and the lattice constant set to unity. First, it is necessary to show that this representation does not change the consideration concerning the operator basis for the iEoM approach in section 2.6. Therefore, each operator in the operator basis has to

be orthonormal with respect to either one of the two Frobenius norms by construction. So a general Frobenius norm between two operators $A_{\mathbf{k}}$ and $B_{\mathbf{k}'}$ in the momentum space representation yields

$$(A_{\mathbf{k}}|B_{\mathbf{k}'}) = \left(\frac{1}{\sqrt{N}} \sum_{\mathbf{l}} A_{\mathbf{l}} e^{i\mathbf{k}\mathbf{l}} \middle| \frac{1}{\sqrt{N}} \sum_{\mathbf{l}'} B_{\mathbf{l}'} e^{i\mathbf{k}'\mathbf{l}'} \right) \quad (3.22)$$

$$= \frac{1}{N} \sum_{\mathbf{l}, \mathbf{l}'} (A_{\mathbf{l}}|B_{\mathbf{l}'}) e^{-i\mathbf{k}\mathbf{l}} e^{i\mathbf{k}'\mathbf{l}'} . \quad (3.23)$$

From equation (2.57) it is known that only $A = B$ and $\mathbf{l} = \mathbf{l}'$ to yield a non-zero result. In the case $A = B$ the Frobenius norm $(A_{\mathbf{l}}|B_{\mathbf{l}'}) = \delta_{\mathbf{l}, \mathbf{l}'}$ and equation (3.23) is further simplified to

$$= \frac{1}{N} \sum_{\mathbf{l}} e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{l}} = \delta_{\mathbf{k}\mathbf{k}'} . \quad (3.24)$$

In the last step the orthogonality relation

$$\sum_{\mathbf{l}} e^{-i(\mathbf{k}-\mathbf{k}')\mathbf{l}} = N \delta_{\mathbf{k}\mathbf{k}'} \quad (3.25)$$

is used to receive the final result

$$(A_{\mathbf{k}}|B_{\mathbf{k}'}) = \begin{cases} 1 & \text{if } A = B \wedge \mathbf{k} = \mathbf{k}' \\ 0 & \text{otherwise} \end{cases} . \quad (3.26)$$

Hence, operators of the form of equation (3.21) fulfill the orthogonality relations under the Frobenius norm and therefore the use of the momentum space representation for the operators in the operator basis is also possible for the iEoM approach. The next steps show how the Liouville operator is calculated and further how a matrix element can be determined for this operator representation. Because of the bilinearity of the Liouville operator, the Liouville operator is calculated for an operator $A_{\mathbf{k}}$ in this representation with the same effort as for an operator in its real space representation $A_{\mathbf{l}}$. So the Liouville operator for $A_{\mathbf{k}}$ reads

$$\mathcal{L}(A_{\mathbf{k}}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{l}} \mathcal{L}(A_{\mathbf{l}}) e^{i\mathbf{k}\mathbf{l}} . \quad (3.27)$$

For a better understanding regarding the benefits of this representation, let the Liouville operator $\mathcal{L}(A_{\mathbf{l}})$ have the partial result

$$\mathcal{L}(A_{\mathbf{l}}) = \alpha A_{\mathbf{l}+\boldsymbol{\delta}} + \beta A_{\mathbf{l}} \dots . \quad (3.28)$$

which the prefactors α and β and the shift $\boldsymbol{\delta}$ acting on all local operators in the cluster of $A_{\mathbf{l}}$. In the real space representation the operator $A_{\mathbf{l}+\boldsymbol{\delta}}$ is part of the operators that are added to the operator basis O_m in the m -loop approach. In contrast, in the momentum space representation when the Liouville operator of equation (3.28) is inserted

in equation (3.27)

$$\mathcal{L}(A_{\mathbf{k}}) = \frac{1}{\sqrt{N}} \sum_{\mathbf{l}} (\alpha A_{\mathbf{l}+\boldsymbol{\delta}} + \beta A_{\mathbf{l}}) e^{i\mathbf{k}\mathbf{l}} + \dots \quad (3.29)$$

$$= \frac{1}{\sqrt{N}} \sum_{\mathbf{l}} \alpha A_{\mathbf{l}+\boldsymbol{\delta}} e^{i\mathbf{k}\mathbf{l}} + \beta \underbrace{\frac{1}{\sqrt{N}} \sum_{\mathbf{l}} A_{\mathbf{l}} e^{i\mathbf{k}\mathbf{l}}}_{A_{\mathbf{k}}} \quad (3.30)$$

$$\stackrel{\mathbf{l}'=\mathbf{l}+\boldsymbol{\delta}}{=} \frac{1}{\sqrt{N}} \alpha \sum_{\mathbf{l}'} A_{\mathbf{l}'} e^{i\mathbf{k}(\mathbf{l}'-\boldsymbol{\delta})} + \beta A_{\mathbf{k}} + \dots \quad (3.31)$$

$$= \alpha e^{i\mathbf{k}\boldsymbol{\delta}} \underbrace{\frac{1}{\sqrt{N}} \sum_{\mathbf{l}'} A_{\mathbf{l}'} e^{i\mathbf{k}\mathbf{l}'}}_{A_{\mathbf{k}}} + \beta A_{\mathbf{k}} + \dots \quad (3.32)$$

$$= (\alpha e^{i\mathbf{k}\boldsymbol{\delta}} + \beta) A_{\mathbf{k}} + \dots \quad (3.33)$$

the result is not a new operator but rather the same operator with a prefactor depending on the shift $\boldsymbol{\delta}$ which occur in the Liouville operator of the real space representation in equation (3.28). The advantages are obvious, although we take along all operator on the lattice in form of $A_{\mathbf{l}}$ in the sum of equation (3.21), the operator basis of the momentum space representation not grow as much as in the real space representation, because known shifted operator are not added to the operator basis. Thus, the diagonal matrix element $\mathbf{M}_{ii}$ for the operator $A_{\mathbf{k}}$ in the Liouville matrix in the momentum space representation yields with equations (3.23) and (3.29)

$$M_{ii} = (A_{\mathbf{k}} | \mathcal{L}(A_{\mathbf{k}})) = \alpha e^{i\mathbf{k}\boldsymbol{\delta}} + \beta. \quad (3.34)$$

While in the real space representation the diagonal element is only β and the factor α is only in non-diagonal entries in the submatrix between all shifted $A_{\mathbf{l}}$ operators used in the operator basis O_m . This submatrix is reduced in the momentum space representation only to the factor $\alpha e^{i\mathbf{k}\boldsymbol{\delta}}$ depending on the momentum vector $\mathbf{k}$. As a result the Liouville matrix in its momentum representation is significant smaller for higher loops and moreover its information content is higher. Since all possible shifts of an operator $A_{\mathbf{l}}$ are represented in the Liouville matrix due to the representation in equation (3.21). In summary, the momentum representation of the operators fulfills all claims for being used in the iEoM approach and furthermore possesses some advantages towards the real space representation. Nevertheless, in the end it is necessary to calculate for every Liouville matrix, despite its representation, the lowest eigenvalue to determine the energy gap. The next section presents a method how this is still possible for a Liouville matrix with increasing dimensions which occur at higher loops in the iEoM approach.

3.5 Matrix diagonalization via Lanczos algorithm

Regardless the used dimension of the local Hilbert space and the different representation for the operators in the operator basis, with each iteration step the amount of operators in the operator basis will increase continuously. Of course, this depends on the number of operators created by the Liouville operator. Some representations damp this effect but ultimately the amount of operators is too large and thus a full diagonalization of the Liouville matrix will be not feasible for higher iteration steps. Additionally, this effect is enhanced for large Liouville operator in terms of the numbers of new operators generated. Fortunately, only the lowest eigenvalue is of interest to determine the energy gap. Hence, the Liouville matrix is constructed to be a Hermitian matrix the Lanczos algorithm [40] is well suited to determine the lowest eigenvalue of the Liouville matrix.

The Lanczos algorithm is an effective method for large sparse matrices to determine extremal eigenvalues and their associated eigenvectors of a given matrix. Thereby the given matrix $\mathbf{M}$ with the dimension $n \times n$ is reduced to tridiagonal matrix $\mathbf{T}$ with the dimension $m \times m$ [41].

$$\mathbf{T} \in \mathbb{C}^{m \times m} \text{ with } m < n \quad (3.35)$$

Since m is much smaller than n and T has a tridiagonal shape, not much effort is required to transform $\mathbf{T}$ into its eigensystem. The resulting extremal eigenvalues of $\mathbf{T}$ give an estimation of $\mathbf{M}$'s extremal eigenvalues, where the estimation becomes progressively more accurate with higher m [41]. At the beginning of the Lanczos algorithm, a start vector $\mathbf{s}$ must be selected, for which the m -dimensional Krylov subspace

$$\mathcal{K}^m(\mathbf{s}) = \text{span}(\mathbf{s}, \mathbf{M}\mathbf{s}, \dots, \mathbf{M}^{m-1}\mathbf{s}) \quad (3.36)$$

is formed. Although we are not interested in the time evolution of the start operator in the iEoM, it is appropriated to use the initial condition of equation (2.27) as a start vector for the Lanczos algorithm

$$\mathbf{s} := \mathbf{h}(t = 0) \quad (3.37)$$

to ensure that the initial conditions (2.27) could be realized if needed. During the Lanczos algorithm an orthonormal basis for the Krylov subspace is build starting with the first basis vector

$$\mathbf{q}_1 = \frac{\mathbf{s}}{\|\mathbf{s}\|} \quad (3.38a)$$

of $\mathcal{K}^m$. After that the algorithm generates further basis vectors by using the following steps

$$\alpha_j = \mathbf{q}_j^\dagger \mathbf{M} \mathbf{q}_j \quad (3.38b)$$

$$\mathbf{r}_j = \mathbf{M} \mathbf{q}_j - \alpha_j \mathbf{q}_j - \beta_{j-1} \mathbf{q}_{j-1} \quad (3.38c)$$

$$\beta_j = \begin{cases} \|\mathbf{r}_j\| & \text{if } j \geq 1 \\ 0 & \text{otherwise} \end{cases} \quad (3.38d)$$

Furthermore, a normalization is performed

$$\mathbf{q}_{j+1} = \frac{\mathbf{r}_j}{\|\mathbf{r}_j\|}. \quad (3.38e)$$

So at the end the all basis vectors $\mathbf{q}_j, j \in \{1, \dots, m\}$ created by the Lanczos algorithm (3.38) are all orthonormal

$$\mathbf{q}_i^\dagger \mathbf{q}_j = \delta_{ij} \quad (3.39)$$

and span the Krylov subspace $\mathcal{K}^m$. It is possible to transformation matrix $\mathbf{M}$ with the unitary transformation determine by the matrix

$$\mathbf{Q} = (\mathbf{q}_1 \quad \dots \quad \mathbf{q}_F) \quad (3.40)$$

where its columns are the vectors $\mathbf{q}_i$ calculated by the algorithm, into a tridiagonal matrix with the dimension $m \times m$

$$\mathbf{Q}^\dagger \mathbf{M} \mathbf{Q} = \mathbf{T} = \begin{pmatrix} \alpha_1 & \beta_1 & 0 & \dots & 0 \\ \beta_1 & \alpha_2 & \beta_2 & \ddots & \vdots \\ 0 & \beta_2 & \alpha_3 & \ddots & \ddots \\ & \ddots & \ddots & \ddots & \ddots & 0 \\ \vdots & & \ddots & \ddots & \alpha_{m-1} & \beta_{m-1} \\ 0 & \dots & 0 & \beta_{m-1} & \alpha_m \end{pmatrix}. \quad (3.41)$$

The final step is to find the eigensystem for the matrix $\mathbf{T}$ with the eigenvalue $\tilde{\lambda}_j$ and eigenvectors $\mathbf{w}$. As mentioned above the extremal eigenvalues of $\tilde{\lambda}_j$ are equal to the extremal eigenvalues λ of the input matrix $\mathbf{M}$ with an accuracy depending on the dimension of the used Krylov subspace. To obtain the eigenvector $\mathbf{v}_j$ to the extremal eigenvalue λ_j of $\mathbf{M}$ the m -dimensional eigenvector $\mathbf{w}_j$ needs to be transformed into n -dimensional one with the transformation

$$\mathbf{v}_j = \mathbf{Q} \mathbf{w}_j. \quad (3.42)$$

Of course, depending on the chosen dimension m of the Krylov subspace finding the eigensystem for $\mathbf{T}$ can take some time but still it is significant faster than a full diagonalization of $\mathbf{M}$. In addition, a relative small dimension of the Krylov subspace is sufficient to achieve reasonable accuracy for the most extreme eigenvalue of $\mathbf{M}$. Considering that we only need to calculate the lowest eigenvalue of the Liouville matrix when we calculate the energy gap, thus the Lanczos algorithm is capable of completing this task within a reasonable time compared to a full diagonalization.

3.6 Addressing calculation of the energy gap and presentation of the results

In this section address the presentations of the results which will be mostly used for all following results in the chapter 4. In general all Hamiltonians which are used in this thesis are of the following form

$$H = \sum_i T_i + H_{\text{int}} \quad (3.43)$$

consisting of various hopping terms T_i and finally the interaction part H_{int} . The issue which initial operator A_0 resolves the energy spectrum of the energy gap for charge excitation is already solved in section 3.1. Therefore, the following paragraphs are addressing Liouville matrices $\mathbf{M}$ where the initial operator A_0 is a local operator creating a charge excitation $A_0 \in \{d_{i,\uparrow}^\dagger, d_{i,\downarrow}^\dagger, h_{i,\uparrow}^\dagger, h_{i,\downarrow}^\dagger\}$ on a site i in the real space representation. Of course, in the momentum space representation A_0 is an operator creating a charge excitation $A_0 \in \{d_{\mathbf{k},\uparrow}^\dagger, d_{\mathbf{k},\downarrow}^\dagger, h_{\mathbf{k},\uparrow}^\dagger, h_{\mathbf{k},\downarrow}^\dagger\}$ with momentum $\mathbf{k}$. With this restriction regarding the initial operator, it is possible to make a statement about the Liouville matrix by analyzing the calculations done of the Liouville operator for each local operator in appendix A respectively in appendix B. Whether T_i it is just simple NN-hopping T_0 or more complex spin dependent NNN-hopping T'_s , the Liouville operator $[T_i, \cdot]$ of a local operator includes not itself. Consequently, since diagonal entries

$$M_{ii} = (A_i | \mathcal{L}(A_i)) \quad (3.44)$$

are only non-zero if the Liouville operator of an operator yields the same operator with any prefactor. Therefore, the Liouville operator $[T_i, \cdot]$ is responsible for off-diagonal elements. Exceptional cases are possible for operators in the momentum space representation, but they are initially left out in these considerations. In contrast to this the commutator of $[H_{\text{int}}, \cdot]$ with a local operator $A_0 \in \{\mathcal{Q}_{10}^i, \mathcal{Q}_{01}^i\}$ creating or annihilating DOs generates only the same local operator with a prefactor, where the prefactors are for an operator $\mathcal{Q}_{10}^i$ equal to $U/2$ and for an operator $\mathcal{Q}_{01}^i$ equal to $-U/2$ as shown in appendix A. Furthermore $[H_{\text{int}}, \cdot] = 0$ for any local operator $\hat{o}_n^i \in \{\mathcal{Q}_{00}^i, \mathcal{Q}_{11}^i\}$ which not change the numbers of DO. Apparently the part of the Liouville operator with $[H_{\text{int}}, \cdot]$ take a huge part for the diagonal entries of the Liouville matrix. Since for any operator A_i applies $[H_{\text{int}}, A_i] = a_i A_i$. For the approach where a two-dimensional local Hilbert space is considered, the prefactors a_i for every operator are equal to $U/2$ since as discussed in section 3.3 the operators A_i consist only of one $\mathcal{Q}_{10}^i$ operator and a queue of non-contributing $\mathcal{Q}_{00}^i$ operators regarding $[H_{\text{int}}, \cdot]$. As well, all prefactors a_i for four-dimensional local Hilbert space are also equal to $U/2$. This is proven via the following brief considerations. New operators rise with the commutator $[T_i, \cdot]$ but since every T_i conserves the number of DOs in the system, the effective number of DO created by any new operator is the same as the initial operator ergo one. Therefore, the commutator $[H_{\text{int}}, \cdot]$ with every operator in the operator basis yields $U/2$ and thus the same as the initial operator. As a consequent, regardless of the local Hilbert used, Liouville matrices for an initial operator $A_0 \in \mathcal{Q}_{10}^i$ can be represented

in a certain form, which is examined below. Henceforth, a Liouville matrix for an initial operator A_0 and a Hamiltonian H in the m -th loop will be denoted as $\mathbf{M}_H^m(A_0)$. To simplify things here the operator $h_{i,\uparrow}^\dagger$ is used as the initial operator A_0 . It follows with the previous considerations that for the operator $h_{i,\uparrow}^\dagger$ the Liouville matrix can be written as

$$\mathbf{M}_H^m(h_{i,\uparrow}^\dagger) = \mathbf{M}_{\sum T_i}^m(h_{i,\uparrow}^\dagger) + \mathbf{M}_{H_{\text{int}}}^m(h_{i,\uparrow}^\dagger) = \mathbf{M}_{\sum T_i}^m(h_{i,\uparrow}^\dagger) + \frac{U}{2} \mathbb{1} . \quad (3.45)$$

Consequently, it is possible to calculate only the eigendecomposition for the matrix $\mathbf{M}_{\sum T_i}^m(h_{i,\uparrow}^\dagger)$ and determine the eigenvalues $\tilde{\lambda}_i^m$ of $\mathbf{M}_H^m(h_{i,\uparrow}^\dagger)$ with the corresponding eigenvalues λ_i^m of $\mathbf{M}_{\sum T_i}^m(h_{i,\uparrow}^\dagger)$ via

$$\lambda_i^m = \tilde{\lambda}_i^m - \frac{U}{2} \quad \Rightarrow \quad \tilde{\lambda}_i^m = \lambda_i^m + \frac{U}{2} . \quad (3.46)$$

Here, the corresponding eigenvectors $\mathbf{v}_i$ and $\mathbf{v}_i^*$ are identical for both matrices. Assuming that every hopping amplitude t_i of the terms T_i can be reduced to a linear ratio with an initial hopping amplitude t there is only a linear t dependence in the matrix $\mathbf{M}_{\sum T_i}^m(h_{i,\uparrow}^\dagger)$. Therefore the eigenvalues λ_i^m are calculated in units of t , which can be direct translated into units of the bandwidth of the interaction-free Hubbard model $W = 2zt$ to allow comparison between different dimensions later on. Then, to calculate $\tilde{\lambda}_i^m$ via equation (3.46), a ratio between W and U needs to be defined. So the energy gap for single charge excitation Δ in which we are interested in is derived from the lowest eigenvalue $\lambda_{\min}^m$ of $\mathbf{M}_H^m(h_{i,\uparrow}^\dagger)$ for which applies

$$\Delta \leq \Delta^m = 2\tilde{\lambda}_{\min}^m = U + 2\lambda_{\min}^m \quad \text{with} \quad \lambda_{\min}^m < 0 . \quad (3.47)$$

As mentioned in section 3.1 it is only possible to calculate an upper bound Δ^m for the energy gap Δ with the eigenvalue $\lambda_{\min}^m$. But it is possible to estimate the true value of Δ , because with each loop the upper bound Δ^m approaches the true value of Δ continuously since $\lambda_{\min}^m$ is a monotonically decreasing sequence for which

$$\lambda_{\min}^m > \lambda_{\min}^{m+1} \quad (3.48)$$

holds. Furthermore, the difference between two sequence elements is

$$|\lambda_{\min}^{m+1} - \lambda_{\min}^m| < |\lambda_{\min}^m - \lambda_{\min}^{m-1}| . \quad (3.49)$$

therefore the sequence is bounded from below with the lower bound

$$\lim_{m \rightarrow \infty} \lambda_{\min}^m = \bar{\lambda}_{\min} . \quad (3.50)$$

It follows that for $m \rightarrow \infty$ the calculated energy gap Δ^m becomes equal to the real energy gap Δ

$$\lim_{m \rightarrow \infty} \Delta^m = \lim_{m \rightarrow \infty} (U + 2\lambda_{\min}^m) = U + 2\bar{\lambda}_{\min} = \Delta . \quad (3.51)$$

Consequently, by determine the lower bound $\bar{\lambda}_{\min}$ the energy gap Δ can be calculated via equation (3.51) for different interaction strength U . Of course, bearing in mind that a higher m is correlated to an exponential increase in the size of the Liouville matrix. In the m -loop approach after a considerable m the computational effort to determine both the Liouville matrix $\mathbf{M}_H^m(\cdot)$ and the eigenvalue $\lambda_{\min}^m$ as well as the storage of the Liouville matrix become a problem. Therefore, one possibility is to extrapolate the value of the lower bound $\bar{\lambda}_{\min}$ with values of $\lambda_{\min}^m$ for computable m . Whereby the function for the extrapolation still has to be examined first. If it is possible to determine $\bar{\lambda}_{\min}$, a critical interaction strength U_c at which the energy gap Δ is expected to open can be calculated by setting the energy gap Δ in equation (3.51) to zero. Thus, the critical interaction strength U_c is determined by

$$U_c = -2\bar{\lambda}_{\min} . \quad (3.52)$$

Now all details for the use of the iEoM approach in the t - J model are clarified. In the following chapter the progress is presented which is made in this thesis for determining the critical interaction strength U_c for single charge excitation with the iEoM approach in the different local Hilbert space cases and different models.

