Control Aspects of a Finite Length Hubbard Chain

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Abstract— **Solid state physics provides a rather new application area for quantum control. Yet, the high dimensional state spaces in this field require a thorough analysis of the underlying Lie algebraic structures for developing efficient control strategies. In this paper, we focus a one-dimensional chain of quantum dots described by the Hubbard model. The model plays an extremely important role in solid state physics since it is the simplest model which explicitly takes into account the interplay between Coulomb repulsion of electrons and their kinetic energy. We begin with an comprehensive description to the mathemtical tools need for the appropriate state space construction. Based on these concepts, we introduce the general Hubbard Hamiltonian and discuss some aspects of is general Lie algebraic structure. Finally, we present a toy example for illustrating the afore established notions.**

The tutorial part of this work is supposed to enhance the collaboration between theoretical physicists and mathematicians in the area of quantum control.

I. INTRODUCTION

While quantum control is a well-established tool in coherent ensemble spectroscopy, e.g. [10], [16], solid state physics provides a new area of applications for geometric ideas from nonlinear control theory [7] or [9]. Existing optimal control algorithms [11], however, are confined to systems with a rather small number of particles. Yet, future applications in solid state physics require control strategies far beyond these limits. A first step towards the development of more efficient numerical methods rests on a comprehensive understanding of the control theoretic properties of the underlying quantum mechanical models.

Here, we focus on a one-dimensional chain of finitely many quantum dots described by the Hubbard model [15] which plays an extremely important role in solid state physics. The Hubbard model is the simplest one that allows for a study of the interplay between kinetic energy, coulomb interaction and lattice structure. There exist variants of the Hubbard model for fermions and for bosons, thus the influence of quantum effects due to the different statistics of the participating particles can be studied. In this paper, we exclusively treat the fermionic case.

In one dimension, various exact results are available, e.g. the groundstate (that is for zero temperature) can be determined analytically [14] and the complete excitation spectra for non-zero temperature are known. The infinite dimensional case or, more precisely, the limit to infinitely high coordination number (which is not the same as passing to infinite lentgh) allows at least a numerical treatment up to arbitrary high precision. An extensive review is given in [8]. The resulting model describes the physics of a so-called Mott insulator — insulators which arise solely from correlation effects. The two and three dimensional Hubbard model is still a subject of intense research since no exact solutions are available. However, if it comes to out-of-equilibria physics and control theory even in one dimension only a few result are known [18].

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A. The one-dimensional Hubbard model

In the following, we briefly sketch the 'ingredients' of the Hubbard model, a thorough introduction will be provided in Section III. For a one-dimensional chain of length L, the Hamiltonian of the model is given by

$$H := -\tau \sum_{\substack{i=1 \\ \sigma=\pm}}^{L} \left(c^\dagger_{i,\sigma} c_{i+1,\sigma} + c^\dagger_{i+1,\sigma} c_{i,\sigma}\right) + u \sum_{i=1}^{L} (c^\dagger_{i,+} c_{i,+} - \tfrac{1}{2})(c^\dagger_{i,-} c_{i,-} - \tfrac{1}{2}), \tag{1}$$

where periodic boundary conditions are imposed, i.e. $c_{L+1,\sigma} := c_{1,\sigma}$ and $c^\dagger_{L+1,\sigma} := c^\dagger_{1,\sigma}$. Moreover, σ is allowed to assume only the two values $+$ and $-$ indicating the two spin eigenstates of an electron. The first sum in (1) involving the scalar t corresponds to the kinetric energy of the system while the second sum with the parameter u models the Coulomb interaction. In this description, we assume that the hopping amplitude t is spin-independent and allow only a hopping between nearest neighbours. Finally, the important parameter is the dimensionless ratio u/τ, as this measures the relative strength of kinetic energy versus interaction energy.

