

## Chapter 6

# Gateway schemes of quantum control for spin networks<sup>\*</sup>

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### 6.1 Motivation and Overview

Towards the full-fledged quantum computing, what do we need? Obviously, the first thing we need is a (many-body) quantum system, which is reasonably isolated from its environment in order to reduce the unwanted effect of noise, and the second might be a good technique to fully control it. Although we would also need a well-designed quantum code for information processing for fault-tolerant computation, from a physical point of view, the primary requisites are a system and a full control for it. Designing and fabricating a controllable quantum system is a hard work in the first place, however, we shall focus on the subsequent steps that cannot be skipped and are highly nontrivial.

Typically, when attempting to control a many-body quantum system, every subsystem of it has to be a subject of accurate and individual access to apply operations and to perform measurements. Such a (near-) full accessibility leads to a problem of not only technical difficulties, but also noise (decoherence), as the system can readily interact with its surrounding environment. In a sense, we are wishing for two inconsistent demands, namely, being able to manipulate a quantum system fully by controlling the field parameters while suppressing its interaction with the field.

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A good news is that the technological progress over the last decades has been so great that we are now able to access and control quantum systems quite well, provided they are not too large. The coherent manipulations of small quantum systems, in addition to the observations of quantum behaviours, have been reported for various systems, e.g., NMR/ESR [1, 2, 3, 4], semiconductor quantum dots [5, 6, 7], superconducting quantum bits (*qubits*) [8, 9, 10], and NV-centres in diamonds [11, 12].

Here, we discuss a possible scheme to bridge the gap between what we wish to achieve and what we can realise today. Namely, we aim at controlling a given many-body quantum system and identifying it by accessing only a small subsystem, i.e., *gateway*. Restricting the size of accessible gateway and minimising the number of control parameters should be of help in suppressing the effects of noise.

This chapter consists of two parts, each of which is devoted to these two topics, full quantum control through a gateway and Hamiltonian identification, respectively. Such situations, in which only a subsystem is accessible, arise for example in networks of ‘dark spins’ in diamond and solid state quantum devices [12, 13, 14] as well as spin networks in NMR and ESR setups [1, 4, 15].

In the first part, we present how a system can be controlled through access to a small gateway. Starting with a general argument on the controllability of a quantum system, we show a possible scheme to control spin networks under limited access. The two major issues of our interest in terms of the controllability concern the algebraic criterion for the form of Hamiltonians and the topological (or graph theoretical) condition for the choice of gateway. While the consideration about these aspects will lead to clear insights into the control of spin-1/2 systems, the theory is general enough to be applied to other systems we encounter in the lab. We shall also discuss a few issues related to efficiency, such as, can we compute a pulse sequence for a certain unitary on the chain by a classical computer within polynomial time? Or how much time would a unitary require to be performed?

All these discussions on the controllability assume the complete knowledge of the system Hamiltonian. The second part of this chapter is devoted to the discussions on how the Hamiltonian can be identified despite the limited access. Without the knowledge of Hamiltonian, we can never control a quantum system at will: it will be like going for treasure hunting without a map and a compass. Having learned the details of the system Hamiltonian, we then attempt to fully control it, enjoying the quantumness of the dynamics. Nonetheless, both the full information acquisition and the full control are still very hard. In addition, the operational complexity of information acquisition (state and process tomographies) grows rapidly (exponentially) with respect to the system size.

Presumably the most straightforward way to estimate the quantum dynamics is to apply quantum process tomography (QPT), which is a method to determine a completely positive map  $\mathcal{E}$  on quantum states. The map  $\mathcal{E}$  on a state  $\rho$  can be written as  $\mathcal{E}(\rho) = \sum_i E_i \rho E_i^\dagger$ , where the operators  $E_i$  satisfy  $\sum_i E_i^\dagger E_i = I$  (if  $\mathcal{E}$  occurs with unit probability) [?]. The complexity of QPT grows exponentially with respect to the system size; for a  $N$  qubit system, we need to specify  $2^{4N}$  parameters for  $\mathcal{E}$  and it is an overwhelming task even for small qubit systems [16, 17, 18]. Moreover, QPT necessitates estimating all the matrix elements of  $\rho$ , the state of the whole

system, which is impossible under a restricted access with zero or little knowledge on the Hamiltonian.

The hardness of the task stems from our complete ignorance about the nature of the dynamics. However, here we will consider the cases in which some a priori knowledge or good plausible assumptions are available to us. In reality, it is natural to have substantial knowledge on a fabricated physical system, which is the subject of our control, due to the underlying physics we intend to exploit. Thus, here we will see how such a priori information on the system can help reduce the complexity of Hamiltonian identification. We will primarily focus on the systems consisting of spin-1/2 particles. This is largely because they have been attracting much attention recently as a promising candidate for the implementation of quantum computers.

Yet, it would not make much sense if the size of the gateway is comparable to that of the entire system. From the viewpoint of noise suppression, the smaller the gateway size, the better. Then how can we find a minimal gateway that suffices to obtain full knowledge on the system? As we will see below, the same graph property we introduce in the first part, i.e., the study of spin network control, comes in to the discussion as a criterion for estimability of the spin network Hamiltonian.

This Chapter is based on the results from [19, 20, 21, 22, 23] as well as some new results.



**Part I**  
**Indirect control of spin networks**



## 6.2 Reachability in Quantum Control

A central question in control theory is provided a system, typically described by states, interactions, and our influence on them, to characterize the operations that can be achieved by suitable controls. In (unitary) quantum dynamics, the usual setup is a time dependent Hamiltonian of the form

$$H(t) = H_0 + \sum_k f_k(t) H_k, \quad (6.1)$$

where the time dependence  $f_k(t)$  can be chosen by the experimentator. While in usual quantum mechanics we solve the Schrödinger equation for a given  $f_k(t)$  to obtain a time evolution unitary  $U$ , the question of control is exactly the inverse: provided a unitary  $U$ , is there a control  $f_k(t)$  which achieves it? The unitaries for which this is true are called *reachable*.

Given a system (6.1), how do we characterize the reachable unitaries? It turns out that it is easier to include those unitaries which are reachable *arbitrarily well* into our consideration, and to describe things in terms of *simulable Hamiltonians*: we call a Hamiltonian  $iH$  simulable if  $\exp(-iHt)$  is reachable arbitrarily well for any  $t \geq 0$ . Clearly,  $iH_0$  is effectively reachable by setting  $f_k \equiv 0$  and letting the system evolve for a suitable time  $t$ . We could also set  $f_1 \equiv 1$  and all others zero, and simulate  $iH_0 + iH_1$ , and so on. Let us call the simulable set  $\mathcal{L}$  and see which rules it obeys:

1.  $A, B \in \mathcal{L} \Rightarrow A + B \in \mathcal{L}$  : this is a simple consequence of Trotter's formula, which says that by switching quickly between  $A$  and  $B$  the system evolves under the average of  $A$  and  $B$ .
2.  $A \in \mathcal{L}, \alpha > 0 \Rightarrow \alpha A \in \mathcal{L}$  : this follows simply from letting a weaker interaction evolve longer to simulate a stronger one, and vice versa.
3.  $A, -A, B, -B \in \mathcal{L} \Rightarrow [A, B] \in \mathcal{L}$  : this follows from a not so well-known variant of Trotter's formula given by

$$\lim_{n \rightarrow \infty} \left( e^{Bt/n} e^{At/n} e^{-Bt/n} e^{-At/n} \right)^{n^2} = e^{-[A, B]t^2} \quad (6.2)$$

4.  $A \in \mathcal{L} \Rightarrow -A \in \mathcal{L}$  : This is a property which heavily relies on finite dimensions, where the quantum recurrence theorem holds,

$$\forall \epsilon, t > 0 \exists T > t : \|e^{-AT} - 1\| \leq \epsilon \quad (6.3)$$

which implies  $e^{-A(T-t)} \approx e^{+At}$ .

If we combine all the above properties we find that the simulable set obeys exactly the properties of a Lie algebra over the reals. This is very useful; in particular, if through rules 1-4 *arbitrary* Hamiltonians can be simulated, then likewise arbitrary unitaries are reachable: the system is *fully controllable* [24, 25, 26] (in fact, this condition is necessary and sufficient). It was shown by Lloyd that it is a generic pro-

perty: in fact two randomly chosen Hamiltonians are universal for quantum computing almost surely. We will not prove this here as we are going to show something stronger: a randomly chosen pair of two-body qubit Hamiltonians is universal for quantum computing almost surely. That is, Lloyd's result holds even when restricting ourselves to *physical* Hamiltonians.

### 6.3 Indirect Control

The above equations do not yet take into account the structure of the controls. As discussed in the introduction, it is interesting to consider the case of composite system  $V = C \cup \bar{C}$  where only a part  $C$  of the system is controlled, while the remainder  $\bar{C}$  is completely untouched. In the light of Eq. (6.1) this means that  $H_k = h_C^{(k)} \otimes 1_{\bar{C}}$ . Control is mediated to  $\bar{C}$  only through the *drift*  $H_0 = H_V$ , which acts on  $C$  and  $\bar{C}$ . If through  $H_V$  the whole system is controllable, it means that we have a case of *weak* controllability: the controls  $H_k$  do not themselves generate all Hamiltonians, the drift evolution is necessary. This implies that  $H_V$  sets a time limit for how quickly the system can be controlled. It also reveals many-body properties of  $H_V$  and is therefore interesting from a fundamental perspective.