4 Results

In the following chapter first calculations with the iterated equation of motion approach are presented. At the beginning calculation are done for a simple hopping of a hole on a one-dimensional chain for both local Hilbert spaces. With this we first get insights into how the approach works and test whether the assumption of section 3.1 holds that it is possible to calculate the band gap Δ with a Liouville matrix built for a creation operator of a hole. Also in one dimension comparing analytic solutions and the solutions given by the iEoM approach is possible, so that a statement about the performance of the iEoM can be made. Further optimizations concerning the operator basis will be discussed. Furthermore, the simple hopping is extended to two dimensions and applied to a two-dimensional square lattice. At the end all the knowledge that we achieved within this thesis towards the iEoM approach is applied to calculate the critical interaction strength U_c for the energy gap for single charge excitation in a t - J model at half-filling and in the limit of $0 < J \ll T \ll \Delta$ via the iEoM approach for both on a one-dimensional chain and on a two-dimensional square lattice. All following values for $\lambda_{\min}^m$ are calculated with the Lanczos algorithm of section 3.5 unless otherwise specified.

4.1 Simple one-dimensional approach

At first, we start with simple Hamiltonian in one dimension and use the operator $h_{i,\uparrow}^\dagger$ in the real space representation as the initial operator to build the operator basis and the corresponding Liouville matrix. The Hamiltonian defining the Liouville operator is

$$H_{1D} = T_0 + H_{\text{int}} \quad (4.1)$$

where T_0 is the nearest neighbor hopping of a DO on a one-dimensional chain and H_{int} is the interaction term. Other terms of the complete Hamiltonian of equation (2.14) are not of interest at first since this serves only as a testbed for the method and moreover the other terms of equation (2.14) apply only partially for the one-dimensional chain and need further evaluation. As discussed in section 3.6, it is only necessary to build the Liouville matrix $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ and use the Lanczos algorithm of section 3.5 to calculate the lowest eigenvalue $\lambda_{\min}^m$ for differences loops m , since this will resolve the energy gap as described in section 3.1. The value $\lambda_{\min}^{m=0}$ is trivial and equals zero in the real space representation for each local Hilbert space choices, since the Liouville operator of $h_{i,\uparrow}^\dagger$ does not reproduce itself. Therefore, $m = 0$ is left out in the results for the real space representation. In section 3.2 the two different choices of local Hilbert spaces were presented, a four-dimensional $\mathcal{H}_4^L$ and a two-dimensional $\mathcal{H}_2^L$ local Hilbert space both having an orthonormal local operator basis with respect to the Frobenius scalar product.

Even though the final aim is to describe a system at the vicinity of half-filling, the $\mathcal{H}_4^L$ case should not be dropped, despite the fact that in the $\mathcal{H}_4^L$ case all four local spin configuration are equally likely. It rather serves as example what happens if half-filling is not considered properly. So results for the simple model of equation (4.1) in the $\mathcal{H}_4^L$ case are presented along with the results for the $\mathcal{H}_2^L$ case in the following and are compared to each other to a limited extent. Concluding, results generated with the $\mathcal{H}_4^L$ case are finally discussed in more detail in section 4.3 After that, the $\mathcal{H}_4^L$ case is dropped. We start with the results for the simple model if the iEoM approach uses the $\mathcal{H}_4^L$ case.

Local four-dimensional Hilbert space $\mathcal{H}_4^L$

The figure 4.1 shows the lowest eigenvalue of the Liouville matrix $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ related to the initial operator $h_{i,\uparrow}^\dagger$ acting on the local four-dimensional Hilbert space $\mathcal{H}_4^L$ for different amounts of loops m . In addition, the corresponding number of operators used to build the matrix $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ are also shown in figure 4.1. If the eigenvalues $\lambda_{\min}^m$ in

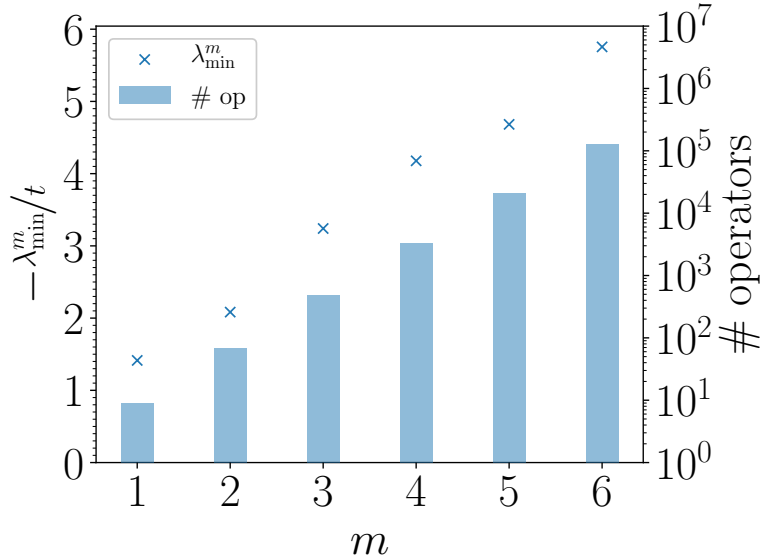


Figure 4.1: Results for the Hamiltonian of (4.1) on a one-dimensional chain with $\mathcal{H}_4^L$. Lowest eigenvalues $\lambda_{\min}^m$ of the Liouville matrix $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ and the size of the corresponding operator basis $\mathcal{O}_m$ for the m -loop are shown.

figure 4.1 are considered, the predicted convergence of $\lambda_{\min}^m$ to a $\bar{\lambda}_{\min}$ cannot be observed up to the highest possible loop for the $\mathcal{H}_4^L$ case. It rather seems that the values of $\lambda_{\min}^m$ increases nearly linearly in the observed range of figure 4.1. Since we are limited in the computational power higher loop result were a convergence of $\lambda_{\min}^m$ could take place are not feasible. The problem becomes apparent when the amount of operators for each loop in figure 4.1 are studied. The exponential increase with each loop is clearly shown in figure 4.1 and already for $m = 7$ the numbers of operator which have to be calculated is expected to be around 10^7 operators. This leads us to the limits of the computational

power and storage used here. Therefore, the next loop step is already not feasible and at first it is not possible to make a statement for higher loops regarding $\lambda_{\min}^m$. As mentioned before the $\mathcal{H}_4^L$ represents not the corrected local Hilbert space for the actual problem. The observation of a non-convergence behavior is likely due to this reason. But what exactly causes this behavior cannot be deduced from the results shown in figure 4.1 alone. In the next step the iEoM approach is now applied with the initial operator acting on the two dimension local Hilbert space $\mathcal{H}_2^L$ so a first comparison of the two local basis choices is possible.

Local two-dimensional Hilbert space $\mathcal{H}_2^L$

Here, the iEoM approach is applied to the Hamiltonian of equation (4.1) with respect to the two-dimensional Hilbert space $\mathcal{H}_2^L$. The Liouville matrix $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ is calculated for with different numbers of loops m and the numbers of operators rise during this process are recorded and displayed together with the lowest eigenvalues $\lambda_{\min}^m$ in figure 4.2. In

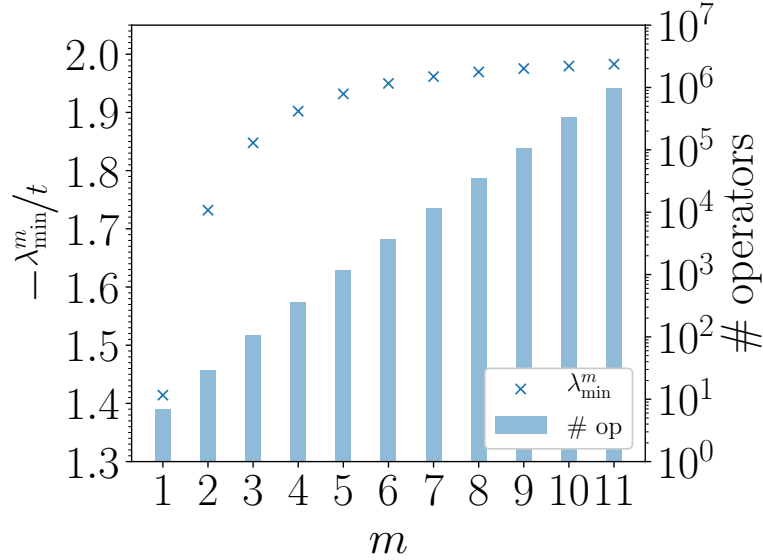


Figure 4.2: Results for the Hamiltonian of (4.1) on a one-dimensional chain with $\mathcal{H}_2^L$. Lowest eigenvalues $\lambda_{\min}^m$ of the Liouville matrix $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ and the size of the corresponding operator basis $\mathcal{O}_m$ for the m -loop are shown.

contrast to case of a four-dimensional local Hilbert space $\mathcal{H}_4^L$, the lowest eigenvalues $\lambda_{\min}^m$ show convergence behavior in the case for a two-dimensional local Hilbert space $\mathcal{H}_2^L$ as described in section 3.1. Furthermore, the feasible loops are higher since with each loop numbers of operators in figure 4.2 not rise as quickly as in figure 4.1. Therefore, in the case of $\mathcal{H}_2^L$ it is possible to build Liouville matrices up to 11-loops but then the numbers of operators reach also the critical area where the numbers of operators exceed the 10^7 threshold. This is easy to comprehend, since for the $\mathcal{H}_2^L$ case the Liouville operator of the head operator only can generate new operators as discussed in section 3.3 in contrast to

the $\mathcal{H}_4^L$ case where every local operator can produce new operators. Now that this has been clarified, we turn to the determination of the lower bound $\bar{\lambda}_{\min}$ and further receive via equation (3.52) a value for the critical interaction strength U_c . Here the objective is to find an asymptotic function which has a sufficient predictive power to estimate values of $\lambda_{\min}^m$ for loops m which are not feasible to calculate with the available calculation power. Once such a function is found the position of the horizontal asymptote of function give a solid estimation for the value of $\bar{\lambda}_{\min}$. Here, different empirical asymptotic functions X with three degrees of freedom were tested. The measure of the predictive power is based on the absolute differences

$$\delta_X = |\bar{\lambda}_{\min}^{\tilde{X}} - \bar{\lambda}_{\min}^{\bar{X}}| . \quad (4.2)$$

The value $\bar{\lambda}_{\min}^{\tilde{X}}$ thereby is determined by using only the values of $\lambda_{\min}^m$ within the first three loops m to determine the function f . Where in the calculation of $\bar{\lambda}_{\min}^{\tilde{X}}$ only the values of $\lambda_{\min}^m$ within the last three possible loops m are used to determine the function X . In following illustration or tables the corresponding functions are label with $\tilde{f}$ and $\bar{f}$. The absolute difference $|\bar{\lambda}_{\min}^{\tilde{X}} - \bar{\lambda}_{\min}^{\bar{X}}|$ not only gives a measurement for the predictive power but also an estimation for the uncertainty with respect to $\bar{\lambda}_{\min}^X$ if the parameters of the function f are determined with a least squares method taking the values of $\lambda_{\min}^m$ in all calculated loops m into account. The uncertainty for the values $\bar{\lambda}_{\min}^X$ which is determined with the function X is estimated to be around two times the value of the difference δ_X

$$\Delta \bar{\lambda}_{\min}^X = 2\delta_X = 2|\bar{\lambda}_{\min}^{\tilde{X}} - \bar{\lambda}_{\min}^{\bar{X}}| . \quad (4.3)$$

Of course, this estimation of the uncertainty only makes sense if more than three values of $\lambda_{\min}^m$ are available. Empirical attempts showed that a general rational function in the form of

$$f(x) = \frac{a}{(x-b)^2} + c \quad (4.4)$$

provides a lower value of δ_X with calculated values of $\lambda_{\min}^m$ than e.g. exponential or other rational functions. In table 4.1 and table 4.2 also the results of the functions

$$g(x) = ae^{-bx} + c \quad h(x) = \frac{a}{x-b} + c \quad (4.5)$$

are given as a reference for this matter. Whereby for all functions the parameter c in equation (4.4) gives the position of the horizontal asymptote, therefore the value of c corresponds to the required value $-\bar{\lambda}_{\min}^X$ which can be used to determine U_c via equation (3.52). In figure 4.3 calculated values of $\lambda_{\min}^m$ are shown together with the LS fit f for all values. Furthermore, the functions $\tilde{f}$ and $\bar{f}$ to estimate the uncertainty are also shown.

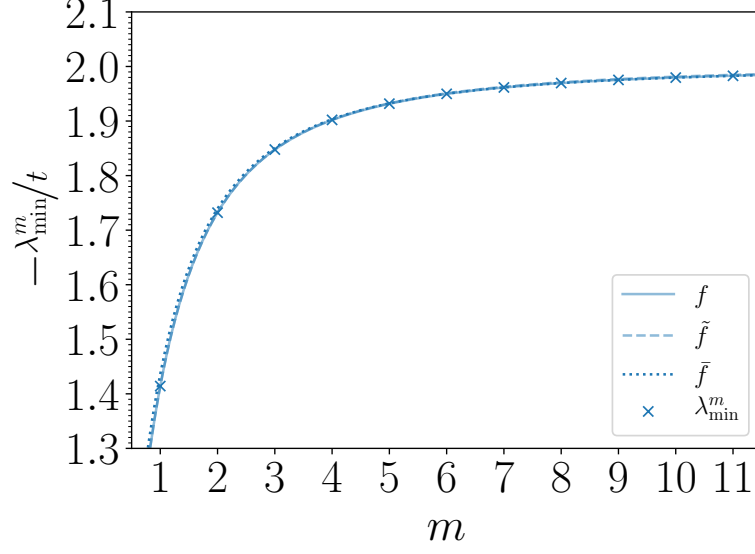


Figure 4.3: Results for the Hamiltonian of (4.1) on a one-dimensional chain with $\mathcal{H}_2^L$. Lowest eigenvalues $\lambda_{\min}^m$ of the Liouville matrix $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ for the m -loop are shown. Also, three LS fits are displayed where f uses all values of $\lambda_{\min}^m$ and $\tilde{f}$ and $\bar{f}$ use the results of the first respectively the last three loops.

The parameters calculated for the corresponding fit of figure 4.3 and the parameters of the other in figure 4.3 not shown functions of equation (4.5) are listed in table 4.1. The resulting values of $\bar{\lambda}_{\min}^X$ together with the values for estimating their uncertainty and the corresponding critical interaction strengths U_c calculated with equation (3.52) are listed in table 4.2.

Table 4.1: Parameters associated with the different functions X of equations (4.4) to (4.5) determined with a least squares method using the values of $\lambda_{\min}^m$. Where f corresponds to the functions displayed in figure 4.3. The errors of the parameters are determined by the least squares method.

Function X	a/t	b	c/t
f	-2.557 ± 0.007	-1.0881 ± 0.0030	2.00061 ± 0.00014
g	-1.18 ± 0.05	0.76 ± 0.04	1.971 ± 0.005
h	-0.58 ± 0.03	0.09 ± 0.04	2.042 ± 0.005

When the results in table 4.2 are compared it is noticeable that the function f gives the best estimation as mentioned previously. The uncertainties in the results with f are significantly smaller than for the other functions tested. So the function f provides the most reliable results among the studied functions. This still holds true in further calculations but here is not explicitly re-examined in this way afterwards. Therefore, f is the only function used for further results. Furthermore, it shows, already with only

Table 4.2: The values of $\bar{\lambda}_{\min}^X$ associated with the different function of equations (4.4) to (4.5). Where f corresponds to the functions displayed in figure 4.3 and the values of U_c/W are calculated via equation (3.52) with $W = 4t$ in one dimension. The values $\bar{\lambda}_{\min}^{\tilde{X}}$ and $\bar{\lambda}_{\min}^{\tilde{X}}$ are determined using only the results of the first respectively the last three loops. With equation (4.3) the uncertainty for $\bar{\lambda}_{\min}^X$ is determined.

Function X	$-\bar{\lambda}_{\min}^{\tilde{X}}/t$	$-\bar{\lambda}_{\min}^{\tilde{X}}/t$	$-\bar{\lambda}_{\min}^X/t$	U_c/W
f	2.003	2.000	2.001 ± 0.005	1.0003 ± 0.0024
g	1.914	1.993	1.97 ± 0.16	0.98 ± 0.08
h	2.096	2.007	2.04 ± 0.18	1.02 ± 0.09

the bare necessary loops like used in the function $\tilde{f}$ the calculated value of $-\bar{\lambda}_{\min}$ only changes for higher used loops only in the order of $1 \cdot 10^{-3}$. This effect also can be observed qualitatively in figure 4.3, because all shown functions show a strong overlap, even if they only use the first three loops like $\tilde{f}$. The result from this analysis is that the value for the critical interaction strength U_c for the $\mathcal{H}_2^L$ case with the simple Hamiltonian of equation (4.1) can be determined with a LS fit of the function f to calculated values of $\lambda_{\min}^m$. The result for U_c is already listed in table 4.2 and reads

$$\frac{U_c}{W} = 1.0003 \pm 0.0024 . \quad (4.6)$$

This result is in perfect agreement with results for the half-filled chain in the limit of strong interaction [25] where the energy gap in zeroth order noted as

$$\Delta(U/t \rightarrow \infty) = U - 4t \Rightarrow U_c/W = 1 . \quad (4.7)$$

To study the energy gap in higher orders the simple model of equation (4.1) will be extended in section 4.6 but for now the results with the simple model in the $\mathcal{H}_2^L$ case are sufficient.

The results obtained with the $\mathcal{H}_2^L$ case are in line with the expectations while the observed non-convergence behavior for the $\mathcal{H}_4^L$ case is only answered with a not suitable Hilbert space. However, this has not been discussed in detail here. The exacted issue leading to this observation is addressed later on in the section section 4.3. While in the next section deals with the iEoM in its momentum space representation when it is applied to the simple Hamiltonian of equation (4.1).