The operator $c_{i,\sigma}$ annihilates an electron at site i with spin σ, whereas $c^\dagger_{i,\sigma}$ creates an electron at site i with spin σ. In particular, they fulfill the canonical fermionic anti-commutation relations:

$$\left[c^\dagger_{i,\sigma}, c^\dagger_{j,\sigma'}\right]_+ = \left[c_{i,\sigma}, c_{j,\sigma'}\right]_+ = 0, \quad \left[c^\dagger_{i,\sigma}, c_{j,\sigma'}\right]_+ = \delta_{i,j}\delta_{\sigma,\sigma'}\mathrm{I}$$

where $[A,B]_+ := AB + BA$ denotes the anti-commutator. The local particle density operator $n_{i,\sigma} := c^\dagger_{i,\sigma} c_{i,\sigma}$, measures how many electrons with spin σ occupy site i. In view of the Pauli principle, $n_{i,\sigma}$, or more precisely, the eigenvalues of $n_{i,\sigma}$ can assume only the numbers 0 or 1. Hence, for an L-site lattice, the underlying Hilbert space $\mathscr{H}$ is 4^L-dimensional.

For later purposes, it is important to point out that there exist several conserved quantities for the above Hubbard

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Hamiltonian (i.e. self-adjoint operators A which commute with H), e.g. the total particle number

$$N := \sum_{i=1}^{L} (n_{i,+} + n_{i,-}), \tag{2}$$

as well as the z-component of the total spin

$$S^z = \sum_{i=1}^{L} (n_{i,+} - n_{i,-}). \tag{3}$$

Moreover, the total momentum is also conserved and the H is invariant under any cyclic permutation of the site-indices $i = 1, \ldots, L$,

B. Control Issues

A characteristic physical observable for distinguishing different states of the system is the so-called (mean) double occupancy

$$D := \tfrac{1}{L} \sum_{i=1}^{L} n_{i,+} n_{i,-}. \tag{4}$$

Here, we always assume that the chain is half-filled, i.e. the number of particles is equal to L (the number of sites). For free electrons (i.e. for the Hubbard model at $u = 0$) its thermal expectation value $\langle D \rangle := \mathrm{Tr}(\rho_0 D)$ is equal to $\frac{1}{4}$. Here, the thermal equilibrium state ρ_0 is given the density matrix

$$\rho_0 := \frac{\mathrm{e}^{-\beta H}}{\mathrm{Tr}(\mathrm{e}^{-\beta H})}, \quad \beta := \frac{1}{kT}, \tag{5}$$

where T denotes the temperature and k the Boltzmann constant. Hence, for $u \neq 0$ the quantity

$$d := |\langle D \rangle - \tfrac{1}{4}| \tag{6}$$

is supposed to characterize the conductivity of the system. So $d = 0$ corresponds to the case of free electrons (perfect metal) and $d = 0.25$ corresponds to a model where the electron spins are somehow entangled such that the system goes into the Mott-insulating phase.

Assuming that our system ($u \neq 0$) is in thermal equilibrium at time $t = 0$, its initial density matrix is given by (5) and thus we have $d > 0$ for $t = 0$. Now, the time evolution of (5) is governed by the Liouille–von Neumann equation

$$\dot{\rho}(t) = \big[\mathrm{iH}, \rho(\mathrm{t})\big], \tag{7}$$

where $[A, B] := AB - BA$ denotes the usual commutator. Clearly, the solution of (7) is given by

$$\rho(t) = U(t) \rho_0 U(t)^{\dagger} \tag{8}$$

and thus confined to the unitary orbit of ρ_0, where $U(t)$ satisfies the lifted equation

$$\dot{U}(t) = \mathrm{iHU(t)}\,, \quad \mathrm{U(0) = I}, \tag{9}$$

which evolves on the corresponding Lie group of unitary transformations. Having fixed the setting so far, a couple of control issues naturally arise once the parameter u in (1) is regarded as a control parameter:

- What are the extremal values of d the system can be driven to (depending on the initial state)?
- What is the best (time-optimal) way to reach these extremal values? Is it by 'turning off' u for $t > 0$, or can a faster decay be constructed by using a different switching procedure?

To answer these questions, a thorough reachability analysis of the Hubbard model is required. In Section III, we will see that these are highly non-trivial control problems even for chains of moderate finite length.