The question is, given  $H_V$  and a split of the system into  $C\bar{C}$ , how can we decide if the system is controllable? Is the general result by Lloyd still correct when restricting ourselves to such a split, and to a physically realistic  $H_V$ ? In the following, we will aim to answer both questions.

Using the results from the last section,  $V$  is controllable if and only if

$$\langle iH_V, \mathcal{L}(C) \rangle = \mathcal{L}(V), \quad (6.4)$$

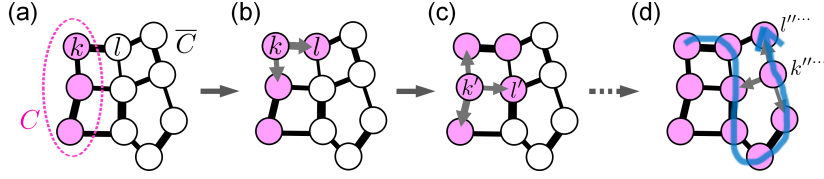
where, for the sake of simplicity, we have assumed the  $ih_C^{(k)}$ 's to be generators of the local Lie algebra  $\mathcal{L}(C)$  of  $C$  and where we use the symbol  $\langle \mathcal{A}, \mathcal{B} \rangle$  to represent the algebraic closure of the operator sets  $\mathcal{A}$  and  $\mathcal{B}$ .  $\mathcal{L}(V)$  denotes the full Lie algebra of the composite system  $V$ . The condition (6.4) can be tested numerically only for relatively small systems. It becomes impractical instead when applied to large many-body systems where  $V$  is a collection of quantum sites (e.g. spins) whose Hamiltonian is described as a summation of two-sites terms. For such configurations, a graph theoretical approach is more fruitful.

### 6.4 Graph infection

The proposed method exploits the topological properties of the graph defined by the coupling terms entering the many-body Hamiltonian  $H_V$ . This allows us to translate the controllability problem into a simple graph property, *infection* [27, 28, 29]. In many-body quantum mechanics this property has many interesting consequences on

the controllability and on relaxation properties of the system [27, 19]. Also, the same property, also called *zero-forcing*, has been studied in fields of mathematics, e.g., graph theory, in a different context [30]. Let us start reviewing this infection property for the most general setup, which will show more clearly where the topological properties come from.

The infection process can be described as follows. Suppose that a subset  $C$  of nodes of the graph is “infected” with some property. This property then spreads, infecting other nodes, by the following rule: an infected node infects a “healthy” (uninfected) neighbour if and only if it is its *unique* healthy neighbour. If eventually all nodes are infected, the initial set  $C$  is called *infecting*. Figure 6.1 would be helpful to grasp the picture.



**Fig. 6.1** An example of graph infection. (a) Initially, three coloured nodes in the region  $C$  are ‘infected’. As the node  $l$  is the only one uninfected node among the neighbours of  $k$ , it becomes infected as in (b). (c) Similarly,  $l'$  becomes infected by  $k'$ . (d) Eventually all nodes will be infected one by one.

Note that the choice of  $C$  that infects  $V$  is not unique. Though we are interested in small  $C$ , finding the smallest one is a nontrivial, and indeed hard, problem. Nevertheless, from a pragmatic point of view, the number of nodes we consider for the purpose of quantum computing would not be too large to deal with as a graph problem.

## 6.5 Controllability of spin networks

The link to quantum mechanics is that each node  $n$  of the graph has a quantum degree of freedom associated with the Hilbert space  $\mathcal{H}_n$ , which describes the  $n$ -th site of the many-body system  $V$  we wish to control. The coupling Hamiltonian determines the edges through

$$H_V = \sum_{(n,m) \in E} H_{nm} , \quad (6.5)$$

where  $H_{nm} = H_{mn}$  are some arbitrary Hermitian operators acting on  $\mathcal{H}_n \otimes \mathcal{H}_m$ . Within this context we call the Hamiltonian (6.5) *algebraically propagating* iff for all  $n \in V$  and  $(n, m) \in E$  one has,

$$\langle [iH_{nm}, \mathcal{L}(n)], \mathcal{L}(n) \rangle = \mathcal{L}(n, m), \quad (6.6)$$

where for a generic set of nodes  $P \subseteq V$ ,  $\mathcal{L}(P)$  is the Lie algebra associated with the Hilbert space  $\bigotimes_{n \in P} \mathcal{H}_n$ <sup>2</sup>. The graph criterion can then be expressed as follows:

**Theorem:** *Assume that the Hamiltonian (6.5) of the composed system  $V$  is algebraically propagating and that  $C \subseteq V$  infects  $V$ . Then  $V$  is controllable acting on its subset  $C$ .*

**Proof:** To prove the theorem we have to show that Eq. (6.4) holds, or equivalently that  $\mathcal{L}(V) \subseteq \langle iH_V, \mathcal{L}(C) \rangle$  (the opposite inclusion being always verified). By infection there exists an ordered sequence  $\{P_k; k = 1, 2, \dots, K\}$  of  $K$  subsets of  $V$

$$C = P_1 \subseteq P_2 \subseteq \dots \subseteq P_k \subseteq \dots \subseteq P_K = V, \quad (6.7)$$

such that each set is exactly one node larger than the previous one,

$$P_{k+1} \setminus P_k = \{m_k\}, \quad (6.8)$$

and there exists an  $n_k \in P_k$  such that  $m_k$  is its unique neighbor *outside*  $P_k$ :

$$N_G(n_k) \cap V \setminus P_k = \{m_k\}, \quad (6.9)$$

with  $N_G(n_k) \equiv \{n \in V | (n, n_k) \in E\}$  being the set of nodes of  $V$  which are connected to  $n_k$  through an element of  $E$ . The sequence  $P_k$  provides a natural structure on the graph which allows us to treat it almost as a chain. In particular, it gives us an index  $k$  over which we will be able to perform inductive proofs showing that  $\mathcal{L}(P_k) \subseteq \langle iH_V, \mathcal{L}(C) \rangle$ .

**Basis:** by Eq. (6.7) we have  $\mathcal{L}(P_1) = \mathcal{L}(C) \subseteq \langle iH_V, \mathcal{L}(C) \rangle$ . **Inductive step:** assume that for some  $k < K$

$$\mathcal{L}(P_k) \subseteq \langle iH_V, \mathcal{L}(C) \rangle. \quad (6.10)$$

We now consider  $n_k$  from Eq. (6.9). We have  $\mathcal{L}(n_k) \subset \mathcal{L}(P_k) \subseteq \langle iH_V, \mathcal{L}(C) \rangle$  and

$$[iH_{n_k, m_k}, \mathcal{L}(n_k)] = [iH_V, \mathcal{L}(n_k)] - \sum_m [iH_{n_k, m}, \mathcal{L}(n_k)],$$

where the sum on the right hand side contains only nodes from  $P_k$  by Eq. (6.9). It is therefore an element of  $\mathcal{L}(P_k)$ . The first term on the right hand side is a commutator of an element of  $\mathcal{L}(P_k)$  and  $iH_V$  and thus an element of  $\langle iH_V, \mathcal{L}(C) \rangle$  by Eq. (6.10). Therefore  $[iH_{n_k, m_k}, \mathcal{L}(n_k)] \subseteq \langle iH_V, \mathcal{L}(C) \rangle$  and by algebraic propagation Eq. (6.6) we have

$$\langle [iH_{n_k, m_k}, \mathcal{L}(n_k)], \mathcal{L}(n_k) \rangle = \mathcal{L}(n_k, m_k) \subseteq \langle iH_V, \mathcal{L}(C) \rangle.$$

<sup>2</sup> Note that the condition (6.6) is a stronger property than the condition of controlling  $n, m$  by acting on  $n$ . According to Eq. (6.4) the latter in fact reads  $\langle iH_{nm}, \mathcal{L}(n) \rangle = \mathcal{L}(n, m)$ , which is implied by Eq. (6.6).

But  $\langle \mathcal{L}(P_k), \mathcal{L}(n_k, m_k) \rangle = \mathcal{L}(P_{k+1})$  by Eq. (6.8) so  $\mathcal{L}(P_{k+1}) \subseteq \langle iH_V, \mathcal{L}(C) \rangle$ . Thus by induction

$$\mathcal{L}(P_K) = \mathcal{L}(V) \subseteq \langle iH_V, \mathcal{L}(C) \rangle \subseteq \mathcal{L}(V). \quad \blacksquare \quad (6.11)$$

The above theorem has split the question of algebraic control into two separate aspects. The first part, the algebraic propagation Eq. (6.6) is a property of the coupling that lives on a small Hilbert space  $\mathcal{H}_n \otimes \mathcal{H}_m$  and can therefore be checked easily numerically. The second part is a topological property of the (classical) graph. An important question arises here if this may be not only a sufficient but also necessary criterion. As we will see below, there are systems where  $C$  does not infect  $V$  but the system is controllable *for specific coupling strengths*. However the topological stability with respect to the choice of coupling strengths is no longer given.