4.2 Momentum space representation for the simple one-dimensional approach

Here, the results are presented for both the $\mathcal{H}_2^L$ and $\mathcal{H}_4^L$ case when the momentum space representation for the creator of a hole $h_{\mathbf{k},\uparrow}^\dagger$ is used as an initial operator for the iEoM approach as described in section 3.4. This time starting with the $\mathcal{H}_2^L$ case, since a non-converging behavior for the $\mathcal{H}_4^L$ case is expected as in the real space representation. Again as in section 4.1 the Hamiltonian of equation (4.1) is used, so this section serves as a test for the iEoM method in its momentum representation.

Local two-dimensional Hilbert space $\mathcal{H}_2^L$

In this representation the operators are dependent on a momentum vector $\mathbf{k}$ so the operator that is used as an initial operator is $h_{\mathbf{k},\uparrow}^\dagger$. This of course leads to a Liouville matrix $\mathbf{M}_{T_0}^m(h_{\mathbf{k},\uparrow}^\dagger)$ dependent on $\mathbf{k}$ and consequently the lowest eigenvalue $\lambda_{\min}^m(\mathbf{k})$ also has this dependence. We are interested in the lowest possible $\lambda_{\min}^m(\mathbf{k})$, therefore the dispersion relation of $\lambda_{\min}^m(\mathbf{k})$ has to be examined first. The lowest value of $\lambda_{\min}^m(\mathbf{k})$ is to be expected on a critical point in the one-dimensional Brillouin zone these are in center or at the edges of the Brillouin zone. The figure 4.4 displays two cases of the dispersion relation for different loops for $\mathbf{k}$ in the first Brillouin zone. Since with the momentum space representation the calculation of $\lambda_{\min}^{m=0}$ is not as trivial as in the real space representation $\lambda_{\min}^{m=0}(\mathbf{k})$ is also examined in figure 4.4. In the first case figure 4.4a as before the initial operator is a creator of a hole $h_{\mathbf{k},\uparrow}^\dagger$ and in the second case figure 4.4b a creator of a doubly occupied site $d_{\mathbf{k},\uparrow}^\dagger$ to check the particle hole symmetry of the system. A distinction between spin orientation is not relevant, since no spin type is preferred by the Hamiltonian of equation (4.1).

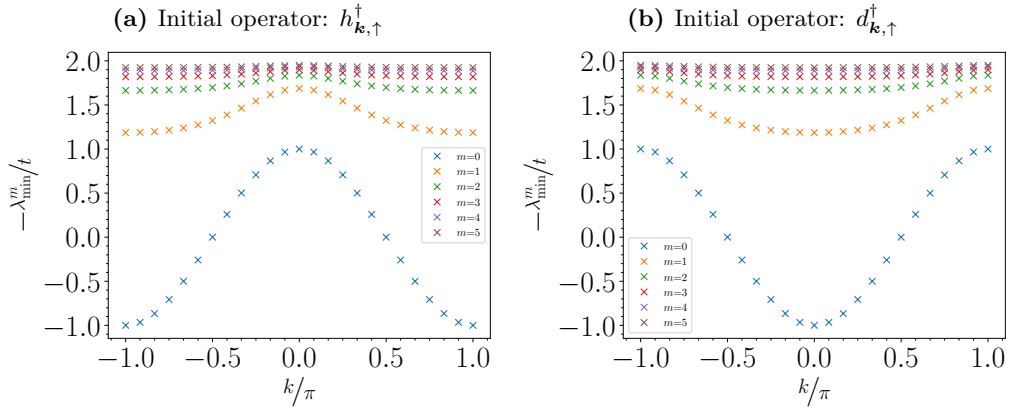


Figure 4.4: Dispersion relation of the lowest eigenvalue $\lambda_{\min}^m(\mathbf{k})$ is displayed in the first Brillouin zone for different loops and initial operators. The Hamiltonian (4.1) is used and the local operators act on $\mathcal{H}_2^L$. In figure 4.4a the initial operator is a creator of a hole $h_{\mathbf{k},\uparrow}^\dagger$ and in figure 4.4b the creator of a double occupation $d_{\mathbf{k},\uparrow}^\dagger$.

The first observation is that for the creator of a hole the lowest value of $\lambda_{\min}^m(\mathbf{k})$ is located in the center of the Brillouin zone at $\mathbf{k} = 0$. Whereas the lowest value for the creator of a doubly occupied site is located at the edges of the Brillouin at $\mathbf{k} = \pm\pi$. While the lowest values of $\lambda_{\min}^m(\mathbf{k})$ in each dispersion have the same value and the dispersion relation of a doubly occupied site is shifted by a value of π compared to the one of a hole. Hence, the particle hole symmetry can also be observed in the results. Furthermore, regardless of the value of the momentum vector $\mathbf{k}$ a convergence of $\lambda_{\min}^m(\mathbf{k})$ for increasing m is already apparent in figure 4.4 but is investigated later on in detail. Another observation is that the dispersion relation flattens with each higher loop m . As a result differences in $\lambda_{\min}^m(\mathbf{k})$ for different momentum direction $\mathbf{k}$ start to vanish for higher values of m and therefore no orientation of $\mathbf{k}$ stands out in higher loops. The next step is to determine $\bar{\lambda}_{\min}^f$ for the momentum representation. Though for higher values of $\lambda_{\min}^m(\mathbf{k})$ the value of $\mathbf{k}$ seems to have no influence, here the $\mathbf{k}$ is chosen to be the value where the lowest value of the dispersion is located for low values of m . In figure 4.5 values of $\lambda_{\min}^m(\mathbf{k})$ are shown for different loops m together with the fit for f and the two functions $\tilde{f}$ and $\bar{f}$ which estimate the uncertainty for $\bar{\lambda}_{\min}^f$. As the initial operator servers the creator of a hole $h_{\mathbf{k},\uparrow}^\dagger$. Consequently, the value of $\mathbf{k}$ is chosen to be $\mathbf{k} = 0$. Since the value of $\lambda_{\min}^m(\mathbf{k} = 0)$ for the loop $m = 0$ is relatively far away from the other values, it is not taken into account to determine $\bar{\lambda}_{\min}$ as in the real space representation. Furthermore, to simplify the comparison between momentum and real space representation the results of the real space calculation displayed in figure 4.3 are also a part of figure 4.5. In figure 4.5 the logarithmic scale for the numbers of operator is omitted in favor for a more visible comparison between the two approaches.

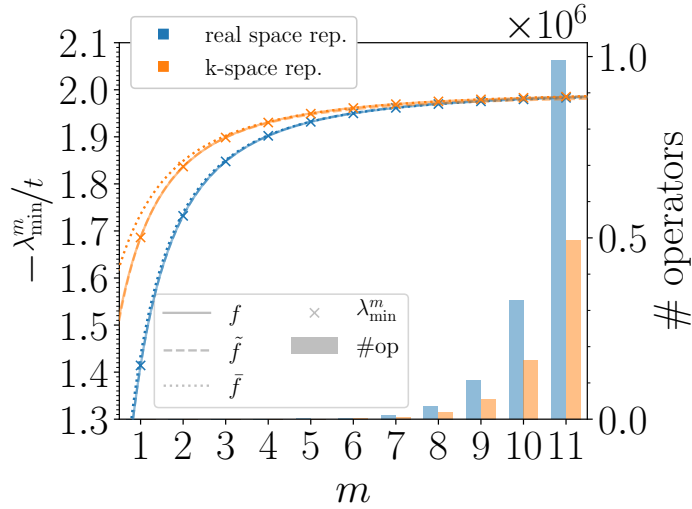


Figure 4.5: Results for the Hamiltonian of (4.1) on a one-dimensional chain with $\mathcal{H}_2^L$, one in real space and the other in momentum space(k-space). Lowest eigenvalues $\lambda_{\min}^m$ of the Liouville matrices $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ and $\mathbf{M}_{T_0}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ and the size of the corresponding operator basis $\mathcal{O}_m$ for the m -loop are shown. Also, three LS fits for each representation are displayed where f uses all values of $\lambda_{\min}^m$ and $\tilde{f}$ and $\bar{f}$ use the results of the first respectively the last three loops.

Starting with the comparison of the numbers of operators in each representation. As expected, the amount of operators in the momentum space representation is significant reduced compared to the real space representation. The operator basis in the real space is almost twice the size and therefore the Liouville matrix in real space representation is nearly four times the size than in the momentum space representation. As expected, the lowest eigenvalues $\lambda_{\min}^m$ show the already in figure 4.4 indicated convergence behavior. Despite the smaller operator basis and Liouville matrix in the momentum space representation the corresponding lowest eigenvalues $\lambda_{\min}^m$ converges more rapidly than in its real space representation since $\lambda_{\min}^m(\mathbf{k} = 0) < \lambda_{\min}^m$ holds in every loop m . Assuming that both $\lambda_{\min}^m$ converge toward an equal $\bar{\lambda}_{\min}$. In the following this assumption is check by using again as in section 4.1 a LS fit with the function f of equation (4.4) to determine $\bar{\lambda}_{\min}^f$. Also for the estimation of the uncertainty of $\bar{\lambda}_{\min}^f$ in the momentum space representation the functions $\tilde{f}$ and $\bar{f}$ are considered as previously discussed. The results received with each fit in figure 4.5 are listed in the table 4.3. The parameters for the real space representation are the same as in 4.2.

Table 4.3: With a least squares method calculated values for $\bar{\lambda}_{\min}^f$ associated with the function of equation (4.4). The values corresponds to the functions displayed in figure 4.5 and the values of U_c/W are calculated via equation (3.52) with $W = 4t$ in one dimension. The values $\bar{\lambda}_{\min}^{\tilde{f}}$ and $\bar{\lambda}_{\min}^{\bar{f}}$ are determined by a LH fit using only the results of the first respectively the last three loops. With equation (4.3) the uncertainty for $\bar{\lambda}_{\min}^f$ is determined.

representation	$-\bar{\lambda}_{\min}^{\tilde{f}}/t$	$-\bar{\lambda}_{\min}^{\bar{f}}/t$	$-\bar{\lambda}_{\min}^f/t$	U_c/W
real space	2.003	2.000	2.001 ± 0.005	1.0003 ± 0.0024
k-space	1.9992	2.000	1.998 ± 0.016	0.999 ± 0.008

The first noticeable observation is that both calculated critical interaction strengths U_c of in each representation in table 4.3 are close to equal. The absolute difference between the two resulting critical interaction strength is only $\Delta U_c/W = 14 \cdot 10^{-4}$ with is smaller than the uncertainty in both values. Therefore, the result obtained with the momentum space representation is in perfect agreement with the result of the real space representation. Consequently, the momentum space representation is better suited than the real space representation since it requires fewer operators for the same result. Another observation concerning the uncertainties in the different results. Compared to the real space representation, the value of the uncertainty of U_c in the momentum space is more than three times as big. Furthermore, already in figure 4.5 slight deviations of the determined functions $\tilde{f}$ and $\bar{f}$ from the calculated values of $\lambda_{\min}^m$ can be noticed in the momentum space representation. This suggests that the used empirical function of equation (4.4) is not as fitting for the momentum space representation as for the real space representation. Despite this, the function f is still the most fitting function among the other function used and the increase in the uncertainty is not so high that this become a problem. Hence, the empirical function in equation (4.4) is still sufficient to determine U_c in the momentum space representation.

Local four-dimensional Hilbert space $\mathcal{H}_4^L$

Now turning to the more so far problematic $\mathcal{H}_4^L$ case. As in the first case, the dispersion for $\lambda_{\min}^m(\mathbf{k})$ is displayed in figure 4.6, when $h_{\mathbf{k},\uparrow}^\dagger$ respectively $d_{\mathbf{k},\uparrow}^\dagger$ is used as an initial operator. Again the spin orientation is not relevant, and we expected the lowest value of $\lambda_{\min}^i(\mathbf{k})$ at critical point in the Brillouin zone. The first noticeable point concerning the

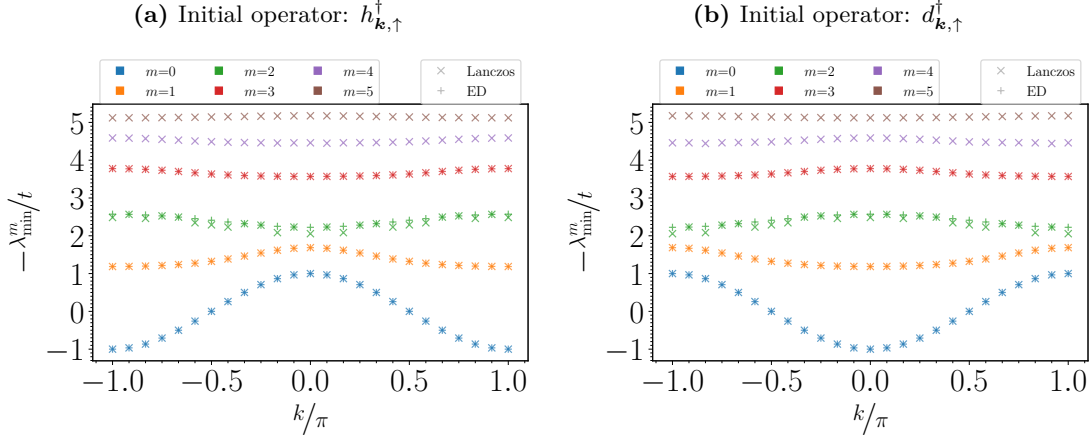


Figure 4.6: Dispersion relation of the lowest eigenvalue $\lambda_{\min}^m(\mathbf{k})$ is displayed in the first Brillouin zone for different loops and initial operators. The Hamiltonian used is from (4.1) and the local operators act on $\mathcal{H}_4^L$. In figure 4.4a the initial operator is a creator of a hole $h_{\mathbf{k},\uparrow}^\dagger$ and in figure 4.4b a creator of a double occupation site $d_{\mathbf{k},\uparrow}^\dagger$. Up to $m = 3$ also results of an exact diagonalization ED are displayed.

two dispersion relations in figure 4.6 is that again no convergence can be observed. While the observation that the dependence of $\lambda_{\min}^m(\mathbf{k})$ on the momentum vector $\mathbf{k}$ decreases with each loop, for both the $\mathcal{H}_2^L$ and the $\mathcal{H}_4^L$ case applies. Also, the shift of π between the two different dispersion relations and therefore the particle-hole symmetry like in the $\mathcal{H}_2^L$ can be observed. Whereas the associated value of $\mathbf{k}$ for the lowest value of $\lambda_{\min}^m(\mathbf{k})$ is not constant with each loop like in the $\mathcal{H}_2^L$ case, even though the position is still either $\mathbf{k} = 0$ or $\mathbf{k} = \pi$. This observation is due to the fact that in the operator basis for both $h_{\mathbf{k},\uparrow}^\dagger$ and $d_{\mathbf{k},\uparrow}^\dagger$ there are also operators from the respective other. Where in the $\mathcal{H}_2^L$ case these operators are strictly separated from each other. Therefore, for further examinations in the momentum space for the $\mathcal{H}_4^L$ we use the results of the $\mathcal{H}_2^L$ case where the lowest value for $h_{\mathbf{k},\uparrow}^\dagger$ is located at 0 and for $d_{\mathbf{k},\uparrow}^\dagger$ at π . Furthermore, figure 4.6 also shows results where the eigenvalue $\lambda_{\min}^i(\mathbf{k})$ are calculated with an exact diagonalization ED of the Liouville matrix, since the values $\lambda_{\min}^{m=2}(\mathbf{k})$ calculated with the Lanczos algorithm show an unusual behavior for the loop $m = 2$ which is the formation of local extrema in the areas between the characteristic points of the Brillouin zone. Compared to the solution with ED the Lanczos algorithm is not able to calculate the correct lowest eigenvalue with the initial vector of equation (3.37). That suggests again that this problem rises due to the operator basis contains both types of operators $h_{\mathbf{k},\uparrow}^\dagger$ and $d_{\mathbf{k},\uparrow}^\dagger$. The figure 4.7 displays the difference between the momentum and real space representations for the creator of a hole, showing in each case the size of the operator basis as well as the corresponding

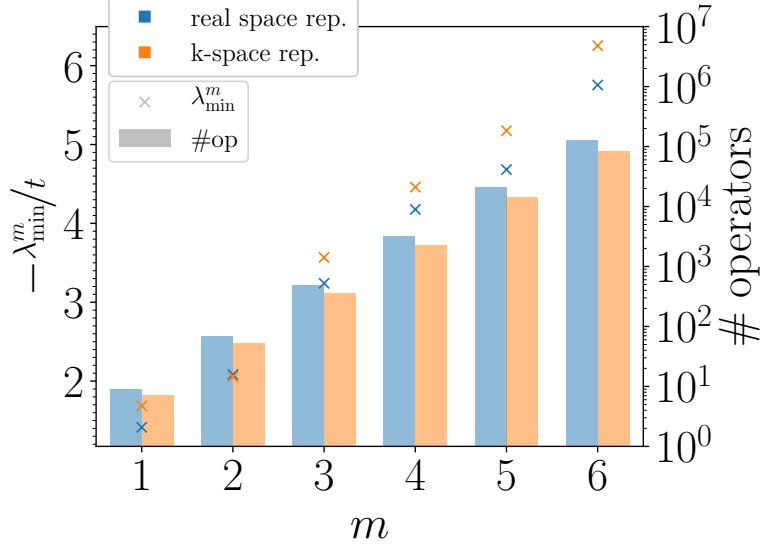


Figure 4.7: Results for the Hamiltonian of (4.1) on a one-dimensional chain with $\mathcal{H}_4^L$, one real space and the other in momentum space(k-space). Lowest eigenvalues $\lambda_{\min}^m$ of the Liouville matrices $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ and $\mathbf{M}_{T_0}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ and the size of the corresponding operator basis $\mathcal{O}_m$ for the m -loop are shown.

lowest eigenvalues $\lambda_{\min}^m$ in each loop m . The figure 4.7 illustrates once again the lack of convergence in $\lambda_{\min}^m$ for the $\mathcal{H}_4^L$ case. Nevertheless, $\lambda_{\min}^m(\mathbf{k} = 0)$ is always higher than $\lambda_{\min}^m$ in the real space representation which also observed for the $\mathcal{H}_2^L$ case indicates that the momentum representation holds more information regarding the energy gap. One exception is the loop $m = 2$ where $\lambda_{\min}^m(\mathbf{k} = 0) > \lambda_{\min}^m$. This is the result of the fact that the lowest $\lambda_{\min}^m(\mathbf{k})$ is not at $\mathbf{k} = 0$, but at $\mathbf{k} = \pi$, as shown in figure 4.6a, which was already discussed above. For other loops, a different $\mathbf{k}$ position of the lowest value also applies, but since the $\mathbf{k}$ dependence is reduced for higher loops, this is only observed at $m = 2$. Another observation regards the size of the operator basis. The size of operator basis in the momentum representation is still lower than in its real space representation. But where for the $\mathcal{H}_2^L$ case the difference was a factor that was approximately equal to 2 between the two representations for the loops observed, the factor for the $\mathcal{H}_4^L$ case is only approximately 1.5.

So for the $\mathcal{H}_4^L$ case the advantages of the momentum representation regarding the size of the operator basis is not high as in the $\mathcal{H}_2^L$ case. After all, the results obtained by the approach with $\mathcal{H}_4^L$ in the two representations still contradict both the results of the $\mathcal{H}_2^L$ case and the predicted behavior of $\lambda_{\min}^m$ described in section 3.1. This discrepancy demands further detailed investigation of the $\mathcal{H}_4^L$ results which is part of the next section.