Recently, we developed an extension of the diagrammatic quantum Monte Carlo method, cf. [1] and [17], that allows for a unified approach to the treatment of correlated initial states. It enables us to study in a first the subsequent time-evolution of the system. Simple observables like the double occupancy are directly accessible in this method. Figure 1 presents some numerical results on its behaviour (for chains up to 64 site) where u is just switched off for $t > 0$.

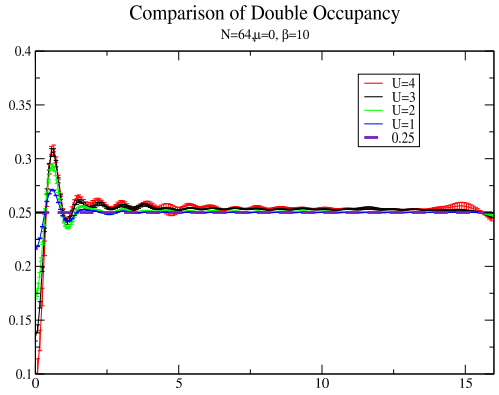

Fig. 1. Here we see the raw behaviour of the $\langle n_{i,+} n_{i,-} \rangle$. Starting from the initial values the double occupancy jumps up to ≈ 0.3 and seems to decay (initially) with some oscillatory behaviour towards the value of free electrons, that is $\frac{1}{4}$.

II. THE MATHEMATICAL SETTING

In this section, we briefly recall the mathematical background of a 'construction' which is called *second quantization* in physics and provides the basic tool to describe many particle quantum systems. Readers interested in more details are referred to [3] or [19].

A. Fock Spaces, Fermions, and Bosons

Let $\mathbb{H}$ be a finite-dimensional Hilbert space with scalar product $\langle \cdot, \cdot \rangle$ modelling the state space of a single particle and let $\mathbb{H}_2 := \mathbb{H} \otimes \mathbb{H}$ denotes the tensor product of $\mathbb{H}$ with itself. Then $\mathbb{H}_2$ is the canonical candidate to model the state space of two interacting particles whose individual state spaces are $\mathbb{H}$. However, for identical particles the quantum mechanical principle of *indistinguishability* requires that any re-numbering of the particles does not effect the output of any measurement. Therefore, the state space of two *indistinguishable* particles is given either by the set of all *symmetric* or *anti-symmetric* 2-tensors. i.e., either by

$$\mathbb{H}_2^s := \mathrm{span}\{\phi \otimes \psi + \psi \otimes \phi \mid \phi, \psi \in \mathbb{H}\} \subset \mathbb{H}_2 \tag{10}$$

or by

$$\mathbb{H}_2^a := \operatorname{span}\{\phi\otimes\psi-\psi\otimes\phi \mid \phi,\psi\in\mathbb{H}\}\subset\mathbb{H}_2. \tag{11}$$

Experimental experience proved that there are two types of elementary particles which behave completely different:

- *Bosons* (particles with integer spin)
- *Fermions* (particles with half-integer spin)

Fermions further have to comply with the *Pauli principle*, i.e. two identical fermions are never allowed to be in the same state. This finally leads to the fact that $\mathbb{H}_2^s$ is the appropriate state space for two identical bosons while $\mathbb{H}_2^a$ is the state space for two identical fermions.

Now, we want to pass to systems which allow a higher number of particles than two. Actually, we are interested in describing systems whose number of particles is not fixed a priori. A reason, why one wants to have this 'degree of freedom', will become clear in a moment. The model space which does achieve this variability in the number of particles is given by the so-called *Fock space*[1]

$$\mathscr{H} := \bigoplus_{k=0}^{\infty}\mathbb{H}_k,\quad \mathbb{H}_k := \mathbb{H}\otimes\cdots\otimes\mathbb{H}, \tag{12}$$

i.e. by the (Hilbert space completion of the) direct sum of all k-fold tensor product of $\mathbb{H}$ with itself. Again, for identical particles one has to restrict to the symmetric (for bosons) or anti-symmetric (for fermions) part of $\mathscr{H}$, i.e. to

$$\mathscr{H}^s := \bigoplus_{k=0}^{\infty}\mathbb{H}_k^s,\quad \mathbb{H}_k^s := \text{symmetric part of } \mathbb{H}_k, \tag{13}$$

and,

$$\mathscr{H}^a := \bigoplus_{k=0}^{\infty}\mathbb{H}_k^a,\quad \mathbb{H}_k^a := \text{anti-symmetric part of } \mathbb{H}_k, \tag{14}$$

respectively. Since $\dim\mathbb{H}_k^a = \binom{\dim\mathbb{H}}{k}$, the direkt sum in (14) is finite. In the sequel, we focus on the case of fermions as electrons in the Hubbard model are spin-$\frac{1}{2}$ particles.