An important example of the above theorem are systems of coupled spin-1/2 systems (qubits). We consider the two-body Hamiltonian given by the following Heisenberg-like coupling,

$$H_{nm} = c_{nm} (X_n X_m + Y_n Y_m + \Delta Z_n Z_m) , \quad (6.12)$$

where the  $c_{nm}$  are arbitrary coupling constants,  $\Delta$  is an anisotropy parameter, and  $X, Y, Z$  are the standard Pauli matrices. The edges of the graph are those  $(n, m)$  for which  $c_{nm} \neq 0$ .

To apply our method we have first shown that the Heisenberg interaction is algebraically propagating. In this case the Lie algebra  $\mathcal{L}(n)$  is associated to the group  $\text{su}(2)$  and it is generated by the operators  $\{iX_n, iY_n, iZ_n\}$ . Similarly the algebra  $\mathcal{L}(n, m)$  is associated with  $\text{su}(4)$  and it is generated by the operators  $\{iX_n I_m, iX_n X_m, iX_n Y_m, \dots, iZ_n Z_m\}$ . The identity (6.6) can thus be verified by observing that

$$\begin{aligned} [X_n, H_{nm}] &= Z_n Y_m - Y_n Z_m \\ [Z_n, Z_n Y_m - Y_n Z_m] &= X_n Z_m \\ [Y_n, X_n Z_m] &= Z_n Z_m \\ [X_n, Z_n Z_m] &= Y_n Z_m, \end{aligned}$$

where for the sake of simplicity irrelevant constants have been removed. Similarly using the cyclicity  $X \rightarrow Y \rightarrow Z \rightarrow X$  of the Pauli matrices we get,

$$\begin{aligned} X_n Z_m &\rightarrow Y_n X_m \rightarrow Z_n Y_m \\ Z_n Z_m &\rightarrow X_n X_m \rightarrow Y_n Y_m \\ Y_n Z_m &\rightarrow Z_n X_m \rightarrow X_n Y_m. \end{aligned}$$

Finally, using

$$[Z_n Z_m, Z_n Y_m] = X_m ,$$

and cyclicity, we obtain all 15 basis elements of  $\mathcal{L}(n, m)$  concluding the proof. According to our Theorem we can thus conclude that *any* network of spins coupled through Heisenberg-like interaction is controllable when operating on the subset  $C$ , if the associated graph can be infected. In particular, this shows that Heisenberg-like chains with arbitrary coupling strengths admits controllability when operated at one end (or, borrowing from [24], that the end of such a chain is a universal quantum interface for the whole system).

## 6.6 General two-body qubit Hamiltonians

Using the graph criterion we found that the dynamical Lie algebra for a Heisenberg spin chain with full local control on the first site

$$H_{\text{Hsbg}} + g(t)Y_1 + f(t)Z_1 \quad (6.13)$$

is  $\text{su}(2^N)$ , where  $H_{\text{Hsbg}}$  is the Hamiltonian describing the Heisenberg-type interaction,  $H_{\text{Hsbg}} = \sum_{(n,m) \in E} H_{nm}$  with  $H_{nm}$  in Eq. (6.12). We can also see that the algebra generated by

$$H_{\text{Hsbg}} + Y_1 + f(t)Z_1 \quad (6.14)$$

is  $\text{su}(2^N)$ .

Extending further, we can consider the Lie algebra generated by  $A = H_{\text{Hsbg}} + Y_1$  and  $B = Z_1 + 1$ . Because  $X_1 = p(A, Z_1)$ , where  $p$  is a (Lie) polynomial in  $A$  and  $Z_1$ , replacing  $Z_1$  with  $Z_1 + 1$  we obtain  $p(A, Z_1 + 1) = X_1 + c1$ . Commuting with  $B$  we find that  $Y_1$  and therefore also  $Z_1$  and 1 separately are in the algebra generated by  $A$  and  $B$ . This has an interesting implication - namely, that the two Hamiltonians  $A = H_{\text{Hsbg}} + Y_1$  and  $B = Z_1 + 1$  generate  $u(2^N)$ . These are *physical* Hamiltonians, because they consist of two-body interactions only. The fact that such pair exists can be used to prove that *almost all pairs of two-body qubit Hamiltonians* are universal: to do so, we first observe that we can construct a basis of  $u(2^N)$  through repeated commutators and linear combinations of  $A$  and  $B$  :

$$\mathfrak{u}(2^N) = \text{span} \{p_1(A, B), \dots, p_{2^{2N}}(A, B)\}$$

where the  $p_k$  are (Lie) polynomials in  $A$  and  $B$ . The fact that this is a basis can be expressed equivalently through

$$D \equiv \det \{|p_1\rangle, \dots, |p_{2^{2N}}\rangle\} \neq 0, \quad (6.15)$$

where  $|p_k\rangle$  is the vector corresponding to the matrix  $p_k(A, B)$ . Now, parametrizing  $A$  and  $B$  through

$$A = \sum_{n,m,\alpha,\beta} a_{\alpha\beta nm} \sigma_n^\alpha \sigma_m^\beta \quad (6.16)$$

$$B = \sum_{n,m,\alpha,\beta} b_{\alpha\beta nm} \sigma_n^\alpha \sigma_m^\beta \quad (6.17)$$

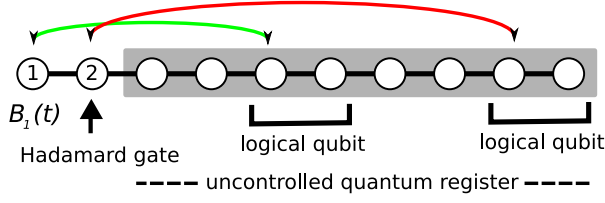
with  $\sigma_n^{(0,1,2,3)} \equiv (1_n, X_n, Y_n, Z_n)$  we can expand  $D$  in Eq. (6.15) as a multinomial in  $a_{\alpha\beta nm}$  and  $b_{\alpha\beta nm}$ . Our result implies that this multinomial is not identical to zero, and therefore its roots have measure zero. Therefore the set of parameters  $(a_{\alpha\beta nm}, b_{\alpha\beta nm})$  for which the system is not controllable is of measure zero. But the parametrization (6.16) holds for arbitrary two-body qubit Hamiltonians, which concludes the argument. We note that this argument is easily extended to general many-body Hamiltonians.

## 6.7 Efficiency considerations

The above results are interesting from the theoretical point of view; however, can they be practically useful from the quantum computing perspective? The two main problems we need to contemplate before attempting to build a large quantum computer using quantum control are as follows. First, the precise sequence of actual controls (or ‘control pulses’) are generally not computable without already simulating the whole dynamics. We need to find an *efficient* mapping from the quantum algorithm (usually presented in the gate model) to the control pulse. Secondly, even if such a mapping can be found, the theory of control tells us nothing about the overall *duration* of the control pulses to achieve a given task, and it might take far too long to be practically relevant.

One approach to circumvent these scaling problems focuses on systems that are sufficiently small, so that we do not already require a quantum computer to check their controllability and to design control pulses. In such a case, the theory of time optimal control [31] can be used to achieve impressive improvements in terms of total time or type of pulses required in comparison with the standard gate model. More complicated desired operations on larger systems are then decomposed (‘compiled’) into sequences of smaller ones. Yet, the feasibility of this approach is ultimately limited by the power of our classical computers, therefore constrained to low-dimensional many-body systems only.

The goal of this section is to provide an example where one can efficiently compute control pulses for a large system, using the full Hilbert space, and to show that the duration of the pulses scales efficiently (i.e., polynomially) with the system size. We will use a Hamiltonian that can be efficiently diagonalized for large systems through the Jordan-Wigner transformation. A similar scheme was developed independently in [32]. The control pulses are applied only to the *first two* spins of a chain (see Fig. 6.2). The control consists of two parts: one where we will use the Jordan-Wigner transformation to efficiently compute and control the information transfer through the chain (thus using it as a quantum data bus), and a second part where we will use some local gates acting on the chain end to implement two-qubit operations. To be efficiently computable, these local gates need to be fast with res-



**Fig. 6.2** (color online) Our approach for universal quantum computation works on a chain of  $N$  spins. By modulating the magnetic field  $B_1(t)$  on qubit 1, we induce information transfer and swap gates on the chain (red and green lines). The states of the qubits from the uncontrolled register can be brought to the controlled part. There, the gates from a quantum algorithm are performed by local operations. Afterward, the (modified) states are swapped back into their original position.

pect to the natural dynamics of the chain. Combining the two actions allows us to implement any unitary operation described in the gate model.

More specifically, we consider a chain of  $N$  spin-1/2 particles coupled by the Hamiltonian

$$H = \frac{1}{2} \sum_{n=1}^{N-1} c_n [(1 + \gamma)XX + (1 - \gamma)YY]_{n,n+1} + \sum_{n=1}^N B_n Z_n,$$

where  $X, Y, Z$  are the Pauli matrices, the  $c_n$  are generic coupling constants, and the  $B_n$  represent a magnetic field. Variation of the parameter  $\gamma$  encompasses a wide range of Hamiltonians, including the transverse Ising model ( $\gamma = 1$ ; for this case we require the fields  $B_n \neq 0$ ) and the  $XX$  model ( $\gamma = 0$ ). We assume that the value of  $B_1$  can be controlled externally. This control will be used to induce information transfer on the chain and realize swap gates between arbitrary spins and the two ‘control’ spins 1, 2 at one chain end. Hence such swap gates are steered *indirectly* by only acting on the first qubit.