4.3 More detailed treatment of the results for the four-dimensional local Hilbert space

In this section we seek for a better understanding of the observation obtained for the $\mathcal{H}_4^L$ case. In contrast to the $\mathcal{H}_2^L$ case the $\mathcal{H}_4^L$ case did not show any of the predicted convergence behavior for the lowest eigenvalue $\lambda_{\min}^m$ of the Liouville matrix in real space as well as in momentum representation for the simple Hamiltonian in equation (4.1).

First we look at the conceptual differences between the $\mathcal{H}_2^L$ and $\mathcal{H}_4^L$ cases. If we recall section 3.2, there is one major difference between the two different case in the operators used which results from the choice of the local Hilbert space. While in the $\mathcal{H}_4^L$ case operators all local operators are allowed due to the fact that all possible states are taken into account, local Operators of the groups $\mathcal{Q}_{10}$ and $\mathcal{Q}_{11}$ are neglected in the $\mathcal{H}_2^L$ case due to the only two possible states in the half-filled system. So in the $\mathcal{H}_4^L$ case operators occur describing processes which are not possible in the half-filled case. This process are in the following labeled as virtual processes. The results of these virtual process are still the same as the initial operator of example for $h_{i,\uparrow}^\dagger$ effectively inserting a DO in the form of a hole in the system. But they require already DOs in the system to yield a non-zero result, which is not the case for half-filling. As a result the operators in the $\mathcal{H}_4^L$ case can be further categorized based on the number u how many DOs they required. Of interest is now the share of operators with different u in the operator basis for various amount of loops m . The figure 4.8 shows this relation for the results of figure 4.8 for both representations. With figure 4.8 it becomes apparent that already after the second

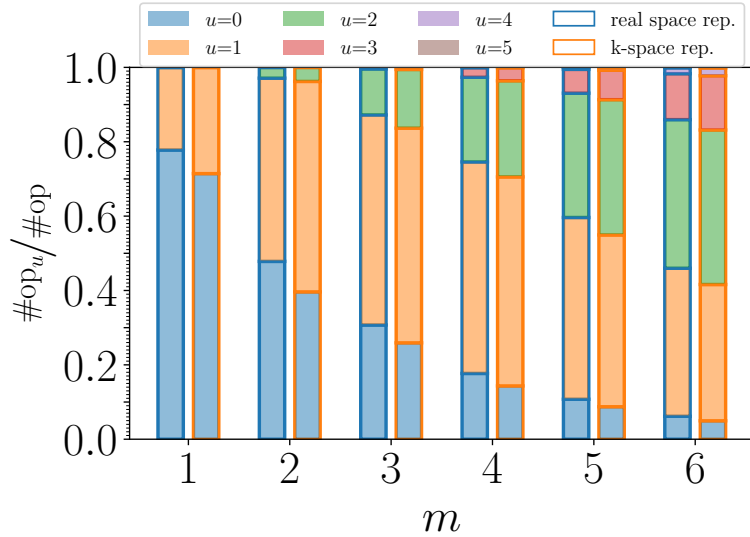


Figure 4.8: Ratio between the number of operators with a certain u and the size of the operator basis $\mathcal{O}_m$ for different loops m . The operators correspond to those used in figure 4.7.

loop operators describing virtual processes ($u > 0$) are dominant in the operator basis for the $\mathcal{H}_4^L$ case in both representations. Whereby in the momentum space representation the share of operators with higher u value are slightly higher than in the real space representation. With these results the missing convergence in the $\mathcal{H}_4^L$ can be interpreted in such a way that with each loop new energy areas connected to the process of inserting an DO in a System where already u DOs are presented. Since with each further loop new operator occur connected to the next higher energy area it is not possible that $\lambda_{\min}^m$ converges. It was not possible to find a subspace in the Liouville matrix where only operators with $u = 0$ contribute. Instead, a convergence behavior for $\lambda_{\min}^m$ in the $\mathcal{H}_4^L$ case could be achieved by dropping simply all operators with $u > 0$ of the operator basis. This approach only serves as a confirmation that those virtual operators take responsibility for the missing observation of the convergence behavior of $\lambda_{\min}^m$ in the $\mathcal{H}_4^L$ case and should not be considered here to determine an U_c . Since the Frobenius scalar product for the $\mathcal{H}_4^L$ cases takes not the strict half-filled disordered system into account. So for this purpose the $\mathcal{H}_2^L$ case should be used instead. Now the issue of whether to use the $\mathcal{H}_4^L$ or the $\mathcal{H}_2^L$ case is resolved, but for now the $\mathcal{H}_4^L$ case is not closed yet. Instead, another analysis possible with the iEoM approach is presented with the results of the $\mathcal{H}_4^L$ case.

So far only the eigenvalues of the Liouville matrix are used but it is also possible to take the eigenvectors v_i to all corresponding eigenvalues λ_i of the Liouville matrix into account. As a consequence, an exact diagonalization ED of the Liouville matrix is necessary, which limits the amount of possible loops m since ED is not as feasible for large matrices as the Lanczos algorithm. When looking at equation (2.20) and equation (2.32), the eigenvectors v_i together with the coefficient α_i contain information about the amplitude of each oscillation with corresponding eigenvalue λ_i for each operator in the operator basis. Therefore, it is possible to assign an eigenvalue λ_i to certain operators in the operator basis according to the corresponding eigenvector. Thereby the absolute square of an element i of an eigenvector v_i serves as a measure of the share of the operator A_i . Furthermore, the coefficients α_i can be determined with the eigenvector v_i and the initial condition in equation (2.27) for the iEoM approach. The square of α_i can be interpreted as a weight of an eigenvalue λ_i towards the time evolution of the operator $A(t)$. If the coefficient α_i is zero, the corresponding eigenvalue λ_i has a vanishing contribution for the time evolution of the operators $A(t)$. Where α_i is calculated via

$$\alpha_i = \mathbf{h}(t=0) \cdot \mathbf{v}_i . \quad (4.8)$$

In the following figure 4.9 α_i^2 is shown for all λ_i for different amount of loops m and in the two representations with a creator of a hole $h_{i,\uparrow}^\dagger$ being the initial operator. Because some eigenvalues are degenerated or tend to be real close together, a histogram is used for better illustration with the width of the bins being $0.1t$. For the momentum representations the initial operator is $h_{\mathbf{k}=0,\uparrow}^\dagger$, since for the band gap in the $\mathcal{H}_2^L$ case, the best result is by $\mathbf{k} = 0$. The results in the real space representation in figures 4.9a-4.9d are all symmetric around zero and show the following behavior. The weights accumulate for values of λ_i in the area around $-2t$ respectively $2t$ for increasing number of loops. For even-numbers of the loop m also a peak is found at $\lambda_i = 0$. Where in higher loops all other eigenvalues $|\lambda_i| > 2t$ have a nearly vanishing weight. So the weight α_i^2 of the eigenvalues which result

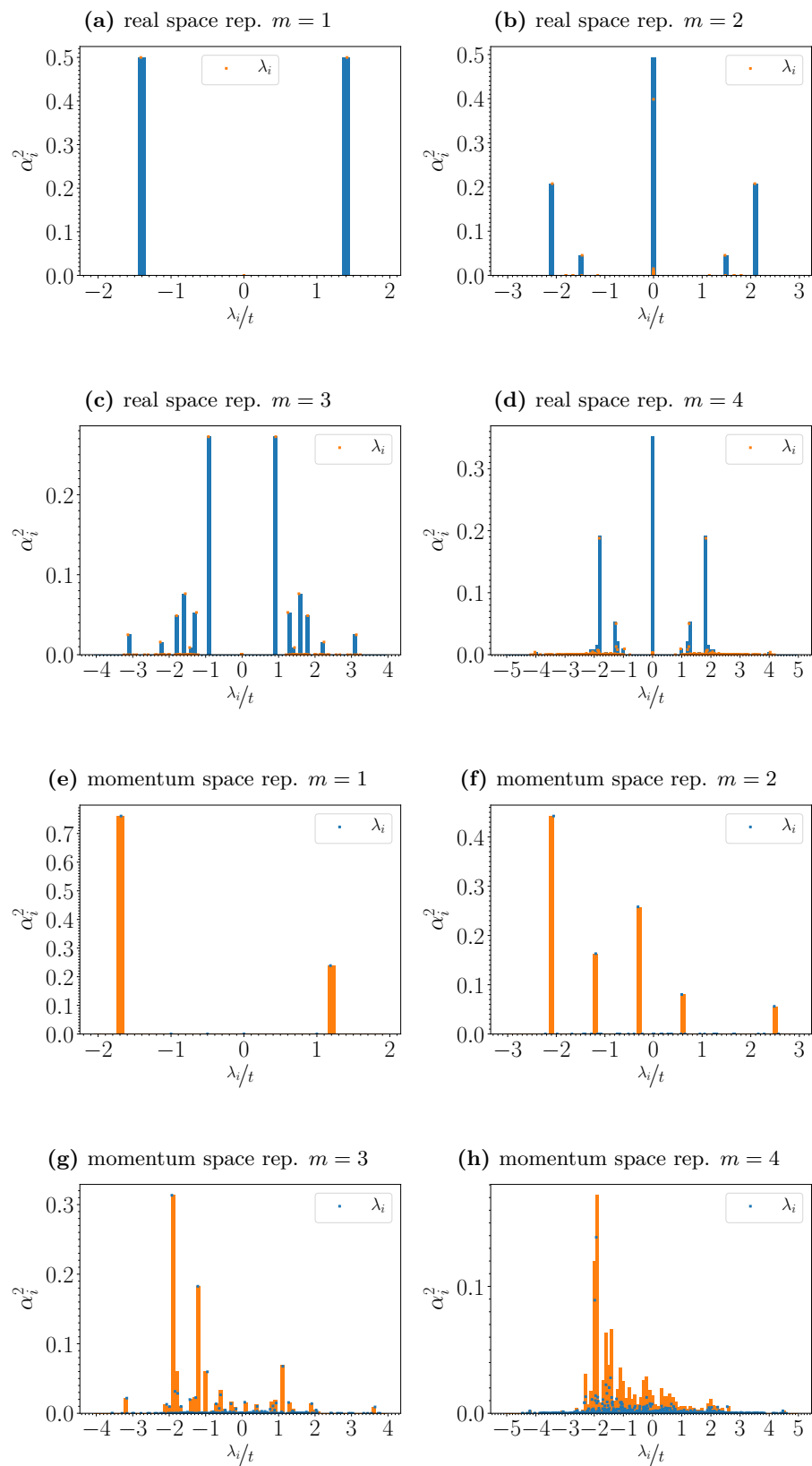


Figure 4.9: The coefficients for the initial condition of the iEoM approach α_i^2 for all eigenvalues λ_i of the Liouville matrix for different loops m for the $\mathcal{H}_4^L$ case together with a histograms accumulating the weights α_i^2 of λ_i within a bin size of $0.1t$ are illustrated. The figures 4.9a-4.9d show λ_i of $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ for the real space representation and figures 4.9e-4.9h show λ_i of $\mathbf{M}_{T_0}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ for the momentum space representation.

in the non-convergence behavior in the $\mathcal{H}_4^L$ case tend to drop in the higher loops. For the results in the momentum space representation in figures 4.9e-4.9h an almost similar observation can be made. With the difference that here the results are not symmetric around zero which applies for the weights α_i^2 as well as the eigenvalues λ_i . Furthermore, the distribution of the α_i^2 weights is shifted so that the eigenvalues $\lambda_i < 0$ have higher weights. Where the dispersion relation in figure 4.6a demands for $m = 2$ a shift in $\mathbf{k}$ to achieve the lowest $\lambda_{\min}^m$. In figure 4.9f a shift to $\mathbf{k} = \pi$ would only results in a shift of the weighs towards higher λ_i . However, since the lowest weighted λ_i is of interest, the observation endorses the assumption already made that the observation in figure 4.6a is due of both operators of holes and operators of doubly occupied sites being both part of the operator basis and $\mathbf{k} = 0$ is the correct value for the creator of a hole. Despite this, the significant weighted eigenvalues λ_i for higher loops are again located in the area of $-2t$ and for all $|\lambda_i| > 2t$ the weights nearly vanish. These observations indicate that the eigenvalues significantly weighted with α_i^2 shows a so far not detected convergence behavior. Though, to investigate this behavior in higher loops, the problem is that the Liouville matrix must be solved with ED, with is simply not feasible for higher loops due to the size of the Liouville matrix. Therefore, it is not clear if these observations still hold for higher loops. Assuming this is the case, the convergence behavior should not be evaluated as a possibility to determine the energy gap for single charge excitation in the half-filled case. Since the $\mathcal{H}_4^L$ case simply does not correctly match the physics for the half-filled case. Rather, the presented result should demonstrate other possibilities which can be used to in the iEoM approach to analyze the properties of the studied system.

In conclusion, the $\mathcal{H}_4^L$ case is not applicable to examine the problem. But a new concept concerning the eigenvalues λ_i of the Liouville matrix was explored with the $\mathcal{H}_4^L$ case where the eigenvalues λ_i were weighted with the factor α_i which are connected to the initial condition and the corresponding eigenvector $\mathbf{v}_i$. Henceforth, only the $\mathcal{H}_2^L$ case is used to calculate the energy gap and the $\mathcal{H}_4^L$ case is no longer treated. But since this section showed the necessity to look at the values of α_i , the next section deals with them in the $\mathcal{H}_2^L$ case.

4.4 Considering initial conditions for the results in the two-dimensional Hilbert space

In the previous section dealt with the impact of the initial conditions in the $\mathcal{H}_4^L$ case towards the eigenvalues' contribution to the time evolution. Here the same examination is done for the $\mathcal{H}_2^L$ case. The figure 4.10 shows the calculated α_i^2 via equation (4.8) in dependence on the corresponding eigenvalue λ_i and also a histogram accumulating the weights of α_i^2 within a bin size of $0.1t$. Again the initial operator is a creator of a hole $h_{i,\uparrow}^\dagger$ and in the momentum representation the operator $h_{\mathbf{k}=0,\uparrow}^\dagger$ is chosen accordingly to the results of the dispersion relation in figure 4.4a. The most important observation in figure 4.10 is that in both representations the weights α_i^2 of $\lambda_{\min}^m$ is for every calculated loop m non-zero in contrast to the $\mathcal{H}_4^L$ case. Therefore, the procedure for determining

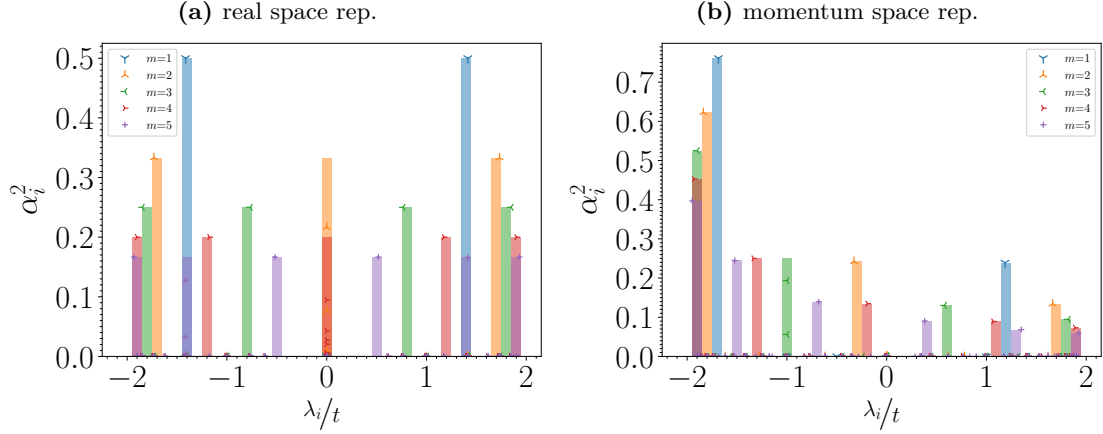


Figure 4.10: The coefficients for the initial condition of the iEoM approach α_i^2 for all eigenvalues λ_i of the Liouville matrix for different loops m for the $\mathcal{H}_2^L$ case together with a histogram accumulating the weights α_i^2 of λ_i within a bin size of $0.1t$ are illustrated. The figure 4.10a shows λ_i of $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ for the real space representation and figure 4.10b shows λ_i of $\mathbf{M}_{T_0}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ for the momentum space representation.

the energy gap, which is described in section 3.6, needs no modification in the $\mathcal{H}_2^L$ case assuming that this behavior carries on for higher loops $m > 5$. For the real space representation in figure 4.10a the distribution of the weights and eigenvalues is again symmetric around zero and for each even loop m a peak shows at zero. But furthermore in each loop m all accumulated non-zero weights in the histogram are equal. Where with each loop m the total weight is only distributed between $m+1$ values of λ_i . This also holds for the momentum space representation although the symmetries for the eigenvalues as well as in the accumulated non-zero weights are broken. Where the weights are shifted in favor of the lowest eigenvalue $\lambda_{\min}^m$. Thus, in the momentum space representation, the lowest eigenvalues is therefore also the most weighted eigenvalue.

All in all the results indicates that the method in section 3.6 is the path to follow for further energy gap calculations in the $\mathcal{H}_2^L$ case. Since the Lanczos algorithm is capable of determine the eigenvector for the lowest eigenvalue $\lambda_{\min}^m$, a calculation of the corresponding α_i^2 can serve as a short check whether the lowest eigenvalue still has a non-zero weight in further calculations.

4.5 Extension of the simple model to a two-dimensional square lattice

In the previous section all calculations take place in one dimension and now in this section the iEoM approach is again applied to a Hamiltonian

$$H_{2D} = T_0 + H_{\text{int}} \quad (4.9)$$

which has the same form as in equation (4.1), but now the simple NN DOs hopping T_0 takes place on a two-dimensional square lattice. As indicated in the previous section for higher dimension the $\mathcal{H}_4^L$ case is no longer part of the calculated cases. Here only the $\mathcal{H}_2^L$ case serves as a tool to determine an energy gap. The fact that a higher dimension Hamiltonian is used has no direct influence on the approach to determine the energy gap. Only the higher dimension most likely increases the size of the used operator basis in each loop. Therefore, the procedure is the same as in the one-dimensional case and thus figure 4.11 displays already both the results in the real space and the momentum space representation. Hence, figure 4.11 shows the lowest eigenvalue $\lambda_{\min}^m$ of $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ and the size of the operator basis for both representations. Again the trivial case for $m = 0$ is not taken into consideration. Of course, for the momentum space representation a value for $\mathbf{k}$ needs to be chosen so that $\lambda_{\min}^m(\mathbf{k})$ is minimal there. Calculation showed that in the

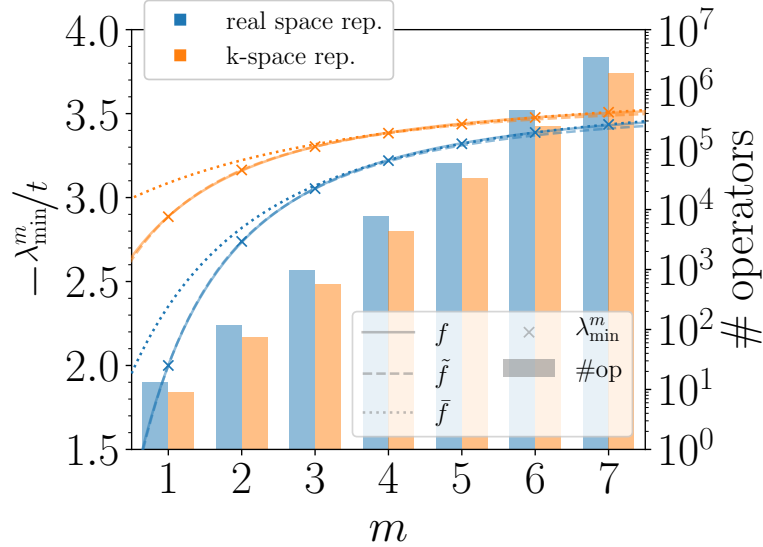


Figure 4.11: Results for the Hamiltonian of (4.9) on a two-dimensional square lattice with $\mathcal{H}_2^L$, one in real space and the other in momentum space(k-space). Lowest eigenvalues $\lambda_{\min}^m$ of the Liouville matrices $\mathbf{M}_{T_0}^m(h_{i,\uparrow}^\dagger)$ and $\mathbf{M}_{T_0}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ and the size of the corresponding operator basis $\mathcal{O}_m$ for the m -loop are shown. Also, three LS fits for each representation are displayed where f uses all values of $\lambda_{\min}^m$ and $\tilde{f}$ and $\bar{f}$ use the results of the first respectively the last three loops.

two-dimensional case for $h_{\mathbf{k},\uparrow}^\dagger$ the minimum is located at the center of the Brillouin zone $\mathbf{k} = (0,0)^T$ and that the dispersion relation is rotationally symmetric around the center of the Brillouin zone. The lowest point of $\lambda_{\min}^m(\mathbf{k})$ for the operator creating a doubly occupied site $d_{\mathbf{k},\uparrow}^\dagger$ is located at the corner points of the Brillouin zone for example $\mathbf{k} = (\pi, \pi)^T$. Also, as in the one dimension case three function are fitted to the calculated values of $-\lambda_{\min}^m(\mathbf{k})$ in the form of equation (4.4) in which the parameters are determined by the least squares method. The functions determined by the LS method are also displayed in figure 4.11. As in one dimension, the uncertainty for $-\bar{\lambda}_{\min}$ is again determined with the functions $\tilde{f}$ and $\bar{f}$. All necessary values of f , $\tilde{f}$ and $\bar{f}$ shown in figure 4.11 to determine U_c and the corresponding uncertainty are listed in table 4.4 for the two different representation.