B. Creation and annihilation operators

Let $\psi_1\wedge\psi_2\wedge\cdots\wedge\psi_k$ denote the normalized element of $\mathbb{H}_k^a$ which corresponds to $\psi_1\otimes\psi_2\otimes\cdots\otimes\psi_k$, i.e.

$$\psi_1\wedge\psi_2\wedge\cdots\wedge\psi_k := \frac{1}{\sqrt{k!}}\sum_{\pi\in\Pi_k}\operatorname{sign}(\pi)\,\psi_{\pi(1)}\otimes\psi_{\pi(2)}\otimes\cdots\otimes\psi_{\pi(k)}, \tag{15}$$

where Π_k denotes the corresponding permutation group. For any $\phi\in\mathbb{H}$ we define operators $c_\phi:\mathbb{H}_k^a\to\mathbb{H}_{k-1}^a$ and $c_\phi^\dagger:\mathbb{H}_k^a\to\mathbb{H}_{k+1}^a$ as follows: Let $\psi_1\wedge\psi_2\wedge\cdots\wedge\psi_k\in\mathbb{H}_k^a$. Then

$$c_\phi(\psi_1\wedge\psi_2\wedge\cdots\wedge\psi_k) := \sum_{i=1}^{k}(-1)^{i+1}\langle\phi,\psi_i\rangle\cdot\psi_1\wedge\cdots\wedge\widehat{\psi}_i\wedge\cdots\wedge\psi_k \tag{16}$$

[1] In mathematics $\mathscr{H}$ is called the *tensor algebra* of $\mathbb{H}$, while $\mathscr{H}^a$ is referred to as the *exterior algebra* of $\mathbb{H}$.

for $k\geq 1$ and $c_\phi(1) := 0$ for $k=0$ and

$$c_\phi^\dagger(\psi_1\wedge\psi_2\wedge\cdots\wedge\psi_k) := \phi\wedge\psi_1\wedge\cdots\wedge\psi_k, \tag{17}$$

where $\psi_1\wedge\cdots\wedge\widehat{\psi}_i\wedge\cdots\wedge\psi_k\in\mathbb{H}_{k-1}^a$ is obtained from $\psi_1\wedge\psi_2\wedge\cdots\wedge\psi_k\in\mathbb{H}_k^a$ by dropping the i-th term. From the above definition, c_ϕ and $c_\phi^\dagger$ now readily extend to linear operators on $\mathscr{H}^a$.

Let $\mathbf{1} := (1,0,\ldots,0)\in\mathscr{H}^a$ be the so-called *vacuum state* and let $\phi_1,\ldots,\phi_d$ be a orthogonal basis of $\mathbb{H}$. Then, one has the canonical anti-commuator relations

$$\big[c_{\phi_i},c_{\phi_j}\big]_+ = \big[c_{\phi_i}^\dagger,c_{\phi_j}^\dagger\big]_+ = 0 \quad\text{and}\quad \big[c_{\phi_i},c_{\phi_j}^\dagger\big]_+ = \delta_{ij}\mathrm{I} \tag{18}$$

and the equalities

$$c_{\phi_i}^\dagger\mathbf{1} = \phi_i \quad\text{and}\quad c_{\phi_i}c_{\phi_j}^\dagger\mathbf{1} = \delta_{ij}\mathbf{1}, \tag{19}$$

where $\big[a,b\big]_+ := ab+ba$. A recursive application of (19) shows that $\mathscr{H}^a$ is spanned by all the state vectors of the from

$$\big(c_{\phi_1}^\dagger\big)^{n_1}\big(c_{\phi_2}^\dagger\big)^{n_2}\cdots\big(c_{\phi_d}^\dagger\big)^{n_d}\mathbf{1} \tag{20}$$

with $n_i\in\{0,1\}$. Due to (19) and (20) the operators $c_{\phi_i}^\dagger$ and c_{ϕ_i} are said to create and, respectively, annihilate the state ϕ_i. Therefore, they are called *creation* and *annihilation operators*, respectively. Note, that the sign of the state vectors in (20) does dependent on the chosen ordering.