In order to focus on the main idea we now present our method for  $\gamma = 0$  and  $B_n = 0$  for  $n > 1$ . The general case follows along the same lines, though more technically involved. Our first task is to show that by only tuning  $B_1(t)$ , we can perform swap gates between arbitrary pairs of qubits. First we rewrite the Hamiltonian using the Jordan-Wigner transformation  $a_n = \sigma_n^+ \prod_{m < n} Z_m$ , into  $H = \sum_{n=1}^{N-1} c_n \{a_n^\dagger a_{n+1} + a_{n+1}^\dagger a_n\}$ . The operators  $a_n$  obey the canonical anticommutation relations  $\{a_n, a_m^\dagger\} = \delta_{nm}$  and  $\{a_n, a_m\} = 0$ . The term we control by modulating  $B_1(t)$  is  $h_1 = Z_1 = 1 - 2a_1^\dagger a_1$ . From Sec 6.2, we know that the reachable set of unitary time-evolution operators on the chain can be obtained from computing the *dynamical Lie algebra* generated by  $ih_1$  and  $iH$ . It contains all possible commutators of these operators, of any order, and their real linear combinations. For example, it contains the anti-Hermitian operators  $ih_{12} \equiv [ih_1, [ih_1, iH]]/(4c_1) = i(a_1^\dagger a_2 + a_2^\dagger a_1)$ ,  $ih_{13} \equiv [iH, ih_{12}]/c_2 = a_1^\dagger a_3 - a_3^\dagger a_1$  and  $ih_{23} \equiv [ih_{12}, ih_{13}] = i(a_2^\dagger a_3 + a_3^\dagger a_2)$ . We observe that taking the commutator with  $h_{12}$  exchanges the index 1 of  $h_{13}$  with 2. Taking the commutator with  $iH$  we find that  $ih_{14} \equiv [ih_{13}, iH] + ic_1 h_{23} - ic_2 h_{12} = i(a_1^\dagger a_4 + a_4^\dagger a_1)$  and  $ih_{24} \equiv a_2^\dagger a_4 - a_4^\dagger a_2$

are also elements of the dynamical Lie algebra. Hence the effect of taking the commutator with  $H$  is raising the index of the  $h_{kl}$ . Generalizing this, we find that the algebra contains the elements  $ih_{kl}$ , with  $k < l$ ,  $ih_{kl} \equiv a_k^\dagger a_l - a_l^\dagger a_k$  for  $(k-l)$  even,  $ih_{kl} \equiv i(a_k^\dagger a_l + a_l^\dagger a_k)$  for  $(k-l)$  odd, and  $h_k = Z_k = 1 - 2a_k^\dagger a_k$ . We thus know that the time evolution operators  $\exp(-\pi ih_{kl}/2)$  (which will turn out to be very similar to swap gates) can be achieved through tuning  $B_1(t)$ . The main point is that because both  $h_1$  and  $H$  are free-Fermion Hamiltonians, the corresponding control functions can be computed *efficiently* in a  $2N$ -dimensional space (we will do so explicitly later). Ultimately, we need to transform the operators back to the canonical spin representation. Using  $a_k^\dagger a_l = \sigma_k^- \sigma_l^+ \prod_{k < j < l} Z_j$ , we find  $\exp(-\pi ih_{kl}/2) = (|00\rangle_{kl}\langle 00| + |11\rangle_{kl}\langle 11|) \otimes 1 + (|01\rangle_{kl}\langle 10| - |10\rangle_{kl}\langle 01|) \otimes L_{kl}$  for  $(k-l)$  even. The operator  $L_{kl} = \prod_{k < j < l} Z_j$  arises from the non-local tail of the Jordan-Wigner transformation and acts only on the state of the spins *between*  $k$  and  $l$ , *controlled* by the state of the qubits  $k, j$  in the odd parity sector.

In order to use the chain as a quantum data bus, our goal is to implement *swap gates*  $S_{kl} = |00\rangle_{kl}\langle 00| + |11\rangle_{kl}\langle 11| + |10\rangle_{kl}\langle 01| + |01\rangle_{kl}\langle 10|$ , so the fact that we have achieved some modified operators with different phases on  $k, l$  instead, and also the controlled non-local phases  $L_{kl}$ , could potentially be worrisome. We will use a method suggested in [32] that allows us to tackle these complications. That is, rather than using the physical qubits, we encode in *logical* qubits, consisting of two neighbouring physical qubits each. They are encoded in the odd parity subspace  $|01\rangle, |10\rangle$ . Although this encoding sacrifices half of the qubits, the Hilbert space remains large enough for quantum computation, and the encoding has the further advantage of avoiding macroscopic superpositions of magnetization, which would be very unstable. Swapping a logical qubit  $n$  to the control end of the chain then consists of two physical swaps  $\exp(-\pi ih_{1\ 2n-1}/2)$  and  $\exp(-\pi ih_{2\ 2n}/2)$ . Since both physical swaps give the same phases, the resulting operation is indeed a full logical swap. Any single-qubit operation on the logical qubits can be implemented by bringing the target qubit to the control end, performing the gate there, and bringing it back again. We could equally decide to perform single logical qubit gates directly, without bringing them to the control end. This is possible because  $\exp(-ih_{2n-1\ 2n}t)$  in the physical picture translates to  $\exp(-iX_{L,n}t)$  in the logical picture, and because  $Z_{2n-1}$  is in the algebra generated by  $Z_1$ , which allows us to perform the operation  $\exp(-iZ_{2n-1}t) = \exp(-iZ_{L,n}t)$ .

For quantum computation, we need to be able to perform at least one entangling two-qubit operation. We choose a controlled-Z operation, which can be performed by operating only on one physical qubit from each of the two logical qubits involved; to perform a controlled-Z between logical qubit  $n$  and  $m$ , we bring the physical qubits  $(2n-1)$  and  $(2m-1)$  to the control end, perform a controlled-Z between them, and bring them back. It is easy to check that again all unwanted phases cancel out. The controlled-Z could not be efficiently computed in the interplay with the many-body Hamiltonian  $H$ , because it cannot be generated by a quadratic Hamiltonian in the Jordan-Wigner picture. Therefore, this gate must be implemented on a time-scale  $t_g$  much faster than the natural evolution of the chain, i.e.,  $t_g \ll \min_j \{1/c_j\}$ . We can soften this requirement by using control theory to generate  $\exp(-iZ_1 X_2 t)$

by modulating  $\beta_1(t)Y_1$  (this is a linear term in the Jordan-Wigner picture), and then using a fast Hadamard gate on the second site to obtain  $\exp(-iZ_1Z_2t)$ , which, together with  $\exp(-iZ_1t)$  and  $\exp(-iZ_2t)$ , gives the controlled-Z gate. This leads to a remarkable conclusion: besides a fast Hadamard gate on the second qubit, all other controls required for quantum computation can be computed efficiently within the framework of optimal control.

The crucial question left open above, is how long does it actually take to implement the gates? In order to evaluate the efficiency, we have numerically simulated a range of chain lengths and studied the scaling of the logical swap operation time  $T$  with the (physical) chain length  $N$ . We set the coupling strength constant, namely  $c_n = J \forall n$ . To provide evidence of a polynomial scaling, we set the simulation time  $T_N = N^2$ , (all times are in units of  $1/J$  and  $\hbar = 1$ ) and verify for each  $N$  that we can find a specific  $B_1^*(t)$  that performs the logical swap.

We quantify our success by calculating the error of the operation  $\varepsilon = 1 - F$ , where  $F = (|\text{tr}U^\dagger U_g|/N)^2$  is the gate fidelity between the time evolution  $U$  and the goal unitary  $U_g$ . This standard choice of fidelity is used for evaluating generic unitaries, and for our case it is well suited confirming that the swap gate  $S_{kl} \otimes 1_{\text{rest}}$  acts as the identity almost everywhere. However the normalization factor  $1/N^2$  could in principle wash out errors in the part of the gate that acts on qubits  $k$  and  $l$  only, resulting in the wrong scaling. Therefore, we checked the reduced gate fidelity (tracing out the rest of the system) on those qubits alone, finding that its fidelity remains above  $1 - 10^{-4}$  for all  $N$  considered.

The function  $B_1(t)$  is obtained using techniques from optimal control theory [31, 33]. Briefly, the procedure is as follows: (1) an initial guess is made for the function  $B_1(t)$ ; (2) we run the optimal control algorithm to generate a new  $B_1(t)$  which decreases the error of our operation; (3) steps 1 and 2 are iterated until the final error reaches a preselected threshold  $\varepsilon$ . In practice, it suffices to choose a threshold which is of the same order of magnitude as the error introduced by the Hadamard gate.