Table 4.4: With a least squares method calculated values for $\bar{\lambda}_{\min}^f$ associated with the function of equation (4.4). The values corresponds to the functions displayed in figure 4.11 and the values of U_c/W are calculated via equation (3.52) with $W = 8t$ in two dimension. The values $\bar{\lambda}_{\min}^{\tilde{f}}$ and $\bar{\lambda}_{\min}^{\bar{f}}$ are determined by a LH fit using only the results of the first respectively the last three loops. With equation (4.3) the uncertainty for $\bar{\lambda}_{\min}^f$ is determined.

representation	$-\bar{\lambda}_{\min}^{\tilde{f}}/t$	$-\bar{\lambda}_{\min}^{\bar{f}}/t$	$-\bar{\lambda}_{\min}^f/t$	U_c/W
real space	3.56	3.64	3.58 ± 0.17	0.90 ± 0.04
k-space	3.58	3.66	3.60 ± 0.23	0.90 ± 0.06

Apparently, the iEoM approach for the simple model on a two-dimensional square lattice for the can only reach 7 loops after that the operator basis size reaches already the critical size. As a consequence, the difference between the last calculate value of $\lambda_{\min}^m$ and the estimated lower bound $\bar{\lambda}_{\min}$ is significantly higher than before in one dimension. Therefore, the influence of the chosen empirical function to $\bar{\lambda}_{\min}$ is higher than in one-dimension. To assess the quality of the empirical function, we look again at the difference between the results for $\bar{\lambda}_{\min}^{\tilde{f}}$ and $\bar{\lambda}_{\min}^{\bar{f}}$ in both representations. The difference for both representations is around an order of $7 \cdot 10^{-2}$. This is noticeably higher than before in one dimension. This indicates that the empirical function which already used in one dimension is not as suitable in two dimension. However, the uncertainty in two dimension is small enough that the function f is still sufficient to give an estimation for $\bar{\lambda}_{\min}$. When comparing the results for the critical interaction strength in the different representation, the absolute difference between them is below the uncertainty for both values. Therefore, the two representations in two dimension as before in one dimension yield identical results. But same as in one dimension the function f tends to yield smaller uncertainties for the results with the real space representation. Despite the slight higher uncertainty, the advantages of the momentum space representation are clearly seen in figure 4.11. With fewer operators in the operator basis, the lowest eigenvalues $\lambda_{\min}^m$ in the momentum space representation are always nearer to the estimate value of $\bar{\lambda}_{\min}$ in each loop m . Whereby the size difference of the operator bases is again approximately a factor of two between the two representations. Hence, the calculated value for the critical interaction strength the simple model on a

two-dimensional square lattice according to the momentum space representation is

$$\frac{U_c}{W} = 0.90 \pm 0.06 . \quad (4.10)$$

The representation of the results as the ratio between the critical interaction strength U_c and the bandwidth W make a comparison between the dimensions possible. Where for the simple model in one dimension the interaction strength is equal the bandwidth $W = 4t$, it might be assumed that this also apply to the simple model in two dimension with the bandwidth $W = 8t$. But apparently, with the results obtained in section 4.5, this not applies for the simple model on a two-dimensional square lattice. Instead, the band gap starts to open already for $U_c = 0.90 \pm 0.06W$ for the simple model in two dimension. The next step is to extend the simple model both in one and two dimension with the spin dependent hopping described in detail in section 2.2. This is part of the next following sections.

4.6 Spin dependent hopping on a one-dimensional chain

As we applied already the iEoM approach to a simple model both in one and in two dimension and determined a critical interaction strength U_c for both dimension, the next step is to expand the simple model by adding terms, which describe simple and spin dependent next nearest neighbor hopping of a DO which are discussed in section 2.2, to the simple Hamiltonian. In this section this is done for the one-dimensional chain. As in section 2.2 already mentioned, not all terms of the complete Hamiltonian of equation (2.14) are present in the one dimension. This includes the terms T'_0 and $T'_{s,0}$ which describe the diagonal NNN hopping. Therefore, the Hamiltonian for spin dependent DO hopping reads as

$$H_{\text{eff}} = T_0 + T''_0 + T''_{s,0} + H_{\text{int}} . \quad (4.11)$$

in one dimension. The amplitudes of the different hopping terms can be expressed in terms of the simple hopping t_0 . Where the exact value for t'' as well as t''_s is extracted from Ref. [21] in the area of $W/U = 1$ with $t'' = -0.05t_0$ and $t''_s = 0.1t_0$. Therefore, to determine the critical interaction strength U_c for the spin dependent system with the iEoM using operators in the momentum space representation, the approach is the same as for the simple model, described in section 4.2 with one difference. Due to equation (4.11), more terms are presented in the Liouville operator of each local operator in the $\mathcal{H}_2^L$ case. As a consequence, the operator base is expected to grow faster in each loop than in the simple case. Since new terms are presented, it seems appropriated to investigate the dispersion relation of the lowest eigenvalue $\lambda_{\min}^m(\mathbf{k})$ of $\mathbf{M}_{\sum T_i}^m(h_{\mathbf{k},\uparrow}^\dagger)$. The figure 4.12 shows the dispersion relation of $\lambda_{\min}^m(k)$ for different loop m and different initial operators $h_{\mathbf{k},\uparrow}^\dagger$ and $d_{\mathbf{k},\uparrow}^\dagger$. Comparing both dispersion relation of figure 4.12 the particle hole symmetry is also presented within the result with the spin dependent Hamiltonian of equation (4.11). However, the dispersion relation of the zeroth loop $m = 0$ takes up a large part in both

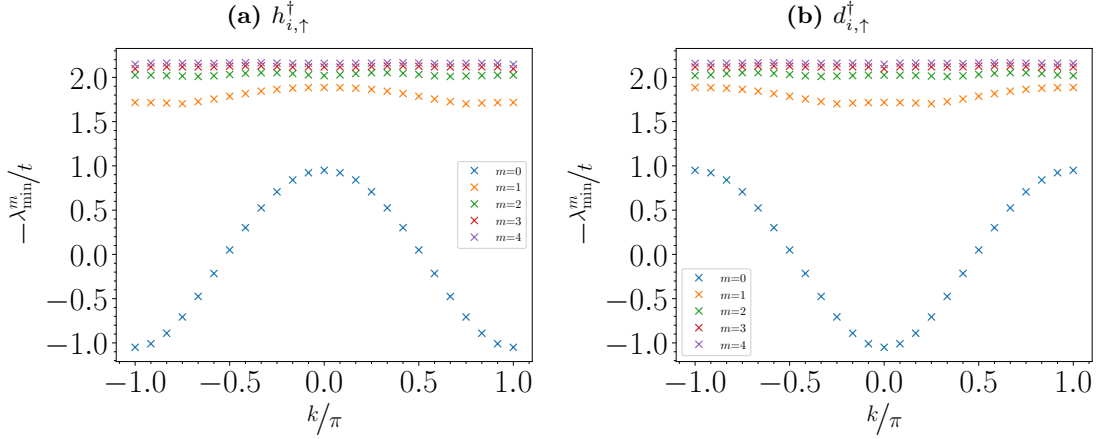


Figure 4.12: Dispersion relation of the lowest eigenvalue $\lambda_{\min}^m(\mathbf{k})$ is displayed in the first Brillouin zone for different loops and initial operators. The Hamiltonian (4.1) is used and the local operators act on $\mathcal{H}_2^L$. In figure 4.12a the initial operator is a creator of a hole $h_{\mathbf{k},\uparrow}^\dagger$ and in figure 4.12b a creator of a double occupation $d_{\mathbf{k},\uparrow}^\dagger$.

figures leaving the behavior of the dispersion relation for higher loops rather hidden. Therefore, in figure 4.13 the dispersion relation of $\lambda_{\min}^m(\mathbf{k})$ for $h_{\mathbf{k},\uparrow}^\dagger$ is shown for $m > 0$. With figure 4.13 it is possible to see that in contrast to the simple case the value of $\mathbf{k}$

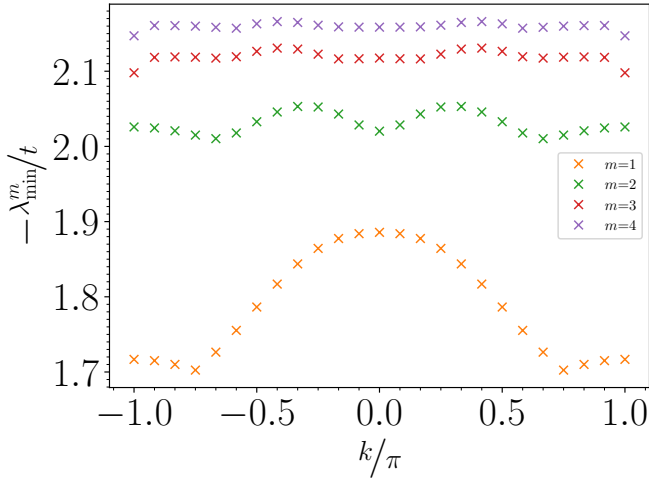


Figure 4.13: Dispersion relation of the lowest eigenvalue $\lambda_{\min}^m(\mathbf{k})$ for $h_{\mathbf{k},\uparrow}^\dagger$ and $m > 0$ is displayed in the first Brillouin zone. The Hamiltonian (4.1) is used and the local operators act on $\mathcal{H}_2^L$.

where $\lambda_{\min}^m(\mathbf{k})$ is minimal tends to move for higher loops. Where for $m = 0$ and $m = 1$ the minimal $\lambda_{\min}^m(\mathbf{k})$ is located at $\mathbf{k} = 0$, the minimal splits up into two separate ones at $m = 2$, which move for higher m towards $\mathbf{k} = -0.5$ respectively $\mathbf{k} = 0.5$. In addition, the effect that for higher loops the dispersion relation flattens is still present. As a consequence, it is still fine to use $\lambda_{\min}^m(\mathbf{k})$ at $k = 0$ to determine $\bar{\lambda}_{\min}$ but the value of $\lambda_{\min}^{m=2}(\mathbf{k} = 0)$ is not considered in the LS method since the effect which flattens the dispersion relation in higher loops is not strong enough for $m = 2$. The figure 4.14 show the values of $\lambda_{\min}^m(\mathbf{k} = 0)$ and

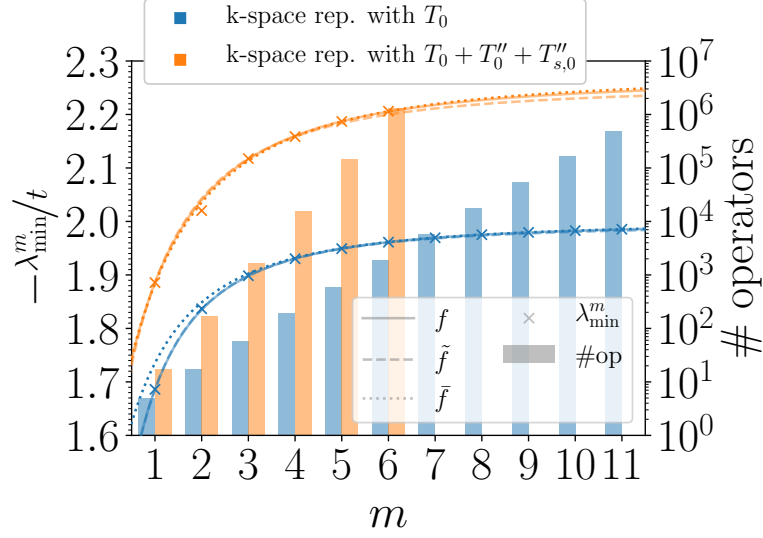


Figure 4.14: Results for the Hamiltonians of (4.11) and (4.1) on a one-dimensional chain with $\mathcal{H}_4^L$, both in moment space(k-space). Lowest eigenvalues $\lambda_{\min}^m$ of the Liouville matrix $\mathbf{M}_{\sum T_i}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ with T_i from the Hamiltonian (4.11) and $\mathbf{M}_{T_0}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ and the size of the corresponding operator basis $\mathcal{O}_m$ for the m -loop are shown. Also, three LS fits for each result are displayed where f uses all values of $\lambda_{\min}^m$ and $\tilde{f}$ and $\bar{f}$ use the results of the first respectively the last three loops.

the size of the operator basis for the iEoM approach using the spin dependent Hamiltonian up to a loop of $m = 6$. For a comparison the previous results for the simple Hamiltonian in one-dimension are also displayed in figure 4.14. The values to determine an estimation for the critical interaction strength U_c are listed in table 4.5 for both sets of parameters used in figure 4.14.

Table 4.5: Values of $\bar{\lambda}_{\min}^f$ associated with the function of equation (4.4). The values corresponds to the functions displayed in figure 4.14 and the values of U_c/W are calculated via equation (3.52) with $W = 8t$ in two dimension. The values $\bar{\lambda}_{\min}^{\tilde{f}}$ and $\bar{\lambda}_{\min}^{\bar{f}}$ are determined by a LH fit using only the results of the first respectively the last three loops. With equation (4.3) the uncertainty for $\bar{\lambda}_{\min}^f$ is determined.

$\sum T_i$	$-\bar{\lambda}_{\min}^{\tilde{f}}/t$	$-\bar{\lambda}_{\min}^{\bar{f}}/t$	$-\bar{\lambda}_{\min}^f/t$	U_c/W
T_0	1.996	2.000	1.998 ± 0.008	0.999 ± 0.004
$T_0 + T_0'' + T_{s,0}''$	2.25	2.27	2.27 ± 0.04	1.13 ± 0.02

Apparently, when the two estimates of U_c listed in table 4.5 are compared to each other, taking the terms T_0'' and $T_{s,0}''$ causes an increase in the critical interaction strength U_c/W of around 13 % compared that of the simple model with only T_0 . Although, the increase in the uncertainty again indicates that the empirical function f does not fit as well

as in the simple case. But the function is retained since the uncertainty is still small. Furthermore, the consequences for more than one hopping term in the Hamiltonian is visible in figure 4.12 regarding the size of the operator basis. The number of operators rises significantly faster so that for $m = 6$ the critical size is already reached. For the one-dimension chain an exact result is available in Ref. [25] which is

$$\frac{U_c}{W} = \frac{\sqrt{3}}{2} \approx 0.866 . \quad (4.12)$$

When the two results are compared, there is a significant relative deviation of 31 % between our and the exact result. Now the question is how to interpret this deviation. Although in Ref. [25] the movement of a hole in a disordered spin background is also considered the main difference is that in the present work correlations between spins of the order t^2/U are completely neglected and only hopping process of a hole are used where the next nearest neighbor hopping is also in the order of t^2/U . This indicates that these spin correlations also have a not negligible impact on the critical interaction strength. Therefore, the terms in the t - J model describing spin correlations should also be considered up to the order t^2/U . This would have a non negligible impact on the approach discussed in section 3.3 for the $\mathcal{H}_2^L$ case since the Liouville operator of a local operator $\mathcal{Q}_{00}$ with non spin correlations neglected has now a non-vanishing contribution. Solving this issue is not part of this thesis and therefore open for further investigations. The question if this observation also holds for the results of the two-dimensional squared lattice is discussed in the next section.

4.7 Spin dependent hopping on a two-dimensional square lattice

In this section the simple and spin dependent next nearest neighbor hopping is taken into consideration in the case of a two-dimensional square lattice as its done before for the one-dimension chain. Now in comparison to the one-dimension chain all terms of the Hamiltonian in equation (2.14) are used the case of the square lattice. Again the parameters for each hopping amplitude is taken from Ref. [21] in the area of $W/U=1$. The parameter for the various hopping terms read as

$$t'_0 = -0.1 \quad t''_0 = -0.05 \quad t'_{s,0} = 0.1 \quad t''_{s,0} = 0.1 . \quad (4.13)$$

Since in one dimension the dispersion relation of $\lambda_{\min}^m(\mathbf{k})$ for the spin dependent hopping showed an unexpected behavior the dispersion relation is also investigated here. In figure 4.15 the dispersion relation is illustrated up to the loop $m = 2$ where the initial operator for the iEoM approach is both $h_{\mathbf{k},\uparrow}^\dagger$ and $d_{\mathbf{k},\uparrow}^\dagger$. As before, particle hole symmetry is still present in the spin dependent Hamiltonian on a squared lattice. In contrast to the results in one dimension the minima of $\lambda_{\min}^m$ not moves and stay in the same position as in the non spin dependent case, which is for $h_{\mathbf{k},\uparrow}^\dagger$ in the center of the Brillouin zone $\mathbf{k} = (0,0)^T$ and for $d_{\mathbf{k},\uparrow}^\dagger$ in the corner points of the Brillouin zone for example $\mathbf{k} = (\pi, \pi)^T$. Therefore, no adjustments are needed and $\bar{\lambda}_{\min}$ is determined as before in section 4.7. In figure 4.16 the different $\lambda_{\min}^m$ of $\mathbf{M}_{\sum T_i}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ with T_i from the spin-dependent Hamiltonian in

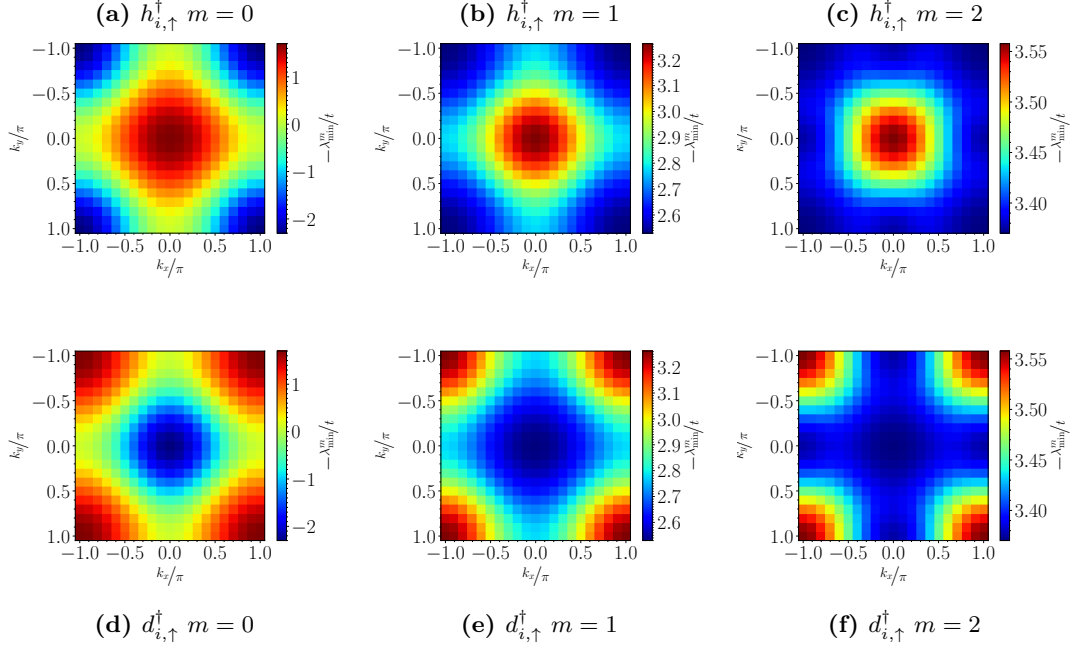


Figure 4.15: Dispersion relation of the lowest eigenvalue $\lambda_{\min}^m(\mathbf{k})$ is displayed in the first Brillouin zone for different loops and initial operators. The Hamiltonian used is from (2.14) and the local operators act on $\mathcal{H}_2^L$. In figures 4.15a-4.15c the initial operator is a creator of a hole and in figures 4.15d-4.15f the creator of a double occupied site is used.

equation (2.14) are shown as well as the results for the simple model of section 4.5 for comparison. For the spin dependent hopping in two dimension on a square lattice the highest possible loop here achieved is $m = 3$. Therefore, the approach to estimate the uncertainty for U_c used before fails. Instead, the uncertainty for U_c is estimated with the determined uncertainty of the simple two dimension model. In table 4.6 the estimation for the critical interaction strength for both results displayed in figure 4.16 is listed together with the values to estimate the corresponding uncertainty if possible.