III. THE ONE-DIMENSIONAL HUBBARD MODEL

Based on the results of the previous section, the Hubbard model and the 'construction' of its underlying Hilbert space can be desrcibed as follows. First, let $\mathbb{H}_{\text{pos}}$ be the state space of single particle which can occupy L different sites (of a chain). In other words, $\mathbb{H}_{\text{pos}}$ is a complex Hilbert space for representing a discrete 'position' operator with L different eigenstates $e_1,\ldots,e_L$. Since an electron also carry a spin, we choose additionally a two dimensional Hilbert space $\mathbb{H}_{\text{spin}}$ to model its spin-$\frac{1}{2}$ property. We denote by e_+ and e_- the corresponding two spin-eigenstates. Thus, we arrive at the state space

$$\mathbb{H} := \mathbb{H}_{\text{pos}}\otimes\mathbb{H}_{\text{spin}}\cong\mathbb{C}^{2L} \tag{21}$$

for a single electron in a chain of length L. Clearly, $\dim\mathbb{H} = 2L$. Now, observing the electrons are fermions, we obtain $\mathbb{H}_k^a$ as the right state space of k electrons in an L-chain. Finally, the complete anti-symmetric Fock space of an L-chain is given by

$$\mathscr{H}_L := \mathbb{C}\oplus\mathbb{H}_1^a\oplus\mathbb{H}_2^a\oplus\cdots\oplus\mathbb{H}_{2L}^a. \tag{22}$$

Hence,

$$\dim\mathscr{H}_L = \sum_{k=0}^{2L}\binom{2L}{k} = 2^{2L} = 4^L. \tag{23}$$

Next, let $c_{i,+}$ and $c_{i,-}$ denote the operators $c_{e_i\otimes e_+}$ and $c_{e_i\otimes e_-}$, respectively, cf. (16). In the same way, we define $c\dagger_{i,+}$ and

$c^\dagger_{i,-}$ by (17). Then, for a one-dimensional chain of length L, the general Hubbard Hamiltonian is given by [15]

$$H := H_{\mathrm{kin}} + H_{\mathrm{u}} := \\ -\sum_{\substack{i,j=1\\ \sigma=\pm}}^{L} \tau_{ij} c^\dagger_{i,\sigma} c_{j,\sigma} + \sum_{i=1}^{L} u_i (c^\dagger_{i,+} c_{i,+} - \tfrac{1}{2})(c^\dagger_{i,-} c_{i,-} - \tfrac{1}{2}). \tag{24}$$

The scalars τ_{ij} from the so-called hopping matrix while the parameters u_i are the Coulomb interaction at each site. They both have dimensions of energy. Restricting to nearest-neighbour actions with $\tau := \tau_{i,i+1} = \tau_{i+1,1}$, site-independent $u := u_i$ and cyclic boundard conditions, finally yields (1).

Now, let us regard $(u_1, \ldots, u_L)$ as control parameters which can be switched on and off or, more generally, which can be time-dependent $u_i(t)$. Thus, a first but fundamental challange — from a control-theoretic point ouf view — is the characterization of the reachable set of the resulting control system

$$\dot{U}(t) = \mathrm{i}\big(\mathrm{H_{kin}} + \mathrm{H_u}\big)\mathrm{U(t)}\,, \quad \mathrm{U(0) = I}, \tag{25}$$