If the algorithm converges for each  $N$  and the corresponding  $T_N$ , giving the optimal pulse sequence  $B_1^*(t)$ , then we can assert that the scaling of the operation time is at least as good as  $T_N = N^2$ , up to a given precision. Simulating chain lengths up to  $N = 40$ , we find that  $T_N = N^2$  can be achieved. We stress here that the chosen scaling law  $T_N$  may not necessarily describe the shortest time on which the physical swap gate can be performed. However, the dynamical Lie algebra of quasi-free fermions has a dimension of the order  $N^2$ , indicating that such scaling might be optimal.

## 6.8 Conclusion

We have seen that control theory provides a powerful framework for indirect control, and therefore for potential control schemes of large many-body systems. We could furthermore show that almost all physical relevant Hamiltonians provide

full control, and that at least in some cases efficient mappings from the gate model to quantum control are possible. Under which conditions this is true, and if - and how - such schemes can furthermore be made fault-tolerant in the presence of noise remains an active area of research. One thing that is clear, however, is that in order to apply such schemes, good knowledge about the system Hamiltonian  $H_0$  is required. In the next part, we will consider how such knowledge can be obtained using similar indirect schemes.



**Part II**  
**Indirect Hamiltonian tomography of spin  
networks**



## 6.9 The gateway scheme of Hamiltonian tomography

It has recently been studied how a priori knowledge on the system could reduce the complexity of quantum process tomography. A noteworthy example is the method developed on the basis of compressed sensing [34, 35], which is originally a scheme to make a best estimation for all elements of a sparse matrix despite limited amount of data. Assuming the sparsity under physically plausible settings has been also a key in other works on indirect Hamiltonian identification. The results on which we base the most of the following description exploited the polynomial dimensionality of a subspace we probe [21, 22]. That is, there is already an exponential reduction for the number of parameters to be determined. While this assumption puts a condition on the type of Hamiltonians, it was shown that a larger class of Hamiltonians (for 1D spin chains) could also be estimated through a gateway Di Carlo et al. [36]. We shall see below that this is a special case of the generic estimation of quadratic Hamiltonians, which might describe the dynamics of either bosons or fermions on not only 1D chains but also more general networks.

Suppose that we have a network consisting of  $N$  spin-1/2 particles, such as the one in Fig 6.3. Our aim is to estimate all the non-zero coupling strengths between spins and the intensities of the local magnetic fields. The assumptions we make are as follows:

1. The topology of the network is known. That is, information on the graph  $G = (V, E)$  corresponding to the network is available, where nodes  $V$  of the graph correspond to spins and edges  $E$  connect spins that are interacting with each other.
2. The type of the interaction between spins, such as the Heisenberg, XX, etc., is a priori known.
3. The inhomogeneous magnetic field is applied in the  $z$ -direction.
4. The values of coupling strengths are all real and their signs are known.

Assumptions 1 and 2 are the key for reducing the complexity of the problem. In many experimental situations, these information are available due to the conditions for fabrication, albeit a number of exceptions. In the following, we describe the estimation scheme assuming Hamiltonians that have the following form:

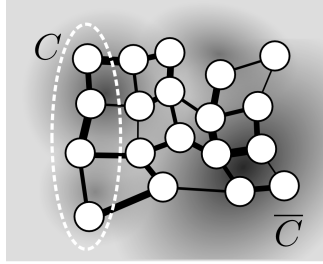
$$H = \sum_{(m,n) \in E} c_{mn} (X_m X_n + Y_m Y_n + \Delta Z_m Z_n) + \sum_{n \in V} b_n Z_n, \quad (6.18)$$

for simplicity. Here,  $X_m, Y_m$ , and  $Z_m$  are the standard Pauli operators for spin-1/2,  $c_{mn}$  are the coupling strengths between the  $m$ -th and  $n$ -th spins,  $b_n$  are the intensity of local magnetic field at the site of  $n$ -th spin, and  $\Delta$  is an anisotropy factor that is common for all interacting pairs.

The Hamiltonians of the type of Eq. (6.18) have a nice property,  $[H, \sum_n Z_n] = 0$ , i.e., the total magnetisation is preserved under the dynamics generated by  $H$ . Thus the whole  $2^N$ -dimensional Hilbert space is decomposed into the direct sum of subspaces, each of which corresponds to a specific number of total magnetisation.

For the purpose of Hamiltonian tomography, analysing the dynamics in the single excitation sector  $\mathcal{H}_1$ , which has only a single up spin  $|\uparrow\rangle$  among  $N$  spins, turns out to be sufficient. We will write a single excitation state as  $|\mathbf{n}\rangle \in \mathcal{H}_1$  when only the spin  $n \in V$  is in  $|\uparrow\rangle$  with all others in  $|\downarrow\rangle$ , and  $|\mathbf{0}\rangle = |\downarrow \dots \downarrow\rangle$ . In Sec. 6.13, we will treat more general cases, i.e., Hamiltonians that do not conserve the total magnetisation, such as the generic XX- or Ising-type Hamiltonians.

The task of Hamiltonian tomography is to estimate  $c_{mn}$  and  $b_n$  under the limited access to a small gateway  $C \subset V$  only. Naturally, the challenge here is to obtain information about the inaccessible spins in  $\bar{C} \equiv V \setminus C$ , which could be a large majority of  $V$ . The question is, however, how small can  $C$  be such that we can (in principle) still learn all the couplings and fields in  $V$ ?



**Fig. 6.3** All coupling strengths (solid lines) and local magnetic fields (background) of a 2-dimensional network  $G = (V, E)$  of spins (white circles) can be estimated *indirectly* by quantum state tomography on a gateway  $C$  (enclosed by the dashed red line). The coupling strengths and field intensities are represented by the width of lines and the density of the background colour, respectively.

This can be answered by using the *infecting* property, which has been introduced in Sec 6.4 for a given graph  $G$  and a subset  $C \subset V$  of nodes. The main theorem about hamiltonian identification under a limited access can be presented in terms of the infection property as follows. That is, *if  $C$  infects  $V$ , then all  $c_{mn}$  and  $b_n$  can be obtained by acting on  $C$  only*. Therefore,  $C$  can be interpreted as an upper bound on the smallest number of spins we need to access for the purpose of Hamiltonian tomography, i.e., given by the cardinality  $|C|$  of the smallest set  $C$  that infects  $V$ . To prove this statement, let us assume that  $C$  infects  $V$  and that all eigenvalues  $E_j$  ( $j = 1, \dots, |V|$ ) in  $\mathcal{H}_1$  are known. Furthermore, assume that for all orthonormal eigenstates  $|E_j\rangle$  in  $\mathcal{H}_1$  the coefficients  $\langle \mathbf{n} | E_j \rangle$  are known for all  $n \in C$ . We show how these information lead to the full Hamiltonian identification, and then in Section 6.10 show how these necessary data,  $E_j (\forall j)$  in  $\mathcal{H}_1$  and  $\langle \mathbf{n} | E_j \rangle$  for all  $j \in 1, \dots, |V|$  and all  $n \in C$ , can be obtained by simple state tomography experiments.

Observe that the coupling strengths between spins *within*  $C$  are easily obtained because of the relation  $c_{mn} = \langle \mathbf{m} | H | \mathbf{n} \rangle = \sum E_k \langle \mathbf{m} | E_k \rangle \langle E_k | \mathbf{n} \rangle$ , where we defined  $c_{mm} \equiv \langle \mathbf{m} | H | \mathbf{m} \rangle$  for the diagonal terms. Since  $C$  infects  $V$  there is a  $k \in C$  and a  $l \in \bar{C} \equiv V \setminus C$  such that  $l$  is the only neighbour of  $k$  outside of  $C$ , i.e.

$$\langle \mathbf{n} | H | \mathbf{k} \rangle = 0 \quad \forall n \in \overline{C} \setminus \{l\}. \quad (6.19)$$

For an example see Fig. 6.1. Using the eigenequation, we obtain for all  $j$

$$E_j |E_j\rangle = H |E_j\rangle = \sum_{m \in C} \langle \mathbf{m} | E_j \rangle H | \mathbf{m} \rangle + \sum_{n \in V \setminus C} \langle \mathbf{n} | E_j \rangle H | \mathbf{n} \rangle.$$

Multiplying with  $\langle \mathbf{k} |$  and using Eq. (6.19) we obtain

$$E_j \langle \mathbf{k} | E_j \rangle - \sum_{m \in C} c_{km} \langle \mathbf{m} | E_j \rangle = c_{kl} \langle \mathbf{l} | E_j \rangle. \quad (6.20)$$

By assumption, the left-hand side (LHS) is known for all  $j$ . This means that up to an unknown constant  $c_{kl}$  the expansion of  $|\mathbf{l}\rangle$  in the basis  $|E_j\rangle$  is known. Through normalisation of  $|\mathbf{l}\rangle$  we then obtain  $c_{kl}^2$ , thus  $c_{kl}$  (by using the assumed knowledge on its sign) and hence  $\langle \mathbf{l} | E_j \rangle$ . Redefining  $C \Rightarrow C \cup \{k\}$ , it follows by induction that all  $c_{mn}$  are known. Finally, we have

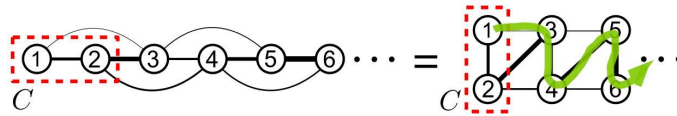
$$c_{mm} = \langle \mathbf{m} | H | \mathbf{m} \rangle = E_0 - \Delta \sum_{n \in N(m)} c_{mn} + 2b_m, \quad (6.21)$$

where  $N(m)$  stands for the (directly connected) neighbourhood of  $m$ , and

$$E_0 = \frac{1}{2} \Delta \sum_{(m,n) \in V} c_{mn} - \sum_{n \in V} b_n \quad (6.22)$$

is the energy of the ground state  $|\mathbf{0}\rangle$ . Summing Eq. (6.21) over all  $m \in V$  and using Eq. (6.22), we can have the value of  $\sum_{n \in V} b_n$ , thus that of  $E_0$  as well, since all other parameters are already known. Then we obtain the strength of each local magnetic field,  $b_m$ , from Eq. (6.21).