Table 4.6: With a least squares method calculated values for $\bar{\lambda}_{\min}^f$ associated with the function of equation (4.4). The values corresponds to the functions displayed in figure 4.16 and the values of U_c/W are calculated via equation (3.52) with $W = 8t$ in two dimension. The values $\bar{\lambda}_{\min}^f$ and $\bar{\lambda}_{\min}^f$ are determined by a LH fit using only the results of the first respectively the last three loops. With equation (4.3) the uncertainty for $\bar{\lambda}_{\min}^f$ is determined.

$\sum T_i$	$-\bar{\lambda}_{\min}^f/t$	$-\bar{\lambda}_{\min}^f/t$	$-\bar{\lambda}_{\min}^f/t$	U_c/W
T_0	3.58	3.69	3.61 ± 0.23	0.90 ± 0.06
$T_0 + T'_0 + T'_{s,0}$ $+ T''_0 + T''_{s,0}$	-	-	3.83 ± 0.23	0.96 ± 0.06

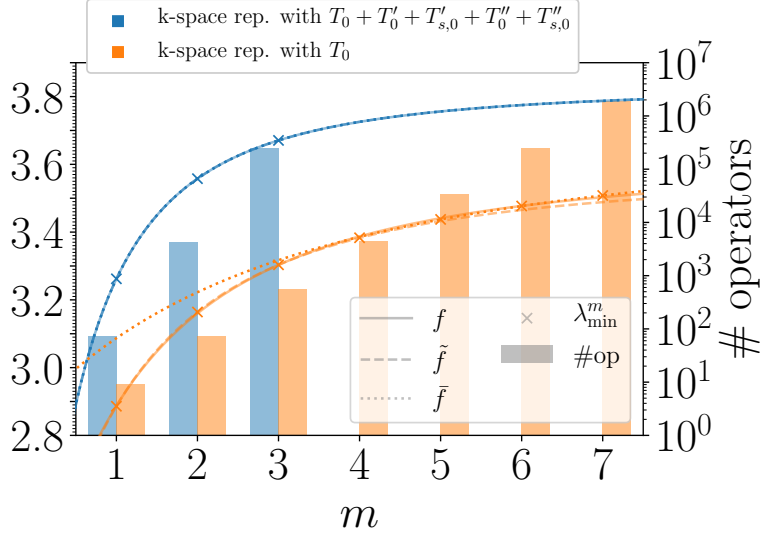


Figure 4.16: Results for the Hamiltonians of (2.14) and (4.1) on a two-dimensional square lattice with $\mathcal{H}_2^L$, both in moment space(k-space). Lowest eigenvalues $\lambda_{\min}^m$ of the Liouville matrices $\mathbf{M}_{\sum T_i}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ with T_i from the Hamiltonian (2.14) and $\mathbf{M}_{T_0}^m(h_{\mathbf{k}=0,\uparrow}^\dagger)$ and the size of the operator basis $\mathcal{O}_m$ for the m -loop are shown. Also three LS fits for the simple Hamiltonian(4.1). Where f uses all values of $\lambda_{\min}^m$. Whereas $\tilde{f}$ and $\bar{f}$ use the results of the first respectively the last three loops.

When the two results for the critical interaction strength in table 4.6 are compared, the expansion of the simple model with simple and spin dependent NNN hopping terms results in an increase of U_c which was also observed in one dimension. The next step is to compare the obtained result of U_c for the Hamiltonian of equation (2.14) on a squared lattice with values of the literature. In Ref. [21] the ratio $W/U_c \approx 0.9$ is determined for the critical interaction strength U_c , which translate to

$$\frac{U_c}{W} \approx 1.11. \quad (4.14)$$

The result was obtained for a generalized t - J model on a two-dimensional square lattice with the Lanczos approach. Although the Hamiltonian of equation (2.14) and the corresponding parameter are taken from the Ref. [21], the relative deviation of 14% raise the question of why the deviation is so high. The difference is that the complete Hamiltonian of Ref. [21] contains spin correlations which are neglected here, since the Hamiltonian of equation (2.14) describes only movements of DOs. This observation confirms the assumption of section 4.6 that the spin correlation should not be neglected. Whether it is possible to reproduce the value of Ref. [21] with the iEoM approach, if also the spin correlations are taken into account cannot be answered here. But this serves as a good test if the approach is extended to consider also spin correlations. This final result concludes the presentation of the results made in this thesis and the next chapter provides a summary of all results as well as an outlook.

5 Summary and outlook

In the course of this thesis the energy gap for single charge excitation in the Fermi-Hubbard model is investigated in a parameter regime where charge fluctuations are suppressed so that a mapping to an effective model namely the t - J model is possible.

As a tool for this purpose the iterated equations of motion approach was introduced. It was discussed how to dissolve the corresponding energy spectrum for a given initial operator by solving the iterated equations of motion. As a result, a necessity for a Hermitian Liouville matrix was identified which was attained with a scalar product preserving unitarity on operator level. In this context a reworked approach of the so called m -loop approach was discussed where operators occurring within a loop are all orthonormal by construction. This was achieved by introducing an orthonormal local operator basis with respect to the Frobenius scalar product.

The solution of the iterated equations of motion for an operator creating a hole respectively a doubly occupied site was established as a possibility to assess the energy gap for single charge excitation in the t - J model. Moreover, two different choices of the local Hilbert space, a four- respectively two-dimensional local Hilbert space, were presented, and different restrictions and advantages for the orthonormal local operator basis regarding the both choices were discussed. The two-dimensional local Hilbert space directly affected the technique discussed for the m -loop approach which resulted in a simplification of the approach. The momentum space representation of the operators used was introduced effectively reducing the size of the operator basis for the iEoM approach around a factor of two without remarkable shortcomings. To cope with the hugely increasing number of operators in the operator basis in higher loops the Lanczos algorithm was introduced. This algorithm was used as a useful tool to evade a full diagonalization, which was not feasible due to the huge size of the Liouville matrices in higher loops, and yet accessing the important features for the estimation of the energy gap even in higher loops.

First results for the two different local Hilbert space choices were obtained for a simple model in one dimension, which only considered simple nearest neighbor hopping of a hole respectively a double occupation. It was not possible to produce converging results towards an energy gap for single charge excitation in the four-dimensional Hilbert space, which was traceable in a detailed analysis of the operators in the operator basis to the missing consideration of half-filling in the four-dimensional space. In contrast, for the two-dimension space this convergence was observed. The estimated values determined with an empirical function for the critical interaction strength were identical in both momentum space and real space representation. Moreover, the results were also in agreement with the zeroth order perturbation theory result in one dimension [25]. Also, results for the simple model applied to a two-dimensional square lattice were calculated but the obtained result

were smaller than the zeroth order result in two dimension. Lastly, next nearest neighbor hopping both simple and spin dependent hopping of a hole and were added to the simple model. Again, the critical interaction strength was examined in both dimensions for the extended model. In one dimension only, an unordinary behavior in the dispersion for the lowest eigenvalue of the Liouville matrix was observed where the minimum of the dispersion was split into two parts which drifted apart from each other. Due to the effect that the dispersion flattened in higher loops and the limited number of possible loops, the drifting of the minima was not examined further here. Compared to the obtained solution for the simple model the adding of the simple and spin dependent next nearest neighbor hopping terms resulted in an increase of the ratio U_c/W between the critical interaction strength U_c and the bare bandwidth W in both dimension. This observation in one dimension is in contradiction to analytical results of Ref. [25] where the ratio is lower than the zeroth order. From this it was concluded that spin correlations have a non-negligible contribution to the critical interaction strength U_c since they were not considered in this approach. In principle this also applies to the two-dimensional model since the difference to the comparable investigation [21] are also the lack of spin correlations. The difference is that the result of [21] determined a higher ration U_c/W than the zeroth order in two dimension. But the estimated ratio is below the zeroth order. Therefore, the consideration of spin correlations is expected to lower the ratio in one dimension where in two dimension it should have an increasing effect on the ratio. To confirm this interpretation, further calculations considering spin correlations in both one and two dimension are therefore mandatory. This in turn is linked to the need to improve the iEoM approach so that more loops are possible. Concepts must be found to limit the size of the operator basis while still allowing the determination of the energy gap. One approach could be to filter operators depending on their weight in the eigenvector of the lowest eigenvalue of the Liouville matrix or to characterize types of operators which have a great weight in the eigenvector of the lowest eigenvalue in each possible loop and look for a pattern which can be used to construct an operator basis which only consists of those operators important for the energy gap.

The strategies to enhance the iEoM approach in this field of application are therefore numerous. However, before these are pursued further, additional studies that consider the spin correlations in the t - J model should be the focus for further development of the iEoM approach in this area.

A Operators of the four-dimensional local Hilbert space

Here all local operators of the four-dimensional local Hilbert space $\mathcal{H}_4^L$ are listed together with corresponding Liouville operators and simplification rules. The normalization factor N for each operator has to be taken separately into consideration for each prefactor α and is not part of the shown operators. As a consequence, the real prefactors $\tilde{\alpha}$ in the case of the Liouville operators in the form

$$\mathcal{L}(\hat{\sigma}_a^i) = \alpha \hat{\sigma}_b^j \hat{\sigma}_c^i. \quad (\text{A.1})$$

reads as

$$\tilde{\alpha} = \alpha \frac{N_a}{N_b N_c}. \quad (\text{A.2})$$

where N_x is the corresponding normalization factor of the operator $\hat{\sigma}_x^i$. For the simplification rules in the form

$$\hat{\sigma}_a^i \hat{\sigma}_b^i = \alpha \hat{\sigma}_c^i. \quad (\text{A.3})$$

the factor is

$$\tilde{\alpha} = \alpha \frac{N_a N_b}{N_c}. \quad (\text{A.4})$$

$d_{i,\uparrow}^\dagger$: **with $N=2$**

Liouville operator: $\mathcal{L}(d_{i,\uparrow}^\dagger) = [T_0, d_{i,\uparrow}^\dagger] + [H_{\text{int}}, d_{i,\uparrow}^\dagger]$

$$[H_{\text{int}}, d_{i,\uparrow}^\dagger] = \frac{U}{2} d_{i,\uparrow}^\dagger \quad (\text{A.5a})$$

$$[T_0, d_{i,\uparrow}^\dagger] = f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger h_{i\pm 1,\downarrow}^\dagger - \sigma_i^+ d_{i\pm 1,\downarrow}^\dagger + \tilde{n}_{i,\downarrow} d_{i\pm 1,\uparrow}^\dagger + \frac{1}{2} d_{i\pm 1,\uparrow}^\dagger \quad (\text{A.5b})$$

simplification rules:

$$d_{i,\uparrow}^\dagger d_{i,\uparrow} = n_i^u + \frac{1}{2} \tilde{n}_{i,\uparrow} + \frac{1}{2} \tilde{n}_{i,\downarrow} + \frac{1}{4} \quad d_{i,\uparrow}^\dagger h_{i,\downarrow} = -f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \quad (\text{A.6a})$$

$$d_{i,\uparrow}^\dagger \tilde{n}_{i,\uparrow} = -\frac{1}{2} d_{i,\uparrow}^\dagger \quad d_{i,\uparrow}^\dagger \tilde{n}_{i,\downarrow} = \frac{1}{2} d_{i,\uparrow}^\dagger \quad (\text{A.6b})$$

$$d_{i,\uparrow}^\dagger \sigma_i^- = -d_{i,\downarrow}^\dagger \quad d_{i,\uparrow}^\dagger n_i^u = -\frac{1}{4} d_{i,\uparrow}^\dagger \quad (\text{A.6c})$$

$d_{i,\downarrow}^\dagger$: **with $N=2$**

Liouville operator: $\mathcal{L}(d_{i,\downarrow}^\dagger) = [T_0, d_{i,\downarrow}^\dagger] + [H_{\text{int}}, d_{i,\downarrow}^\dagger]$

$$[H_{\text{int}}, d_{i,\downarrow}^\dagger] = \frac{U}{2} d_{i,\downarrow}^\dagger \quad (\text{A.7a})$$

$$[T_0, d_{i,\downarrow}^\dagger] = -f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger h_{i\pm 1, \uparrow}^\dagger - \sigma_i^- d_{i\pm 1, \uparrow}^\dagger + \tilde{n}_{i,\uparrow} d_{i\pm 1, \downarrow}^\dagger + \frac{1}{2} d_{i\pm 1, \downarrow}^\dagger \quad (\text{A.7b})$$

simplification rules:

$$d_{i,\downarrow}^\dagger d_{i,\downarrow} = n_i^u + \frac{1}{2} \tilde{n}_{i,\uparrow} + \frac{1}{2} \tilde{n}_{i,\downarrow} + \frac{1}{4} \quad d_{i,\downarrow}^\dagger h_{i,\uparrow} = f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \quad (\text{A.8a})$$

$$d_{i,\downarrow}^\dagger \tilde{n}_{i,\uparrow} = \frac{1}{2} d_{i,\downarrow}^\dagger \quad d_{i,\downarrow}^\dagger \tilde{n}_{i,\downarrow} = -\frac{1}{2} d_{i,\downarrow}^\dagger \quad (\text{A.8b})$$

$$d_{i,\downarrow}^\dagger \sigma_i^+ = -d_{i,\uparrow}^\dagger \quad d_{i,\downarrow}^\dagger n_i^u = -\frac{1}{4} d_{i,\downarrow}^\dagger \quad (\text{A.8c})$$

$d_{i,\uparrow}$: **with $N=2$**

Liouville operator: $\mathcal{L}(d_{i,\uparrow}) = [T_0, d_{i,\uparrow}] + [H_{\text{int}}, d_{i,\uparrow}]$

$$[H_{\text{int}}, d_{i,\uparrow}] = \frac{U}{2} d_{i,\uparrow} \quad (\text{A.9a})$$

$$[T_0, d_{i,\uparrow}] = f_{i,\downarrow} f_{i,\uparrow} h_{i\pm 1, \downarrow} + \sigma_i^- d_{i\pm 1, \downarrow} - \tilde{n}_{i,\downarrow} d_{i\pm 1, \uparrow} - \frac{1}{2} d_{i\pm 1, \uparrow} \quad (\text{A.9b})$$

simplification rules:

$$d_{i,\uparrow} d_{i,\uparrow}^\dagger = -n_i^u - \frac{1}{2} \tilde{n}_{i,\uparrow} + \frac{1}{2} \tilde{n}_{i,\downarrow} + \frac{1}{4} \quad d_{i,\uparrow} d_{i,\downarrow}^\dagger = -\sigma_i^- \quad (\text{A.10a})$$

$$d_{i,\uparrow} f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger = -h_{i,\downarrow} \quad d_{i,\uparrow} \tilde{n}_{i,\downarrow} = \frac{1}{2} d_{i,\uparrow} \quad (\text{A.10b})$$

$$d_{i,\uparrow} \tilde{n}_{i,\uparrow} = \frac{1}{2} d_{i,\uparrow} \quad d_{i,\uparrow} n_i^u = \frac{1}{4} d_{i,\uparrow} \quad (\text{A.10c})$$

$d_{i,\downarrow}$: **with $N=2$**

Liouville operator: $\mathcal{L}(d_{i,\downarrow}) = [T_0, d_{i,\downarrow}] + [H_{\text{int}}, d_{i,\downarrow}]$

$$[H_{\text{int}}, d_{i,\downarrow}] = \frac{U}{2} d_{i,\downarrow} \quad (\text{A.11a})$$

$$[T_0, d_{i,\downarrow}] = -f_{i,\downarrow} f_{i,\uparrow} h_{i\pm 1, \uparrow} + \sigma_i^+ d_{i\pm 1, \uparrow} - \tilde{n}_{i,\uparrow} d_{i\pm 1, \downarrow} - \frac{1}{2} d_{i\pm 1, \downarrow} \quad (\text{A.11b})$$

simplification rules:

$$d_{i,\downarrow} d_{i,\downarrow}^\dagger = -n_i^u + \frac{1}{2}\tilde{n}_{i,\uparrow} - \frac{1}{2}\tilde{n}_{i,\downarrow} + \frac{1}{4} \quad d_{i,\downarrow} d_{i,\uparrow}^\dagger = -\sigma_i^+ \quad (\text{A.12a})$$

$$d_{i,\downarrow} f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger = h_{i,\uparrow} \quad d_{i,\downarrow} \tilde{n}_{i,\uparrow} = \frac{1}{2}d_{i,\downarrow} \quad (\text{A.12b})$$

$$d_{i,\downarrow} \tilde{n}_{i,\downarrow} = \frac{1}{2}d_{i,\downarrow} \quad d_{i,\downarrow} n_i^u = \frac{1}{4}d_{i,\downarrow} \quad (\text{A.12c})$$