Since system (25) evolves on the unitary group of $\mathscr{H}_L$, which is a compact Lie group, the reachable sets are in principle completely determined by the system Lie algebra of (25), i.e. by the Lie algebra spanned by all iterated Lie brackets of the form

$$H_{\mathrm{kin}}, H_{\mathrm{u}}, [H_{\mathrm{kin}}, H_{\mathrm{u}}], \big[H_{\mathrm{kin}}, [H_{\mathrm{kin}}, H_{\mathrm{u}}]\big], \big[H_{\mathrm{u}}, [H_{\mathrm{kin}}, H_{\mathrm{u}}]\big], \ldots,$$

cf. [9]. However, due to the high dimensional state space the computation is rather involved and time-consuming even for chains of moderate size. Therefore, a deep analysis of the Lie algebraic structure of such systems is necessary. A first step in this direction is provided by the following subsection on quadratic Hamiltonians. More on the interplay between Lie theory and quantum control can be found in [2], [5], [6] and [13].

A. Supplementary material on quadratic Hamiltonians

The kinetic part H_{kin} of the (general) Hubbard Hamiltonian, has the structure of a so-called quadratic fermionic Hamiltonian. In the sequel, we briefly summarize some useful Lie algebraic results on such quadratic Hamiltonians. Similar results can be obtained for bosons. Some of the these ideas are sketched in [12], a rigorous mathematical presentation is provided by [4]. Although these results immediately apply only to H_{kin}, they play an essential role for analysing the system algebra of (25).

For $i = 1, \ldots, d$, let $c_i := c_{\phi_i}$ and $c^\dagger_i := c^\dagger_{\phi_i}$ be defined as in the previous subsection. A operator of the form

$$H := \sum_{ij}^{d} \big(x_{ij} c_i c_j + r_{ij} c_i c^\dagger_j + s_{ij} c^\dagger_i c_j + y_{ij} c^\dagger_i c^\dagger_j\big), \tag{26}$$

where $X := (x_{ij}), Y := (y_{ij}), R := (r_{ij}), S := (s_{ij})$ are arbitrary complex $d \times d$ matrices, is called a (formal) *fermionic quadratic Hamiltonian*. Clearly, any H of this form is a linear operator acting on $\mathscr{H}^a$, i.e. $H \in \mathrm{L}(\mathscr{H}^a)$, where $\mathrm{L}(\mathscr{H}^a)$ denotes the set of all linear operators from $\mathscr{H}^a$ to itself. For the following results it is convenient to introduce the operators

$$a_i := \begin{cases} \frac{1}{\sqrt{2}}(c^\dagger_i + c_i) & \text{for } 1 \le i \le d, \\ \frac{\mathrm{i}}{\sqrt{2}}(c^\dagger_i - c_i) & \text{for } d+1 \le i \le 2d, \end{cases} \tag{27}$$

which are often called *Majorana operators* in the literature. They satisfy the anti-commutator relations

$$\big[a_i, a_j\big]_+ = \delta_{ij}\mathrm{I}. \tag{28}$$

Thus, we can alternatively write H as follows

$$H := \mathrm{i}\sum_{\mathrm{ij}}^{\mathrm{2d}} \omega_{\mathrm{ij}} \mathrm{a_i a_j}, \tag{29}$$

where the $2d \times 2d$ matrices $\Omega := (\omega_{ij})$ and $\begin{bmatrix} X & R \\ S & Y \end{bmatrix}$ are related by a straightforward unitary conjugation. By (28), we observe

$$H := \mathrm{i}\sum_{\mathrm{ij}}^{\mathrm{2d}} \omega_{\mathrm{ij}} \mathrm{a_i a_j} = \mathrm{i}\sum_{\substack{\mathrm{ij}\\ \mathrm{i}\neq\mathrm{j}}}^{\mathrm{2d}} \omega_{\mathrm{ij}} \mathrm{a_i a_j} + \frac{\mathrm{i}}{2}\mathrm{Tr}(\Omega)\,\mathrm{I}. \tag{30}$$

Therefore, we restrict the following discussion to the case $\mathrm{Tr}(\Omega) = 0$. Now, consider the linear map

$$\rho : \mathfrak{sl}_{\mathbb{C}}(2d) \to \mathrm{L}(\mathscr{H}^a), \quad \Omega \mapsto \mathrm{iH} := -\sum_{\mathrm{ij}}^{\mathrm{2d}} \omega_{\mathrm{ij}} \mathrm{a_i a_j}. \tag{31}$$