An interesting application of the above scheme is a one-dimensional(1D) spin chain with non-nearest neighbour interactions [37]. If spins interact with the next-nearest neighbours in addition to the nearest ones, the whole graph can be infected by setting the two end spins as  $C$ , as shown in Fig.6.4. Similarly, if spins interact with up to  $r$ -th nearest neighbours, all coupling strengths can be estimated by including the  $r$  spins at the chain end, from the first to the  $r$ -th, in  $C$ .



**Fig. 6.4** An example of graphs for non-nearest neighbour interactions. The graph for next-nearest interaction (left) can be infected by  $C$  as it is easily seen after deforming (right).

## 6.10 Data acquisition

In order to perform the above estimation procedure, we need to know the energy eigenvalues  $E_j$  in  $\mathcal{H}_1$  and the coefficients  $\langle \mathbf{n} | E_j \rangle$  for all  $n \in C$  by controlling/measuring the spins in  $C$ . Suppose the spin 1 is in  $C$ . To start, we initialise the system as  $|0\rangle$  and apply a fast  $\pi/2$ -pulse on the spin 1 to make  $\frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)$ . This can be done efficiently by acting on the spin 1 only; the basic idea is that by measuring the spin 1, and flipping it quickly every time when it was found in  $|\uparrow\rangle$ , the state of the network becomes  $|0\rangle$  within a polynomial time with respect to the network size  $N = |V|$ . The reason for this is two-fold: the excitation-preserving property of the Hamiltonian guarantees that an up-spin cannot be observed more than  $N$  times and the propagation time of up-spins in the network is polynomial in  $N$  [38]. Then, we perform quantum state tomography on the spin  $n \in C$  after a time lapse  $t$ . By repeating the preparation and measurements on spin  $n$ , we obtain the following matrix elements of the time evolution operator as a function of  $t$ :

$$e^{iE_0 t} \langle \mathbf{n} | U(t) | 1 \rangle = \sum_j \langle \mathbf{n} | E_j \rangle \langle E_j | 1 \rangle e^{-i(E_j - E_0)t}. \quad (6.23)$$

If we take  $n = 1$  and Fourier-transform Eq. (6.23) we can get information on the energy spectrum in  $\mathcal{H}_1$ . Up to an unknown constant  $E_0$ , which turns out to be irrelevant, we learn the values of all  $E_j$  from the peak positions. The height of the  $j$ -th peak gives us the value of  $|\langle 1 | E_j \rangle|^2$  for *all* eigenstates. Thanks to the arbitrariness of the global phase, we can set  $\langle 1 | E_j \rangle > 0$ . Hence observing the *decay/revival* of an excitation at  $n = 1$  we can learn some  $E_j$  and all the  $\langle 1 | E_j \rangle$ .

In order to determine  $\langle \mathbf{n} | E_j \rangle$  for other  $n \in C$ , we prepare a state at 1 and measure at  $n$ . Namely, setting  $n (\neq 1)$  in Eq. (6.23) allows us to extract the coefficient  $\langle \mathbf{n} | E_j \rangle$  correctly, including their relative phase with respect to  $\langle 1 | E_j \rangle$ . Continuing this analysis over all sites in  $C$ , we get all information necessary for the Hamiltonian tomography. It could be problematic if there were eigenstates in  $\mathcal{H}_1$  that have no overlap with *any*  $n \in C$ , i.e.,  $\langle \mathbf{n} | E_j \rangle = 0$ . Fortunately, such eigenstates do not exist, as shown in [27]. Therefore we can conclude that all eigenvalues in the  $\mathcal{H}_1$  can be obtained. Although tomography cannot determine the extra phase shift  $E_0$ , it does not affect the estimation procedure (it is straightforward to check that it cancels out in the above estimation).

Note that in order for the information about  $\langle \mathbf{n} | E_j \rangle$  ( $n \in C$ ) to be attained there should be no degeneracies in the spectrum of Eq. (6.23). For example, suppose there are two orthogonal states  $|E_k^{(1)}\rangle$  and  $|E_k^{(2)}\rangle$ , both of which are the eigenstates of  $H$  corresponding to the same eigenvalue  $E_k$ . The height of the peak at  $E_k$  in the Fourier transform of  $\langle 1 | U(t) | 1 \rangle$  would be  $|\langle 1 | E_k^{(1)} \rangle|^2 + |\langle 1 | E_k^{(2)} \rangle|^2$ . There is no means to estimate the value of each term from this sum, let alone the values of  $\langle \mathbf{n} | E_k^{(1)} \rangle$  and  $\langle \mathbf{n} | E_k^{(2)} \rangle$ . Also even if there are no degeneracies, thus if  $E_j$  are all distinct, the peaks need to be sharp enough to be resolved. The issues on degeneracies and resolving peaks are discussed in the following sections 6.11 and 6.11.

## 6.11 Degeneracy

What if there were degenerate energy levels in the single excitation subspace  $\mathcal{H}_1$ ? While 1D spin chains have no degeneracies [39], there could be in general spin networks. Of course “exact degeneracy” is highly unlikely; however approximate degeneracy could make the scheme less efficient. In this section, we show that there *always* exists an operator  $B_C$ , which represents extra fields applied on  $C$ , such that it lifts all degeneracies of  $H$  in  $\mathcal{H}_1$ . Because  $C$  is only a small subset, the existence of such an operator is not a trivial problem at all. In the following, we demonstrate the existence of such a  $B_C$  by explicitly constructing it, assuming the full knowledge about  $H$ . Without the full knowledge of  $H$  (as is the case in the estimation scenario), we could only guess a  $B_C$  and have it right probabilistically. Nevertheless, as it is clear from the discussion below, the parameter space for  $B_C$  that does not lift all the degeneracies has only a finite volume. Thus even choosing  $B_C$  randomly can make the probability of lifting the degeneracies to converge exponentially fast to one.

Once all degeneracies are lifted, we can estimate the full Hamiltonian  $H + \lambda B_C \otimes I_{\bar{C}}$  and subtracting the known part  $\lambda B_C \otimes I_{\bar{C}}$  completes our identification task. Here,  $\lambda$  is a parameter for the strength of the fields. Although the extra fields on  $C$  do not necessarily have to be a small perturbation, let us consider a small  $\lambda$  to see the effect of  $\lambda B_C$  on the energy levels, making use of the perturbation theory.

Let us denote the eigenvalues of  $H$  as  $E_k$  and the eigenstates as  $|E_k^d\rangle$ , where  $d = 1, \dots, D(k)$  is a label for the  $D(k)$ -fold degenerate states. Let us first look at one specific eigenspace  $\{|E_k^d\rangle, d = 1, \dots, D(k)\}$  corresponding to an eigenvalue  $E_k$ . Since the eigenstates considered here are in  $\mathcal{H}_1$ , we can always decompose them as

$$|E_k^d\rangle_{C\bar{C}} = |\phi_k^d\rangle_C \otimes |\mathbf{0}\rangle_{\bar{C}} + |\mathbf{0}\rangle_C \otimes |\psi_k^d\rangle_{\bar{C}},$$

where the unnormalised states  $|\phi_k^d\rangle_C$  and  $|\psi_k^d\rangle_{\bar{C}}$  are in the single excitation subspace on  $C$  and  $\bar{C}$ , respectively. The state  $|\phi_k^d\rangle_C$  ( $\forall d$ ) cannot be null, i.e.,  $|\phi_k^d\rangle_C \neq 0$ , because if there was an eigenstate in the form of  $|\mathbf{0}\rangle_C \otimes |\psi_k^d\rangle_{\bar{C}}$  then applying  $H$  repeatedly on it will necessarily introduce an excitation to the region  $C$ , in contradiction to being an eigenstate [27]. Furthermore, the set  $\{|\phi_k^d\rangle_C, d = 1, \dots, D(k)\}$  must be linearly independent: for, if there were complex numbers  $\alpha_{kd}$  such that  $\sum_d \alpha_{kd} |\phi_k^d\rangle_C = 0$ , then a state in this eigenspace  $\sum_d \alpha_{kd} |E_k^d\rangle_{C\bar{C}} = \sum_d \alpha_{kd} |\mathbf{0}\rangle_C \otimes |\psi_k^d\rangle_{\bar{C}}$  would be an eigenstate with no excitation in  $C$ , again contradicting the above statement. This leads to an interesting observation that the degeneracy of each eigenspace can be maximally  $|C|$ -fold, because there can be only  $|C|$  linearly independent vectors at most in  $\mathcal{H}_1$  on  $C$ . Thus, the minimal infecting set of a graph, a topological property, is related to some bounds on possible degeneracies, a somewhat algebraic property of the Hamiltonian.