$h_{i,\uparrow}^\dagger$: **with $N=2$**

Liouville operator: $\mathcal{L}(h_{i,\uparrow}^\dagger) = [T_0, h_{i,\uparrow}^\dagger] + [H_{\text{int}}, h_{i,\uparrow}^\dagger]$

$$[H_{\text{int}}, h_{i,\uparrow}^\dagger] = \frac{U}{2}h_{i,\uparrow}^\dagger \quad (\text{A.13a})$$

$$[T_0, h_{i,\uparrow}^\dagger] = -f_{i,\downarrow} f_{i,\uparrow} d_{i\pm 1,\downarrow}^\dagger - \sigma_i^- h_{i\pm 1,\downarrow}^\dagger + \tilde{n}_{i,\downarrow} h_{i\pm 1,\uparrow}^\dagger - \frac{1}{2}h_{i\pm 1,\uparrow}^\dagger \quad (\text{A.13b})$$

simplification rules:

$$h_{i,\uparrow}^\dagger d_{i,\downarrow} = -f_{i,\downarrow} f_{i,\uparrow} \quad h_{i,\uparrow}^\dagger h_{i,\uparrow} = n_i^u - \frac{1}{2}\tilde{n}_{i,\uparrow} - \frac{1}{2}\tilde{n}_{i,\downarrow} + \frac{1}{4} \quad (\text{A.14a})$$

$$h_{i,\uparrow}^\dagger \tilde{n}_{i,\downarrow} = -\frac{1}{2}h_{i,\uparrow}^\dagger \quad h_{i,\uparrow}^\dagger \tilde{n}_{i,\uparrow} = \frac{1}{2}h_{i,\uparrow}^\dagger \quad (\text{A.14b})$$

$$h_{i,\uparrow}^\dagger \sigma_i^+ = h_{i,\downarrow}^\dagger \quad h_{i,\uparrow}^\dagger n_i^u = -\frac{1}{4}h_{i,\uparrow}^\dagger \quad (\text{A.14c})$$

$h_{i,\downarrow}^\dagger$: **with $N=2$**

Liouville operator: $\mathcal{L}(h_{i,\downarrow}^\dagger) = [T_0, h_{i,\downarrow}^\dagger] + [H_{\text{int}}, h_{i,\downarrow}^\dagger]$

$$[H_{\text{int}}, h_{i,\downarrow}^\dagger] = \frac{U}{2}h_{i,\downarrow}^\dagger \quad (\text{A.15a})$$

$$[T_0, h_{i,\downarrow}^\dagger] = f_{i,\downarrow} f_{i,\uparrow} d_{i\pm 1,\uparrow}^\dagger - \sigma_i^+ h_{i\pm 1,\uparrow}^\dagger + \tilde{n}_{i,\uparrow} h_{i\pm 1,\downarrow}^\dagger - \frac{1}{2}h_{i\pm 1,\downarrow}^\dagger \quad (\text{A.15b})$$

simplification rules:

$$h_{i,\downarrow}^\dagger d_{i,\uparrow} = f_{i,\downarrow} f_{i,\uparrow} \quad h_{i,\downarrow}^\dagger h_{i,\downarrow} = n_i^u - \frac{1}{2}\tilde{n}_{i,\uparrow} - \frac{1}{2}\tilde{n}_{i,\downarrow} + \frac{1}{4} \quad (\text{A.16a})$$

$$h_{i,\downarrow}^\dagger \tilde{n}_{i,\downarrow} = \frac{1}{2}h_{i,\downarrow}^\dagger \quad h_{i,\downarrow}^\dagger \tilde{n}_{i,\uparrow} = -\frac{1}{2}h_{i,\downarrow}^\dagger \quad (\text{A.16b})$$

$$h_{i,\downarrow}^\dagger \sigma_i^- = h_{i,\uparrow}^\dagger \quad h_{i,\downarrow}^\dagger n_i^u = -\frac{1}{4}h_{i,\downarrow}^\dagger \quad (\text{A.16c})$$

$h_{i,\uparrow}$: **with $N=2$**

Liouville operator: $\mathcal{L}(h_{i,\uparrow}) = [T_0, h_{i,\uparrow}] + [H_{\text{int}}, h_{i,\uparrow}]$

$$[H_{\text{int}}, h_{i,\uparrow}] = \frac{U}{2} h_{i,\uparrow} \quad (\text{A.17a})$$

$$[T_0, h_{i,\uparrow}] = -f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger d_{i\pm 1,\downarrow} + \sigma_i^+ h_{i\pm 1,\downarrow} - \tilde{n}_{i,\downarrow} h_{i\pm 1,\uparrow} + \frac{1}{2} h_{i\pm 1,\uparrow} \quad (\text{A.17b})$$

simplification rules:

$$h_{i,\uparrow} h_{i,\uparrow}^\dagger = -n_i^u + \frac{1}{2} \tilde{n}_{i,\uparrow} - \frac{1}{2} \tilde{n}_{i,\downarrow} + \frac{1}{4} \quad h_{i,\uparrow} h_{i,\downarrow}^\dagger = \sigma_i^+ \quad (\text{A.18a})$$

$$h_{i,\uparrow} f_{i,\downarrow} f_{i,\uparrow} = -d_{i,\downarrow} \quad h_{i,\uparrow} \tilde{n}_{i,\downarrow} = -\frac{1}{2} h_{i,\uparrow} \quad (\text{A.18b})$$

$$h_{i,\uparrow} \tilde{n}_{i,\uparrow} = -\frac{1}{2} h_{i,\uparrow} \quad h_{i,\uparrow} n_i^u = \frac{1}{4} h_{i,\uparrow} \quad (\text{A.18c})$$

$h_{i,\downarrow}$: **with $N=2$**

Liouville operator: $\mathcal{L}(h_{i,\downarrow}) = [T_0, h_{i,\downarrow}] + [H_{\text{int}}, h_{i,\downarrow}]$

$$[H_{\text{int}}, h_{i,\downarrow}] = \frac{U}{2} h_{i,\downarrow} \quad (\text{A.19a})$$

$$[T_0, h_{i,\downarrow}] = f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger d_{i\pm 1,\uparrow} + \sigma_i^- h_{i\pm 1,\uparrow} - \tilde{n}_{i,\uparrow} h_{i\pm 1,\downarrow} + \frac{1}{2} h_{i\pm 1,\downarrow} \quad (\text{A.19b})$$

simplification rules:

$$h_{i,\downarrow} h_{i,\uparrow}^\dagger = \sigma_i^- \quad h_{i,\downarrow} h_{i,\downarrow}^\dagger = -n_i^u - \frac{1}{2} \tilde{n}_{i,\uparrow} + \frac{1}{2} \tilde{n}_{i,\downarrow} + \frac{1}{4} \quad (\text{A.20a})$$

$$h_{i,\downarrow} f_{i,\downarrow} f_{i,\uparrow} = d_{i,\uparrow} \quad h_{i,\downarrow} \tilde{n}_{i,\downarrow} = -\frac{1}{2} h_{i,\downarrow} \quad (\text{A.20b})$$

$$h_{i,\downarrow} \tilde{n}_{i,\uparrow} = -\frac{1}{2} h_{i,\downarrow} \quad h_{i,\downarrow} n_i^u = \frac{1}{4} h_{i,\downarrow} \quad (\text{A.20c})$$

$f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger$: **with $N=2$**

Liouville operator: $\mathcal{L}(f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger) = [T_0, f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger] + [H_{\text{int}}, f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger]$

$$[H_{\text{int}}, f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger] = \frac{U}{2} f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \quad (\text{A.21a})$$

$$[T_0, f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger] = -d_{i,\uparrow}^\dagger h_{i\pm 1,\downarrow} - h_{i,\uparrow}^\dagger d_{i\pm 1,\downarrow}^\dagger + d_{i,\downarrow}^\dagger h_{i\pm 1,\uparrow} + h_{i,\downarrow}^\dagger d_{i\pm 1,\uparrow}^\dagger \quad (\text{A.21b})$$

simplification rules:

$$f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger h_{i,\uparrow}^\dagger = d_{i,\downarrow}^\dagger \quad f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger h_{i,\downarrow}^\dagger = -d_{i,\uparrow}^\dagger \quad (\text{A.22a})$$

$$f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger f_{i,\downarrow} f_{i,\uparrow} = -n_i^u - \frac{1}{2}\tilde{n}_{i,\uparrow} - \frac{1}{2}\tilde{n}_{i,\downarrow} - \frac{1}{4} \quad f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \tilde{n}_{i,\downarrow} = -\frac{1}{2}f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \quad (\text{A.22b})$$

$$f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \tilde{n}_{i,\uparrow} = -\frac{1}{2}f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \quad f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger n_i^u = \frac{1}{4}f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \quad (\text{A.22c})$$

$f_{i,\downarrow} f_{i,\uparrow}$: **with $N=2$**

Liouville operator: $\mathcal{L}(f_{i,\downarrow} f_{i,\uparrow}) = [T_0, f_{i,\downarrow} f_{i,\uparrow}] + [H_{\text{int}}, f_{i,\downarrow} f_{i,\uparrow}]$

$$[H_{\text{int}}, f_{i,\downarrow} f_{i,\uparrow}] = \frac{U}{2} f_{i,\downarrow} f_{i,\uparrow} \quad (\text{A.23a})$$

$$[T_0, f_{i,\downarrow} f_{i,\uparrow}] = d_{i,\uparrow} h_{i\pm 1,\downarrow}^\dagger + h_{i,\uparrow}^\dagger d_{i\pm 1,\downarrow} - d_{i,\downarrow} h_{i\pm 1,\uparrow}^\dagger - h_{i,\downarrow}^\dagger d_{i\pm 1,\uparrow} \quad (\text{A.23b})$$

simplification rules:

$$f_{i,\downarrow} f_{i,\uparrow} d_{i,\uparrow}^\dagger = h_{i,\downarrow}^\dagger \quad f_{i,\downarrow} f_{i,\uparrow} d_{i,\downarrow}^\dagger = -h_{i,\uparrow}^\dagger \quad (\text{A.24a})$$

$$f_{i,\downarrow} f_{i,\uparrow} f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger = -n_i^u + \frac{1}{2}\tilde{n}_{i,\uparrow} + \frac{1}{2}\tilde{n}_{i,\downarrow} - \frac{1}{4} \quad f_{i,\downarrow} f_{i,\uparrow} \tilde{n}_{i,\downarrow} = \frac{1}{2}f_{i,\downarrow} f_{i,\uparrow} \quad (\text{A.24b})$$

$$f_{i,\downarrow} f_{i,\uparrow} \tilde{n}_{i,\uparrow} = \frac{1}{2}f_{i,\downarrow} f_{i,\uparrow} \quad f_{i,\downarrow} f_{i,\uparrow} n_i^u = \frac{1}{4}f_{i,\downarrow} f_{i,\uparrow} \quad (\text{A.24c})$$

σ_i^- : **with $N=2$**

Liouville operator: $\mathcal{L}(\sigma_i^-) = [T_0, \sigma_i^-] + [H_{\text{int}}, \sigma_i^-]$

$$[H_{\text{int}}, \sigma_i^-] = \frac{U}{2} \sigma_i^- \quad (\text{A.25a})$$

$$[T_0, \sigma_i^-] = -h_{i,\downarrow} h_{i\pm 1,\uparrow}^\dagger - h_{i,\uparrow}^\dagger h_{i\pm 1,\downarrow} - d_{i,\downarrow}^\dagger d_{i\pm 1,\uparrow} - d_{i,\uparrow}^\dagger d_{i\pm 1,\downarrow} \quad (\text{A.25b})$$

simplification rules:

$$\sigma_i^- d_{i,\downarrow} = -d_{i,\uparrow} \quad \sigma_i^- h_{i,\uparrow} = h_{i,\downarrow} \quad (\text{A.26a})$$

$$\sigma_i^- \tilde{n}_{i,\downarrow} = -\frac{1}{2}\sigma_i^- \quad \sigma_i^- \tilde{n}_{i,\uparrow} = \frac{1}{2}\sigma_i^- \quad (\text{A.26b})$$

$$\sigma_i^- \sigma_i^+ = -n_i^u - \frac{1}{2}\tilde{n}_{i,\uparrow} + \frac{1}{2}\tilde{n}_{i,\downarrow} + \frac{1}{4} \quad \sigma_i^- n_i^u = -\frac{1}{4}\sigma_i^- \quad (\text{A.26c})$$

σ_i^+ : **with $N=2$**

Liouville operator: $\mathcal{L}(\sigma_i^+) = [T_0, \sigma_i^+] + [H_{\text{int}}, \sigma_i^+]$

$$[H_{\text{int}}, \sigma_i^+] = \frac{U}{2} \sigma_i^+ \quad (\text{A.27a})$$

$$[T_0, \sigma_i^+] = -h_{i,\uparrow} h_{i\pm 1,\downarrow}^\dagger - h_{i,\downarrow}^\dagger h_{i\pm 1,\uparrow} - d_{i,\uparrow}^\dagger d_{i\pm 1,\downarrow} - d_{i,\downarrow} d_{i\pm 1,\uparrow}^\dagger \quad (\text{A.27b})$$

simplification rules:

$$\sigma_i^+ d_{i,\uparrow} = -d_{i,\downarrow} \quad \sigma_i^+ h_{i,\downarrow} = h_{i,\uparrow} \quad (\text{A.28a})$$

$$\sigma_i^+ \tilde{n}_{i,\downarrow} = \frac{1}{2} \sigma_i^+ \quad \sigma_i^+ \tilde{n}_{i,\uparrow} = -\frac{1}{2} \sigma_i^+ \quad (\text{A.28b})$$

$$\sigma_i^+ \sigma_i^- = -n_i^u - \frac{1}{2} \tilde{n}_{i,\uparrow} + \frac{1}{2} \tilde{n}_{i,\downarrow} + \frac{1}{4} \quad \sigma_i^+ n_i^u = -\frac{1}{4} \sigma_i^+ \quad (\text{A.28c})$$

$\tilde{n}_{i,\uparrow}$: **with $N=2$**

Liouville operator: $\mathcal{L}(\tilde{n}_{i,\uparrow}) = [T_0, \tilde{n}_{i,\uparrow}] + [H_{\text{int}}, \tilde{n}_{i,\uparrow}]$

$$[H_{\text{int}}, \tilde{n}_{i,\uparrow}] = \frac{U}{2} \tilde{n}_{i,\uparrow} \quad (\text{A.29a})$$

$$[T_0, \tilde{n}_{i,\uparrow}] = -h_{i,\uparrow} h_{i\pm 1,\uparrow}^\dagger - h_{i,\uparrow}^\dagger h_{i\pm 1,\uparrow} - d_{i,\uparrow}^\dagger d_{i\pm 1,\uparrow} - d_{i,\uparrow} d_{i\pm 1,\uparrow}^\dagger \quad (\text{A.29b})$$

simplification rules:

$$\tilde{n}_{i,\uparrow} d_{i,\uparrow}^\dagger = \frac{1}{2} d_{i,\uparrow}^\dagger \quad \tilde{n}_{i,\uparrow} d_{i,\downarrow}^\dagger = \frac{1}{2} d_{i,\downarrow}^\dagger \quad \tilde{n}_{i,\uparrow} h_{i,\uparrow}^\dagger = -\frac{1}{2} h_{i,\uparrow}^\dagger \quad (\text{A.30a})$$

$$\tilde{n}_{i,\uparrow} h_{i,\downarrow}^\dagger = -\frac{1}{2} h_{i,\downarrow}^\dagger \quad \tilde{n}_{i,\uparrow} d_{i,\uparrow} = -\frac{1}{2} d_{i,\uparrow} \quad \tilde{n}_{i,\uparrow} d_{i,\downarrow} = \frac{1}{2} d_{i,\downarrow} \quad (\text{A.30b})$$

$$\tilde{n}_{i,\uparrow} h_{i,\uparrow} = \frac{1}{2} h_{i,\uparrow} \quad \tilde{n}_{i,\uparrow} h_{i,\downarrow} = -\frac{1}{2} h_{i,\downarrow} \quad \tilde{n}_{i,\uparrow} f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger = \frac{1}{2} f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \quad (\text{A.30c})$$

$$\tilde{n}_{i,\uparrow} f_{i,\downarrow} f_{i,\uparrow} = -\frac{1}{2} f_{i,\downarrow} f_{i,\uparrow} \quad \tilde{n}_{i,\uparrow} \sigma_i^- = -\frac{1}{2} \sigma_i^- \quad \tilde{n}_{i,\uparrow} \sigma_i^+ = \frac{1}{2} \sigma_i^+ \quad (\text{A.30d})$$

$$\tilde{n}_{i,\uparrow} \tilde{n}_{i,\uparrow} = \frac{1}{4} \quad \tilde{n}_{i,\uparrow} \tilde{n}_{i,\downarrow} = n_i^u \quad \tilde{n}_{i,\uparrow} n_i^u = \frac{1}{4} \tilde{n}_{i,\downarrow} \quad (\text{A.30e})$$

$\tilde{n}_{i,\downarrow}$: **with $N=2$**

Liouville operator: $\mathcal{L}(\tilde{n}_{i,\downarrow}) = [T_0, \tilde{n}_{i,\downarrow}] + [H_{\text{int}}, \tilde{n}_{i,\downarrow}]$

$$[H_{\text{int}}, \tilde{n}_{i,\downarrow}] = \frac{U}{2} \tilde{n}_{i,\downarrow} \quad (\text{A.31a})$$

$$[T_0, \tilde{n}_{i,\downarrow}] = -h_{i,\downarrow} h_{i\pm 1,\downarrow}^\dagger - h_{i,\downarrow}^\dagger h_{i\pm 1,\downarrow} - d_{i,\downarrow}^\dagger d_{i\pm 1,\downarrow} - d_{i,\downarrow} d_{i\pm 1,\downarrow}^\dagger \quad (\text{A.31b})$$

simplification rules:

$$\tilde{n}_{i,\downarrow} d_{i,\uparrow}^\dagger = \frac{1}{2} d_{i,\uparrow}^\dagger \quad \tilde{n}_{i,\downarrow} d_{i,\downarrow}^\dagger = \frac{1}{2} d_{i,\downarrow}^\dagger \quad \tilde{n}_{i,\downarrow} h_{i,\uparrow}^\dagger = -\frac{1}{2} h_{i,\uparrow}^\dagger \quad (\text{A.32a})$$

$$\tilde{n}_{i,\downarrow} h_{i,\downarrow}^\dagger = -\frac{1}{2} h_{i,\downarrow}^\dagger \quad \tilde{n}_{i,\downarrow} d_{i,\uparrow} = \frac{1}{2} d_{i,\uparrow} \quad \tilde{n}_{i,\downarrow} d_{i,\downarrow} = -\frac{1}{2} d_{i,\downarrow} \quad (\text{A.32b})$$

$$\tilde{n}_{i,\downarrow} h_{i,\uparrow} = -\frac{1}{2} h_{i,\uparrow} \quad \tilde{n}_{i,\downarrow} h_{i,\downarrow} = \frac{1}{2} h_{i,\downarrow} \quad \tilde{n}_{i,\downarrow} f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger = \frac{1}{2} f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \quad (\text{A.32c})$$

$$\tilde{n}_{i,\downarrow} f_{i,\downarrow} f_{i,\uparrow} = -\frac{1}{2} f_{i,\downarrow} f_{i,\uparrow} \quad \tilde{n}_{i,\downarrow} \sigma_i^- = \frac{1}{2} \sigma_i^- \quad \tilde{n}_{i,\downarrow} \sigma_i^+ = -\frac{1}{2} \sigma_i^+ \quad (\text{A.32d})$$

$$\tilde{n}_{i,\downarrow} \tilde{n}_{i,\downarrow} = \frac{1}{4} \quad \tilde{n}_{i,\downarrow} \tilde{n}_{i,\uparrow} = n_i^u \quad \tilde{n}_{i,\downarrow} n_i^u = \frac{1}{4} \tilde{n}_{i,\uparrow} \quad (\text{A.32e})$$

n_i^u : with $N=4$

Liouville operator: $\mathcal{L}(n_i^u) = [T_0, n_i^u] + [H_{\text{int}}, n_i^u]$

$$[H_{\text{int}}, n_i^u] = \frac{U}{2} n_i^u \quad (\text{A.33a})$$

$$\begin{aligned} [T_0, n_i^u] = & \frac{1}{2} h_{i,\downarrow} h_{i\pm 1,\downarrow}^\dagger + \frac{1}{2} h_{i,\downarrow}^\dagger h_{i\pm 1,\downarrow} + \frac{1}{2} h_{i,\uparrow} h_{i\pm 1,\uparrow}^\dagger + \frac{1}{2} h_{i,\uparrow}^\dagger h_{i\pm 1,\uparrow} \\ & - \frac{1}{2} d_{i,\downarrow}^\dagger d_{i\pm 1,\downarrow} - \frac{1}{2} d_{i,\downarrow} d_{i\pm 1,\downarrow}^\dagger - \frac{1}{2} d_{i,\uparrow}^\dagger d_{i\pm 1,\uparrow} - \frac{1}{2} d_{i,\uparrow} d_{i\pm 1,\uparrow}^\dagger \end{aligned} \quad (\text{A.33b})$$

simplification rules:

$$n_i^u d_{i,\uparrow}^\dagger = \frac{1}{4} d_{i,\uparrow}^\dagger \quad n_i^u d_{i,\downarrow}^\dagger = \frac{1}{4} d_{i,\downarrow}^\dagger \quad n_i^u h_{i,\uparrow}^\dagger = \frac{1}{4} h_{i,\uparrow}^\dagger \quad (\text{A.34a})$$

$$n_i^u h_{i,\downarrow}^\dagger = \frac{1}{4} h_{i,\downarrow}^\dagger \quad n_i^u d_{i,\uparrow} = -\frac{1}{4} d_{i,\uparrow} \quad n_i^u d_{i,\downarrow} = -\frac{1}{4} d_{i,\downarrow} \quad (\text{A.34b})$$

$$n_i^u h_{i,\uparrow} = -\frac{1}{4} h_{i,\uparrow} \quad n_i^u h_{i,\downarrow} = -\frac{1}{4} h_{i,\downarrow} \quad n_i^u f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger = \frac{1}{4} f_{i,\downarrow}^\dagger f_{i,\uparrow}^\dagger \quad (\text{A.34c})$$

$$n_i^u f_{i,\downarrow} f_{i,\uparrow} = \frac{1}{4} f_{i,\downarrow} f_{i,\uparrow} \quad n_i^u \sigma_i^- = -\frac{1}{4} \sigma_i^- \quad n_i^u \sigma_i^+ = -\frac{1}{4} \sigma_i^+ \quad (\text{A.34d})$$

$$n_i^u \tilde{n}_{i,\downarrow} = \frac{1}{4} \tilde{n}_{i,\uparrow} \quad n_i^u \tilde{n}_{i,\uparrow} = \frac{1}{4} \tilde{n}_{i,\downarrow} \quad n_i^u n_i^u = \frac{1}{8} \quad (\text{A.34e})$$

B Operators of the two-dimensional local Hilbert space

Here, all local operators of the two-dimensional local Hilbert space $\mathcal{H}_2^L$ are listed together with corresponding Liouville Operators and simplification rules. All Liouville operator and simplification rules the normalization N is not part of the operator and therefore the prefactor need to be corrected according to equation (A.2) respectively equation (A.4).