Exploiting (28), we obtain the kernel of ρ as follows

$$\ker\rho = \{\Omega \in \mathfrak{sl}_{\mathbb{C}}(2d) \mid \Omega^\top = \Omega\}. \tag{32}$$

Hence restricting ρ to the complementary space

$$\mathfrak{so}_{\mathbb{C}}(2d) := \{\Omega \in \mathfrak{sl}_{\mathbb{C}}(2d) \mid \Omega^\top = -\Omega\} \tag{33}$$

yields an isomorphism from $\mathfrak{so}_{\mathbb{C}}(2d)$ to the set of all (formal) fermionic quadratic Hamiltonians. Again, the anti-commutation relations (28), imply that this isomorphism is actually a Lie algebra isomorphism, i.e.

$$\rho\big([\Omega, \Omega']\big) = \big[\rho(\Omega), \rho(\Omega')\big] \tag{34}$$

for all $\Omega, \Omega' \in \mathfrak{so}_{\mathbb{C}}(2d)$. Moreover, requiring that $H := \mathrm{i}\rho(\Omega)$ is a self-adjoint operator on $\mathscr{H}^a$ translates to the condition that Ω is additionally real and thus ρ establishes a Lie algebra isomorphism from $\mathfrak{so}_{\mathbb{R}}(2d)$ to $\mathrm{iHam}_2(\mathscr{H}^{\mathrm{a}})$, where $\mathrm{Ham}_2(\mathscr{H}^a)$ denotes the set of all self-adjoint fermionic quadratic Hamiltonians. If we further assume that the subspaces $\mathbb{H}^a_k$, $k = 0, \ldots, d$ are invariant under $H := \mathrm{i}\rho(\Omega)$ (which means that H particle number preserving) then the matrix Ω reduces to the form

$$\Omega = \begin{bmatrix} A & B \\ -B & A \end{bmatrix} \tag{35}$$

with A real skew-symmetric and B real symmetric. In this case, Ω can even be identified with a skew-hermitian $d \times d$ matrix via the Lie algebra isomorphism

$$\mathfrak{u}(d) \ni A + \mathrm{iB} \mapsto \begin{bmatrix} A & B \\ -B & A \end{bmatrix} \in \mathfrak{so}_{\mathbb{R}}(\mathrm{2d}). \tag{36}$$

In a subsequent paper we will study the impact of the presented material to the introduced control problem (25). In particular, we aim at a full characterization of the corresponding system Lie algebra.

B. A Toy Example: $L = 2$

We discuss the lowest dimensional non-trival example, i.e. a Hubbard chain of length $L = 2$, with Hamiltonian given by (1). According to (23), the full state space $\mathscr{H}_2$ is 16-dimensional. The existence of conservation laws implies that the system cannot be controllable on the unitary group $\mathrm{U}(16)$. Hence, we concentrate on the half-filled case, i.e. on the subspace $\mathbb{H}_2^a$ which is invariant due to (2). Since (3) provides another conserved quantity, we expect that $\mathbb{H}_2^a$ decomposes further into an orthogonal sum of two invariant subspaces. Next, we choose a basis of $\mathbb{H}_2^a$ adapted to this decompostion