Now suppose that  $\lambda_k B_{kC}$  is a perturbation that we will construct so that it lifts all the degeneracies for an energy eigenvalue  $E_k$ . Assuming  $B_{kC} |\mathbf{0}\rangle_C = 0$  turns out to be sufficient for our purpose. The energy shifts due to  $B_{kC}$  in the first order are given as the eigenvalues of the perturbation matrix  ${}_{C\bar{C}} \langle E_k^d | B_{kC} \otimes I_{\bar{C}} | E_k^{d'} \rangle_{C\bar{C}} = {}_C \langle \phi_k^d | B_{kC} | \phi_k^{d'} \rangle_C$ . We want the shifts to be different from each other to lift the dege-

neracy. To this end, recall that  $\{|\phi_k^d\rangle_C\}$  are linearly independent, which means that there is a similarity transform  $S_k$  (not necessarily unitary, but invertible) such that the vectors  $|\chi_k^d\rangle_C \equiv S_k^{-1}|\phi_k^d\rangle_C$  are orthonormal. The perturbation matrix can then be written as  ${}_C\langle\chi_k^d|S_k^\dagger B_{kC} S_k|\chi_k^{d'}\rangle_C$ . If we set  $S_k^\dagger B_{kC} S_k = \sum_d \epsilon_{kd} |\chi_k^d\rangle_C \langle\chi_k^d|$  the Hermitian operator

$$B_{kC} \equiv \sum_d \epsilon_{kd} \left(S_k^\dagger\right)^{-1} |\chi_k^d\rangle_C \langle\chi_k^d| S_k^{-1} \quad (6.24)$$

gives us energy shifts  $\epsilon_{kd}$ . Therefore, as long as we choose mutually different  $\epsilon_{kd}$ , the degeneracy in this eigenspace is lifted by  $B_{kC}$ . This happens for an arbitrarily small perturbation  $\lambda_k$ . So we choose  $\lambda_k$  such that the lifting is large while *no new degeneracies* are created, i.e.  $||\lambda_k B_{kC}|| \neq \Delta E_{ij}$ , where  $\Delta E_{ij} = E_i - E_j$  are the energy gaps of  $H$ .

There may be some remaining degenerate eigenspaces of the perturbed Hamiltonian  $H' = H + \lambda_k B_{kC}$ . Fortunately, since  $B_{kC}$  conserves the number of excitations (see Eq. (6.24)), we can still consider only  $\mathcal{H}_1$  and repeat the above procedure to find operators  $B_{k'C}$  to lift degeneracy in each eigenspace spanned by  $|E_{k'}^{d'}\rangle$ . Eventually we can form a total perturbation  $B_C = \sum_k B_{kC}$  that lifts *all* degeneracies in  $\mathcal{H}_1$ . By perturbation theory a ball of finite volume around  $B_C$  has the same property. In practice, we expect that almost all operators will lift the degeneracy, with a good candidate being a simple homogeneous magnetic field on  $C$ . This is confirmed by numerical simulations [22].

## 6.12 Efficiency

The efficiency of the coupling estimation can be studied using standard properties of the Fourier transform (see [40] for an introduction). In experiments, the function  $\langle \mathbf{n} | U(t) | \mathbf{m} \rangle$  ( $m, n \in C$ ) is sampled for discrete times  $t_k$ , rather than for continuous time  $t$ , with an interval  $\Delta t = t_{k+1} - t_k$ . Therefore an important cost parameter is the total number of measured points, being proportional to the sampling frequency,  $f = 1/\Delta t$ . The minimal sampling frequency is given by the celebrated Nyquist-Shannon sampling theorem as  $2f_{min} = E_{max}$ , where  $E_{max}$  is the maximal eigenvalue of  $H$  in the first excitation sector.

Due to decoherence and dissipation, the other important parameter is the total time length  $T (= \max(t_k))$  over which the functions need to be sampled to obtain a good resolution. This is given by the classical uncertainty principle that states that the frequency resolution is proportional to  $1/T$ . Hence the minimal time duration over which we should sample scales as  $T_{min} = 1/(\Delta E)_{min}$ , where  $(\Delta E)_{min}$  is the minimal gap between the eigenvalues of the Hamiltonian. Also, in order for all peaks in the Fourier transform to be resolved, the height of the peaks, which are given by  $|\langle \mathbf{n} | E_j \rangle \langle E_j | \mathbf{m} \rangle|$ , should be high enough. That is, all energy eigenstates need to be well delocalised, otherwise most of  $\langle E_j | \mathbf{m} \rangle$  would have almost zero modulus.

Although a coherence time that is as long as  $T_{min}$  has been assumed so far to make the scheme work by letting the signal propagate back and forth many times, the gateway scheme is also applicable to systems with short coherence times by modifying it. For example, as shown in [41], instead of measuring the spin state in the accessible area, we may be able to measure in the energy eigenbasis  $|E_n\rangle$ , and then the Hamiltonian can be estimated. Such a global measurement is actually easier in some cases than measuring the state of a single component. With this modification to the scheme, however, the graph condition for the accessible area  $C$  needs to be slightly changed; it should be expanded, depending on the graph structure.

Another potential concern is the (Anderson) localisation. The localisation of excitation (or spin-up) will take place, if there is too much disorder in the coupling strengths (see, for example, [42]). Then couplings far away from the controlled region  $C$  can no longer be probed. In turn, this suggests a way of obtaining information on localisation lengths indirectly. That we cannot ‘see’ beyond the localisation length would not be a serious problem as our primary purpose is to identify a quantum system we can control.

When localisation is negligible, the numerical algorithm to obtain the coupling strengths from the Fourier transform is very stable [39]. The reason is that the couplings are obtained from a linear system of equations, so errors in the quantum-state tomography or effects of noise degrade the estimation only linearly.

Let us also look at the scaling of the problem with the number of spins. Typically the dispersion relation in one-dimensional systems of length  $N$  is  $\cos kN$ , which means that the minimal energy difference scales as  $(\Delta E)_{min} \sim N^{-2}$  and thus the total time interval should be chosen as  $T_{min} \sim N^2$ . This agrees well with our numerical results tested up to  $N = 100$ . For each sampling point a quantum-state tomography of a signal of an average height of  $N^{-1}$  needs to be performed. Since the error of tomography scales inverse proportionally to the square root of the number of measurements, roughly  $N^2$  measurements are required for each tomography.

## 6.13 Quadratic Hamiltonians

So far, we have focused on the Hamiltonians that preserve the total magnetisation. Nevertheless, it is possible to generalise the above argument to a more general class. They are those that are quadratic in terms of annihilation and creation operators, that is

$$H = \sum_{m,n \in E} A_{mn} a_m^\dagger a_n + \frac{1}{2} (B_{mn} a_m^\dagger a_n^\dagger + B_{mn}^* a_n a_m), \quad (6.25)$$

which does not preserve the number of quasi-particles  $\sum a_n^\dagger a_n$ . Here,  $E$  is again the set of interacting nodes as in Eq. (6.18). For  $H$  to be Hermitian we must have  $A = A^\dagger$  and  $B^T = -\epsilon B$ , where  $\epsilon = 1$  for fermions and  $\epsilon = -1$  for bosons, depending on the particle statistics described by  $a$  and  $a^\dagger$ . For one-dimensional spin chains, the operators  $a$  and  $a^\dagger$  are defined with the standard spin (Pauli) operators

through the Jordan-Wigner transformation [43, 44],

$$a_n^\dagger a_n = \sigma_n^+ \prod_{m < n} Z_m, \text{ and } a_n^\dagger = \left( \prod_{m < n} Z_m \right) \sigma_n^-, \quad (6.26)$$

where  $\sigma_n^\pm = (X_n \pm iY_n)/2$ . The operators hereby defined,  $a_n$  and  $a_n^\dagger$ , satisfy the canonical anti-commutation relations for fermions, i.e.,  $\{a_m, a_n\} = 0$  and  $\{a_m, a_n^\dagger\} = \delta_{mn}$ . A 1D XX-type Hamiltonian

$$H = \sum_{m=1}^{N-1} c_m [(1 + \gamma)X_m X_{m+1} + (1 - \gamma)Y_m Y_{m+1}] + \sum_{m=1}^N b_m Z_m \quad (6.27)$$

with anisotropy factor  $\gamma \in [0, 1]$  can be rewritten in the form of Eq. (6.25) through the Jordan-Wigner transformation, and the matrices  $A$  and  $B$  will look like

$$A = \begin{pmatrix} -2b_1 & c_1 & & \\ c_1 & -2b_2 & c_2 & \\ & c_2 & -2b_3 & \\ & & & \ddots \end{pmatrix}, \text{ and } B = \begin{pmatrix} 0 & \gamma c_1 & & \\ -\gamma c_1 & 0 & \gamma c_2 & \\ & -\gamma c_2 & 0 & \\ & & & \ddots \end{pmatrix}.$$

A physically important example of quadratic Hamiltonians is the Ising chain of spins with transverse magnetic fields, which is expressed by Eq. (6.27) with  $\gamma = 1$  and is relevant for systems, such as superconducting qubits [9] and NMR. Note also that once the Hamiltonian of a given system is described in quadratic form, the operators  $a$  and  $a^\dagger$  can represent not only fermions, but also bosons by requiring them to obey the bosonic commutation relations,  $[a_m, a_n] = 0$  and  $[a_m, a_n^\dagger] = \delta_{mn}$ . In the following, we shall consider the problem of Hamiltonian tomography of Eq. (6.25) for 1D chains for simplicity, although the generalisation to more complex graphs is possible.