$d_{i,\uparrow}^\dagger$: **with** $N=\sqrt{2}$

Liouville operator:

$$\begin{aligned} \mathcal{L} \left(d_{i,\uparrow}^\dagger \right) &= [H_{\text{int}}, d_{i,\uparrow}^\dagger] + [T_0, d_{i,\uparrow}^\dagger] + [T'_0, d_{i,\uparrow}^\dagger] \\ &\quad + [T'_{s,0}, d_{i,\uparrow}^\dagger] + [T''_0, d_{i,\uparrow}^\dagger] + [T''_{s,0}, d_{i,\uparrow}^\dagger] \end{aligned} \quad (\text{B.1a})$$

$$[H_{\text{int}}, d_{i,\uparrow}^\dagger] = \frac{U}{2} d_{i,\uparrow}^\dagger \quad (\text{B.1b})$$

$$[T_0, d_{i,\uparrow}^\dagger] = t_0 \sum_{j|\langle i,j \rangle} \left(-d_{j,\downarrow}^\dagger \sigma_i^+ - \frac{1}{2} d_{j,\uparrow}^\dagger \sigma_i^z + \frac{1}{2} d_{j,\uparrow}^\dagger \right) \quad (\text{B.1c})$$

$$[T'_0, d_{i,\uparrow}^\dagger] = t' \sum_{j|\langle \langle i,j \rangle \rangle_d} \left(d_{j,\downarrow}^\dagger \sigma_i^+ + \frac{1}{2} d_{j,\uparrow}^\dagger \sigma_i^z - \frac{1}{2} d_{j,\uparrow}^\dagger \right) \quad (\text{B.1d})$$

$$[T''_0, d_{i,\uparrow}^\dagger] = t'' \sum_{j|\langle \langle i,j \rangle \rangle_l} \left(d_{j,\downarrow}^\dagger \sigma_i^+ + \frac{1}{2} d_{j,\uparrow}^\dagger \sigma_i^z - \frac{1}{2} d_{j,\uparrow}^\dagger \right) \quad (\text{B.1e})$$

$$\begin{aligned} [T'_{s,0}, d_{i,\uparrow}^\dagger] &= t'_s \sum_{j,k|\langle i,k,j \rangle_d} \left(\frac{1}{2} d_{j,\downarrow}^\dagger \sigma_k^+ - \frac{1}{2} d_{j,\downarrow}^\dagger \sigma_k^+ \sigma_i^z - d_{j,\uparrow}^\dagger \sigma_k^- \sigma_i^+ \right. \\ &\quad \left. + \frac{1}{4} d_{j,\uparrow}^\dagger \sigma_k^z - \frac{1}{4} d_{j,\uparrow}^\dagger \sigma_k^z \sigma_i^z + \frac{1}{2} d_{j,\downarrow}^\dagger \sigma_k^z \sigma_i^+ \right) \end{aligned} \quad (\text{B.1f})$$

$$\begin{aligned} [T''_{s,0}, d_{i,\uparrow}^\dagger] &= t''_s \sum_{j,k|\langle i,k,j \rangle_l} \left(\frac{1}{2} d_{j,\downarrow}^\dagger \sigma_k^+ - \frac{1}{2} d_{j,\downarrow}^\dagger \sigma_k^+ \sigma_i^z - d_{j,\uparrow}^\dagger \sigma_k^- \sigma_i^+ \right. \\ &\quad \left. + \frac{1}{4} d_{j,\uparrow}^\dagger \sigma_k^z - \frac{1}{4} d_{j,\uparrow}^\dagger \sigma_k^z \sigma_i^z + \frac{1}{2} d_{j,\downarrow}^\dagger \sigma_k^z \sigma_i^+ \right) \end{aligned} \quad (\text{B.1g})$$

simplification rules:

$$d_{i,\uparrow}^\dagger \sigma_i^z = -d_{i,\uparrow}^\dagger \quad d_{i,\uparrow}^\dagger \sigma_i^- = -d_{i,\downarrow}^\dagger \quad (\text{B.2a})$$

$h_{i,\uparrow}^\dagger$: **with** $N=\sqrt{2}$

Liouville operator:

$$\begin{aligned} \mathcal{L}(h_{i,\uparrow}^\dagger) = & [H_{\text{int}}, h_{i,\uparrow}^\dagger] + [T_0, h_{i,\uparrow}^\dagger] + [T'_0, h_{i,\uparrow}^\dagger] \\ & + [T'_{s,0}, h_{i,\uparrow}^\dagger] + [T''_0, h_{i,\uparrow}^\dagger] + [T''_{s,0}, h_{i,\uparrow}^\dagger] \end{aligned} \quad (\text{B.3a})$$

$$[H_{\text{int}}, h_{i,\uparrow}^\dagger] = \frac{U}{2} h_{i,\uparrow}^\dagger \quad (\text{B.3b})$$

$$[T_0, h_{i,\uparrow}^\dagger] = t_0 \sum_{j|\langle i,j \rangle} \left(-h_{j,\downarrow}^\dagger \sigma_i^- - \frac{1}{2} h_{j,\uparrow}^\dagger \sigma_i^z - \frac{1}{2} h_{j,\uparrow}^\dagger \right) \quad (\text{B.3c})$$

$$[T'_0, h_{i,\uparrow}^\dagger] = t' \sum_{j|\langle\langle i,j \rangle\rangle_d} \left(-h_{j,\downarrow}^\dagger \sigma_i^- - \frac{1}{2} h_{j,\uparrow}^\dagger \sigma_i^z - \frac{1}{2} h_{j,\uparrow}^\dagger \right) \quad (\text{B.3d})$$

$$[T''_0, h_{i,\uparrow}^\dagger] = t'' \sum_{j|\langle\langle i,j \rangle\rangle_l} \left(-h_{j,\downarrow}^\dagger \sigma_i^- - \frac{1}{2} h_{j,\uparrow}^\dagger \sigma_i^z - \frac{1}{2} h_{j,\uparrow}^\dagger \right) \quad (\text{B.3e})$$

$$\begin{aligned} [T'_{s,0}, h_{i,\uparrow}^\dagger] = t'_s \sum_{j,k|\langle i,k,j \rangle_d} & \left(-\frac{1}{2} h_{j,\downarrow}^\dagger \sigma_k^- - \frac{1}{2} h_{j,\downarrow}^\dagger \sigma_k^- \sigma_i^z - h_{j,\uparrow}^\dagger \sigma_k^+ \sigma_i^- \right. \\ & \left. - \frac{1}{4} h_{j,\uparrow}^\dagger \sigma_k^z - \frac{1}{4} h_{j,\uparrow}^\dagger \sigma_k^z \sigma_i^z + \frac{1}{2} h_{j,\downarrow}^\dagger \sigma_k^z \sigma_i^- \right) \end{aligned} \quad (\text{B.3f})$$

$$\begin{aligned} [T''_{s,0}, h_{i,\uparrow}^\dagger] = t''_s \sum_{j,k|\langle i,k,j \rangle_l} & \left(-\frac{1}{2} h_{j,\downarrow}^\dagger \sigma_k^- - \frac{1}{2} h_{j,\downarrow}^\dagger \sigma_k^- \sigma_i^z - h_{j,\uparrow}^\dagger \sigma_k^+ \sigma_i^- \right. \\ & \left. - \frac{1}{4} h_{j,\uparrow}^\dagger \sigma_k^z - \frac{1}{4} h_{j,\uparrow}^\dagger \sigma_k^z \sigma_i^z + \frac{1}{2} h_{j,\downarrow}^\dagger \sigma_k^z \sigma_i^- \right) \end{aligned} \quad (\text{B.3g})$$

simplification rules:

$$h_{i,\uparrow}^\dagger \sigma_i^z = h_{i,\uparrow}^\dagger \quad h_{i,\uparrow}^\dagger \sigma_i^- = h_{i,\downarrow}^\dagger \quad (\text{B.4a})$$

$d_{i,\downarrow}^\dagger$: **with** $N=\sqrt{2}$

Liouville operator:

$$\begin{aligned} \mathcal{L} \left(d_{i,\downarrow}^\dagger \right) &= [H_{\text{int}}, d_{i,\downarrow}^\dagger] + [T_0, d_{i,\downarrow}^\dagger] + [T'_0, d_{i,\downarrow}^\dagger] \\ &\quad + [T'_{s,0}, d_{i,\downarrow}^\dagger] + [T''_0, d_{i,\downarrow}^\dagger] + [T''_{s,0}, d_{i,\downarrow}^\dagger] \end{aligned} \quad (\text{B.5a})$$

$$[H_{\text{int}}, d_{i,\downarrow}^\dagger] = \frac{U}{2} d_{i,\downarrow}^\dagger \quad (\text{B.5b})$$

$$[T_0, d_{i,\downarrow}^\dagger] = t_0 \sum_{j|\langle i,j \rangle} \left(-d_{j,\uparrow}^\dagger \sigma_i^- + \frac{1}{2} d_{j,\downarrow}^\dagger \sigma_i^z + \frac{1}{2} d_{j,\downarrow}^\dagger \right) \quad (\text{B.5c})$$

$$[T'_0, d_{i,\downarrow}^\dagger] = t'_0 \sum_{j|\langle\langle i,j \rangle\rangle_d} \left(d_{j,\uparrow}^\dagger \sigma_i^- - \frac{1}{2} d_{j,\downarrow}^\dagger \sigma_i^z - \frac{1}{2} d_{j,\downarrow}^\dagger \right) \quad (\text{B.5d})$$

$$[T''_0, d_{i,\downarrow}^\dagger] = t''_0 \sum_{j|\langle\langle i,j \rangle\rangle_l} \left(d_{j,\uparrow}^\dagger \sigma_i^- - \frac{1}{2} d_{j,\downarrow}^\dagger \sigma_i^z - \frac{1}{2} d_{j,\downarrow}^\dagger \right) \quad (\text{B.5e})$$

$$\begin{aligned} [T'_{s,0}, d_{i,\downarrow}^\dagger] &= t'_s \sum_{j,k|\langle i,k,j \rangle_d} \left(\frac{1}{2} d_{j,\uparrow}^\dagger \sigma_k^- + \frac{1}{2} d_{j,\uparrow}^\dagger \sigma_k^- \sigma_i^z - d_{j,\downarrow}^\dagger \sigma_k^+ \sigma_i^- \right. \\ &\quad \left. - \frac{1}{4} d_{j,\downarrow}^\dagger \sigma_k^z - \frac{1}{4} d_{j,\downarrow}^\dagger \sigma_k^z \sigma_i^z - \frac{1}{2} d_{j,\uparrow}^\dagger \sigma_k^z \sigma_i^- \right) \end{aligned} \quad (\text{B.5f})$$

$$\begin{aligned} [T''_{s,0}, d_{i,\downarrow}^\dagger] &= t''_s \sum_{j,k|\langle i,k,j \rangle_l} \left(\frac{1}{2} d_{j,\uparrow}^\dagger \sigma_k^- + \frac{1}{2} d_{j,\uparrow}^\dagger \sigma_k^- \sigma_i^z - d_{j,\downarrow}^\dagger \sigma_k^+ \sigma_i^- \right. \\ &\quad \left. - \frac{1}{4} d_{j,\downarrow}^\dagger \sigma_k^z - \frac{1}{4} d_{j,\downarrow}^\dagger \sigma_k^z \sigma_i^z - \frac{1}{2} d_{j,\uparrow}^\dagger \sigma_k^z \sigma_i^- \right) \end{aligned} \quad (\text{B.5g})$$

simplification rules:

$$d_{i,\downarrow}^\dagger \sigma_i^z = d_{i,\downarrow}^\dagger \quad d_{i,\downarrow}^\dagger \sigma_i^+ = -d_{i,\uparrow}^\dagger \quad (\text{B.6a})$$

$h_{i,\downarrow}^\dagger$: **with** $N=\sqrt{2}$

Liouville operator:

$$\begin{aligned} \mathcal{L}(h_{i,\downarrow}^\dagger) = & [H_{\text{int}}, h_{i,\downarrow}^\dagger] + [T_0, h_{i,\downarrow}^\dagger] + [T'_0, h_{i,\downarrow}^\dagger] \\ & + [T'_{s,0}, h_{i,\downarrow}^\dagger] + [T''_0, h_{i,\downarrow}^\dagger] + [T''_{s,0}, h_{i,\downarrow}^\dagger] \end{aligned} \quad (\text{B.7a})$$

$$[H_{\text{int}}, h_{i,\downarrow}^\dagger] = \frac{U}{2} h_{i,\downarrow}^\dagger \quad (\text{B.7b})$$

$$[T_0, h_{i,\downarrow}^\dagger] = t_0 \sum_{j|\langle i,j \rangle} \left(-h_{j,\uparrow}^\dagger \sigma_i^+ + \frac{1}{2} h_{j,\downarrow}^\dagger \sigma_i^z - \frac{1}{2} h_{j,\downarrow}^\dagger \right) \quad (\text{B.7c})$$

$$[T'_0, h_{i,\downarrow}^\dagger] = t' \sum_{j|\langle\langle i,j \rangle\rangle} \left(-h_{j,\uparrow}^\dagger \sigma_i^+ + \frac{1}{2} h_{j,\downarrow}^\dagger \sigma_i^z - \frac{1}{2} h_{j,\downarrow}^\dagger \right) \quad (\text{B.7d})$$

$$[T''_0, h_{i,\downarrow}^\dagger] = t'' \sum_{j,k|\langle\langle i,j \rangle\rangle} \left(-h_{j,\uparrow}^\dagger \sigma_i^+ + \frac{1}{2} h_{j,\downarrow}^\dagger \sigma_i^z - \frac{1}{2} h_{j,\downarrow}^\dagger \right) \quad (\text{B.7e})$$

$$\begin{aligned} [T'_{s,0}, h_{i,\downarrow}^\dagger] = t'_s \sum_{j,k|\langle i,k,j \rangle_d} & \left(-\frac{1}{2} h_{j,\uparrow}^\dagger \sigma_k^+ + \frac{1}{2} h_{j,\uparrow}^\dagger \sigma_k^+ \sigma_i^z - h_{j,\downarrow}^\dagger \sigma_k^- \sigma_i^+ \right. \\ & \left. + \frac{1}{4} h_{j,\downarrow}^\dagger \sigma_k^z - \frac{1}{4} h_{j,\downarrow}^\dagger \sigma_k^z \sigma_i^z - \frac{1}{2} h_{j,\uparrow}^\dagger \sigma_k^z \sigma_i^+ \right) \end{aligned} \quad (\text{B.7f})$$

$$\begin{aligned} [T''_{s,0}, h_{i,\downarrow}^\dagger] = t''_s \sum_{j,k|\langle i,k,j \rangle_l} & \left(-\frac{1}{2} h_{j,\uparrow}^\dagger \sigma_k^+ + \frac{1}{2} h_{j,\uparrow}^\dagger \sigma_k^+ \sigma_i^z - h_{j,\downarrow}^\dagger \sigma_k^- \sigma_i^+ \right. \\ & \left. + \frac{1}{4} h_{j,\downarrow}^\dagger \sigma_k^z - \frac{1}{4} h_{j,\downarrow}^\dagger \sigma_k^z \sigma_i^z - \frac{1}{2} h_{j,\uparrow}^\dagger \sigma_k^z \sigma_i^+ \right) \end{aligned} \quad (\text{B.7g})$$

simplification rules:

$$h_{i,\downarrow}^\dagger \sigma_i^z = -h_{i,\downarrow}^\dagger \quad h_{i,\downarrow}^\dagger \sigma_i^+ = h_{i,\uparrow}^\dagger \quad (\text{B.8a})$$

σ_i^z : **with** $N=1$

Liouville operator:

$$\mathcal{L}(\sigma_i^z) = 0 \quad (\text{B.9a})$$

simplification rules:

$$\sigma_i^z \sigma_i^z = 1 - \sigma_i^z \quad \sigma_i^z \sigma_i^+ = \sigma_i^+ \quad \sigma_i^z \sigma_i^- = \sigma_i^- \quad (\text{B.10a})$$

σ_i^+ : **with** $N=\sqrt{2}$

Liouville operator:

$$\mathcal{L}(\sigma_i^+) = 0 \quad (\text{B.11a})$$

simplification rules:

$$\sigma_i^+ \sigma_i^z = -\sigma^+ \quad \sigma_i^+ \sigma_i^- = \frac{1}{2} \sigma_i^z + \frac{1}{2} \quad (\text{B.12a})$$

σ_i^- : **with** $N=\sqrt{2}$

Liouville operator:

$$\mathcal{L}(\sigma_i^-) = 0 \quad (\text{B.13a})$$

simplification rules:

$$\sigma_i^- \sigma_i^z = \sigma^- \quad \sigma_i^- \sigma_i^+ = -\frac{1}{2} \sigma_i^z + \frac{1}{2} \quad (\text{B.14a})$$

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