$$
\begin{aligned}
|1\rangle &:= \tfrac{1}{\sqrt{2}}\left(c_{1,+}^\dagger c_{2,-}^\dagger - c_{1,-}^\dagger c_{2,+}^\dagger\right)\mathbf{1} \\
&= \tfrac{1}{\sqrt{2}}\big((e_1\otimes e_+)\wedge e_2\otimes e_-) - (e_1\otimes e_-)\wedge(e_2\otimes e_+)\big)\,, \\
|2\rangle &:= c_{1,+}^\dagger c_{1,-}^\dagger \mathbf{1} = (e_1\otimes e_+)\wedge(e_1\otimes e_-)\,, \\
|3\rangle &:= c_{2,+}^\dagger c_{2,-}^\dagger \mathbf{1} = (e_2\otimes e_+)\wedge(e_2\otimes e_-)\,, \\
|4\rangle &:= \tfrac{1}{\sqrt{2}}\left(c_{1,+}^\dagger c_{2,-}^\dagger + c_{1,-}^\dagger c_{2,+}^\dagger\right)\mathbf{1} \\
&= \tfrac{1}{\sqrt{2}}\big((e_1\otimes e_+)\wedge(e_2\otimes e_-) + (e_1\otimes e_-)\wedge(e_2\otimes e_+)\big)\,, \\
|5\rangle &:= c_{1,+}^\dagger c_{2,+}^\dagger \mathbf{1} = (e_1\otimes e_+)\wedge(e_2\otimes e_+)\,, \\
|6\rangle &:= c_{1,-}^\dagger c_{2,-}^\dagger \mathbf{1} = (e_1\otimes e_-)\wedge(e_2\otimes e_-)\,,
\end{aligned}
$$

where $\mathbf{1}$ denotes the vacuum state. Applying the Hamiltonian H to these six states yields

$$
\begin{gathered}
H|1\rangle = -\tau\sqrt{2}\big(|2\rangle+|3\rangle\big) - u\tfrac{3}{4}|1\rangle,\ H|2\rangle = -\tau\sqrt{2}|1\rangle + u\tfrac{1}{4}|2\rangle, \\
H|3\rangle = -\tau\sqrt{2}|1\rangle + u\tfrac{1}{4}|3\rangle,\ H|4\rangle = -u\tfrac{3}{4}|4\rangle, \\
H|5\rangle = -u\tfrac{3}{4}|5\rangle,\ H|6\rangle = -u\tfrac{3}{4}|5\rangle.
\end{gathered}
$$

Here, we exploited the fact that the H_{u} coincides with $u\big(\sum_{i=1}^L c_{i,+}^\dagger c_{i,+} c_{i,-}^\dagger c_{i,-} - \frac{3}{4}\big)$ on $\mathbb{H}_2^a$. Moreover, note that the first four basis vectors are eigenvectors of the total z-spin operator S^z, cf. (3), to the eigenvalue zero, while the last two correspond to the eigenvalues ± 2. Now, the matrix representation of H restricted to the subspace $\mathbb{H}_2^a$ reads as

$$
H = H_{\mathrm{kin}} + H_{\mathrm{u}} = \tau\begin{bmatrix} 0 & -\sqrt{2} & -\sqrt{2} & 0 & 0 & 0 \\ -\sqrt{2} & 0 & 0 & 0 & 0 & 0 \\ -\sqrt{2} & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} + u\begin{bmatrix} -\frac{3}{4} & 0 & 0 & 0 & 0 & 0 \\ 0 & \frac{1}{4} & 0 & 0 & 0 & 0 \\ 0 & 0 & \frac{1}{4} & 0 & 0 & 0 \\ 0 & 0 & 0 & -\frac{3}{4} & 0 & 0 \\ 0 & 0 & 0 & 0 & -\frac{3}{4} & 0 \\ 0 & 0 & 0 & 0 & 0 & -\frac{3}{4} \end{bmatrix}.
$$

Then, a brute-force calculation shows that the system algebra is a 4-dimensional subalgebra $\mathfrak{g}$ of $\mathfrak{u}(6)$. More precisely, it is obtained by a non-trivial, but highly reducible representation of $\mathfrak{u}(2)$. Hence, the reachable sets of the equation

$$
\dot\rho(t) = \Big[\mathrm{i}\big(\mathrm{H}_{\mathrm{kin}} + \mathrm{H}_{\mathrm{u}}\big), \rho(\mathrm{t})\Big], \quad \rho(\mathrm{t}) = \rho_0,
$$

are given by the orbits $\{\mathrm{e}^{t\Omega}\rho_0\mathrm{e}^{-t\Omega} \mid \Omega\in\mathfrak{g}\}$, where ρ_0 is any density operator on $\mathbb{H}_2^a$. Therefore, even for this toy example, the reachable sets exhibits a rather non-trivial orbit structure.

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