Since the Hamiltonian Eq. (6.25) does not preserve the number of particles, initialising the chain to be  $|0\dots 0\rangle$  just by accessing the end node appears to be impossible. Nevertheless, this difficulty can be circumvented by making use of the property of such Hamiltonians. The quadratic Hamiltonian above can be diagonalised as  $H = \sum_k E_k b_k^\dagger b_k + \text{const.}$  by transforming  $\alpha = (a_1, \dots, a_N, a_1^\dagger, \dots, a_N^\dagger)^t$  into  $\beta = (b_1, \dots, b_N, b_1^\dagger, \dots, b_N^\dagger)^t$  as  $\beta = T\alpha$ , so that operators  $b$  and  $b^\dagger$  still satisfy the canonical (anti-)commutation relations. So, the quasi-particles described by  $b$  and  $b^\dagger$  behave as free particles that almost do not interact with each other.

The ‘initialisation’ works then as follows. Suppose we can initialise the chain to be in a fixed, but not necessarily known, state  $\rho_0$ . Though  $\rho_0$  can be any state, a realistically plausible one might be a thermal state. We prepare two different states  $\psi_1$  and  $\psi_2$  locally at the end site after initialising the chain to be  $\rho_0$ . For each initial state we observe the time evolution at the same end site to get a reduced density matrix  $\rho(t|\psi_i)$  ( $i = 1, 2$ ) as a function of time. Because the evolution of internal state of the chain is independent of that of the state at the chain end and vice versa (thanks

to the insensitivity between quasi-particles), we can extract the pure response of the chain due to the difference between  $\psi_1$  and  $\psi_2$ , by comparing  $\rho(t|\psi_1)$  and  $\rho(t|\psi_2)$ .

The Hamiltonian of Eq. (6.25) can be rewritten as

$$H = \frac{1}{2} \alpha^\dagger M \alpha,$$

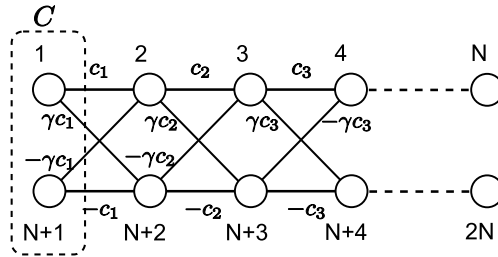
where  $M$  is a  $2N \times 2N$  matrix

$$M \equiv \begin{pmatrix} A & B \\ -\epsilon B^* & -\epsilon A^* \end{pmatrix}, \quad (6.28)$$

with  $\epsilon = 1$  for fermions and  $\epsilon = -1$  for bosons. As in the previous case of the magnetisation-preserving Hamiltonians, we assume that all coupling strengths are real and their signs are known. Also the factor  $\gamma = B_{n,n+1}/A_{n,n+1}$  (anisotropy) is assumed to be constant and known.

Now that we can take it for granted that this  $2N \times 2N$  matrix  $M$  is symmetric and its entries are all real, a key observation is to reinterpret  $M$  as a Hamiltonian that describes the hopping of excitations over a graph of  $2N$  nodes [23]. That is, the ‘Hamiltonian’  $M$  preserves the number of excitations in the  $2N$ -‘spin’ network, therefore we can apply the scheme discussed in previous sections. Of course, the state on which the Hamiltonian  $M$  acts is not a physical spin network, instead it is a fictitious state represented by a  $2N \times 1$  vector,  $(a_1, \dots, a_1^\dagger, \dots)^T$ . So the eigenvectors of  $M$  are something different from physical state vectors.

The graph for a 1D spin chain of Eq. (6.27) is shown in Fig. 6.5. Accessing the spin 1 in the real chain corresponds to accessing the nodes 1 and  $N + 1$ , since what we obtain from the measurement (and Fourier transform) are the values of  $E_j$ ,  $\langle 1|E_j\rangle$ , and  $\langle N + 1|E_j\rangle$  [23]. Here the state  $|\mathbf{n}\rangle$  stands for the localised state on the fictitious  $2N$ -node graph.



**Fig. 6.5** A graph corresponding to the matrix  $M$  with  $A$  and  $B$  of Eq. (6.28) and  $\epsilon = 1$  (fermionic). For bosonic systems, there will be additional edges connecting nodes  $m$  ( $1 \leq m \leq N$ ) and  $N + m$ , because  $B$  is symmetric, rather than antisymmetric. For both fermionic and bosonic cases, there are edges extruding and returning to the same node, corresponding to the diagonal elements of  $A$ , which are not shown here to illustrate the principal structure of the graph.

Let us take an Ising chain of  $N$  spins with transverse magnetic fields, i.e.,  $\gamma = 1$  in Eq. (6.27), as a specific example to demonstrate how the estimation goes. To

make use of the symmetry the graph in Fig. 6.5 possesses, let us define

$$|n^\pm\rangle := \frac{1}{\sqrt{2}}(|\mathbf{n}\rangle + |\mathbf{N} + \mathbf{n}\rangle).$$

We already have the information about  $\langle 1^\pm | E_j \rangle$ , as well as  $E_j$ , from the measurement on the spin 1. The estimation procedure proceeds as in Sec 6.9, namely, by looking at  $\langle 1^+ | M | E_j \rangle$  we have

$$E_j \langle 1^+ | E_j \rangle = -2b_1 \langle 1^- | E_j \rangle,$$

whose LHS is known, thus  $b_1$  can be obtained through the normalisation condition for  $\langle 1^- | E_j \rangle$ . Similarly, evaluating  $\langle 1^- | M | E_j \rangle$  gives

$$E_j \langle 1^- | E_j \rangle = 2c_1 \langle 2^+ | E_j \rangle - 2b_1 \langle 1^+ | E_j \rangle,$$

from which  $c_1$  and  $\langle 2^+ | E_j \rangle$  can be known. Also, from  $E_j \langle 2^+ | E_j \rangle = 2c_1 \langle 1^- | E_j \rangle - 2b_2 \langle 2^- | E_j \rangle$  we have  $b_2$  and  $\langle 2^- | E_j \rangle$ , therefore we have obtained all parameters up to the second spin, so effectively expanded the accessible area to two spins. Then, this procedure can go on one by one till we reach the other end of the chain, i.e., the  $N$ -th spin, identifying all the parameters in the matrix  $M$ .

A remark on the initialisation follows. It was shown in [36] that, in the case of 1D XX chains of spins-1/2, the estimation of Hamiltonian parameters is possible without initialising the chain state. The smart trick there was that the spin 1 was initialised so that the average value of the  $z$ -component of spin, i.e.,  $\langle Z_1 \rangle$ , was made zero at  $t = 0$ . The rationale behind it stems from the Jordan-Wigner transform. Since  $a_n = \sigma_n^+ \prod_{m < n} Z_m$ , if we set  $\langle Z_1 \rangle = 0$ , the averages of all  $a_n$  and  $a_n^\dagger$  ( $n > 1$ ) at  $t = 0$  become zero. Their time evolution is expressed as (in the form of the vector  $\alpha$ )

$$\alpha_n(t) = \sum_{m,k} e^{-iE_k t} T_{nk}^{-1} (T^{-1})_{km}^\dagger \alpha_m(0), \quad (6.29)$$

from which we can see that, in the Jordan-Wigner picture, the initial state of spins from the second to the  $N$ -th gives no effect on the measurement result of the first spin. Here,  $T$  is a matrix that transforms  $\alpha$  into  $\beta = T\alpha$  as mentioned above to diagonalise the Hamiltonian. Hence the above initialisation of the first spin is equivalent to that of the whole chain in the Jordan-Wigner (fermionic) picture, and thus corresponds to a special case of our description on initialisation.

## 6.14 Conclusions

We have seen that despite a severe restriction on our accessibility a large quantum system can be controlled and its Hamiltonian can be identified. As a matter of fact, it is unrealistic for any existing control scheme to have a full access to the system, i.e., a full modulability for the  $d^2 - 1$  parameters for independent Hamiltonians with

$d$  being the system dimensionality. In the case of methods based on electron/nuclear spin resonance, for instance, all we modulate is the external magnetic field and we do not have a full control over all inter-spin couplings. Therefore, a guiding theory of quantum control is needed to systematically understand and design feasible control schemes under a limited access. The results we have reviewed in this chapter are an example towards the more generic theory, already showing how powerful a restricted access can be. Although the limitation for the control in laboratories would vary, the same or modified methods as what we have seen here will be of help in making a shortcut towards the realisation of the full quantum control.

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