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Indirect quantum tomography of quadratic Hamiltonians

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Abstract. A number of many-body problems can be formulated using Hamiltonians that are quadratic in the creation and annihilation operators. Here, we show how such quadratic Hamiltonians can be efficiently estimated indirectly, employing very few resources. We found that almost all the properties of the Hamiltonian are determined by its surface and that these properties can be measured even if the system can only be initialized to a mixed state. Therefore, our method can be applied to various physical models, with important examples including coupled nano-mechanical oscillators, hopping fermions in optical lattices and transverse Ising chains.

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1. Introduction

There has been considerable interest in the problem of Hamiltonian identification through indirect probing, thereby developing various quantum mechanical versions of classical system tomography or classical ‘inverse scattering’ problems [1]. For certain types of interaction, it was found [2]–[7] that only a few resources are required to obtain an accurate model of the system. Indirect Hamiltonian estimation is therefore an interesting problem for both pragmatic purposes and fundamental insights. We are interested in the following questions. How can we obtain precise information about a Hamiltonian under restricted access? What can we learn about the ‘inside’ of a large system by only looking at a subsystem of it? Under what conditions is such indirect probing possible? When is it efficient?

Recent studies have focused on this problem for cases of chains and networks of spin-1/2 particles. The common question addressed can be formulated as follows—can we estimate all parameters, such as coupling strengths and local fields, by accessing only one or a few spins? It should be emphasized that even direct Hamiltonian estimation or, more generally, process tomography, is hard, because the required number of measurements and the complexity of the post-processing both scale exponentially with the system size. However, in realistic situations, we usually have a priori knowledge based on the underlying physics. It has been shown that such knowledge can be used to develop compressed sensing protocols [8, 9], which greatly reduce the complexity of process tomography. Various works on indirect Hamiltonian estimation have relied on similar assumptions; namely, that the dynamics is restricted to a subspace of polynomial dimension [2]–[4]. In [2], the efficiency of the estimation in terms of the required time and the number of measurements is discussed. An interesting example that does not rely on a subspace was analysed by Di Franco et al [5]. We will see here that this is a special case of the generic estimation of quadratic Hamiltonians, which can be estimated efficiently due to a simple description of their dynamics in the Heisenberg picture. Di Franco et al [5] also found that the estimation is quite robust against noise. In [3], the one-dimensional (1D) methods were generalized to arbitrary graphs, and the possible elimination of degeneracies was discussed. Also, Wieśniak and Markiewicz [4] went beyond the simplest subspace in order to study quasi-1D systems. Table 1 summarizes the results obtained so far in terms of the settings and assumptions considered. However, the analysis of physically important cases, such
Table 1. Overview of indirect Hamiltonian estimation schemes. The interaction types represent the Pauli matrices involved in the spin–spin coupling, e.g. $XX + YY + ΔZZ + Z$ stands for a Hamiltonian of the form $\sum_{n,m} A_{nm} (XX + YY + ΔZZ)_{n,m} + \sum_n B_n Z_n$.

<table>
<thead>
<tr>
<th>Interaction type</th>
<th>Needs preparation</th>
<th>Geometry</th>
<th>Obtain</th>
<th>Reference</th>
</tr>
</thead>
<tbody>
<tr>
<td>$XX + YY + ΔZZ$</td>
<td>Specific state</td>
<td>1D</td>
<td>Couplings</td>
<td>[2]</td>
</tr>
<tr>
<td>$(1 + \gamma)XX + (1 - \gamma)YY$</td>
<td>No</td>
<td>1D</td>
<td>Couplings</td>
<td>[5]</td>
</tr>
<tr>
<td>$XX + YY + ΔZZ + Z$</td>
<td>Specific state</td>
<td>Arbitrary</td>
<td>Couplings and fields</td>
<td>[3]</td>
</tr>
<tr>
<td>$XX + YY + Z$</td>
<td>Specific state</td>
<td>Quasi-1D</td>
<td>Couplings and partial topology</td>
<td>[4]</td>
</tr>
<tr>
<td>$a^\dagger a + γaa + h.c.$ (fermions or bosons); and</td>
<td>Arbitrary state</td>
<td>Arbitrary</td>
<td>Couplings and fields</td>
<td>This paper</td>
</tr>
<tr>
<td>$(1 + \gamma)XX + (1 - \gamma)YY + Z$</td>
<td></td>
<td></td>
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</tbody>
</table>

Figure 1. Indirect classical system tomography of a quadratic Hamiltonian. In this example, the spring constants $k_i$ and masses $m_i$ of a chain of coupled harmonic oscillators can be determined by monitoring the dynamics of a single particle at the chain end (in red). See [1] for details.

as the transverse Ising model and the XY model with a magnetic field, has remained open. The solutions to both cases will be presented in this paper.

Our main goal in this paper is to develop a method to perform indirect quantum tomography for many-body systems of identical particles. Even though the method is analogous to the spin case, the Hamiltonians considered here have a higher number of parameters, and it is surprising that they can still be estimated in a similar fashion. The class of Hamiltonians we study here comprises those of quadratic form in bosonic or fermionic operators. There has been tremendous progress in experiments on quantum random walks [10], optical lattices [11], coupled cavities [12], nano-mechanical oscillators [13], etc, which can be modelled by such quadratic Hamiltonians. Thus, the indirect estimation scheme we present here will be of use in reducing the necessary resources for modelling such systems. For the case of bosons, it is the most direct translation of the work by Gladwell [1] to the quantum case. Gladwell studied how the spring constants and masses of coupled classical harmonic oscillator chains can be estimated by looking at the movement of only one particle (see also figure 1). Furthermore, our protocol gives a natural generalization of spin chain estimation, since quadratic Hamiltonians of fermions also describe a certain class of spin system, such as the transverse Ising model.

The main method of indirect estimation is summarized as follows. Firstly, the system is initialized to an arbitrary but fixed state. This can even be, for example, a thermal state,
which can be reached naturally via relaxation. Then, some simple single-particle properties are initialized and, after some quantum evolution, measured again. Finally, the accumulated data are Fourier transformed, and the parameters are extracted through a set of linear equations. This simple method is outlined in figure 2 for the 1D case. The procedure is analogous to an ‘inverse scattering’ problem because the perturbation introduced in one edge of the sample (e.g. rotation of the first qubit) propagates through the sample, ‘scattering’ with the inner structure of the Hamiltonian and then this information encodes the structure of the system. While it is obvious that this procedure provides some information on the system, the surprising result here is that all information can be uniquely identified from observed data without relying on inconclusive methods, e.g. fitting curves on plots. Since this paper extends the applicability of our earlier results in [2, 3] to a much wider class of Hamiltonians, the present method inherits robustness against errors in measurements, numerics and decoherence. The problem of Hamiltonian estimation is thereby mapped to a standard problem of Fourier analysis and data processing.

The paper is structured as follows. Firstly, in section 2 we introduce the necessary notation for quadratic Hamiltonians and some techniques for their diagonalizations. Although these are well-established methods, we present them to facilitate the discussion of the estimation procedure in the following part. Readers who feel familiar enough with them can simply skip
this section. In section 3, we first discuss the simplest case of estimation, namely when the system is a chain of hopping particles, and then generalize it to arbitrary graphs. Finally, in section 4 we discuss how the results apply to 1D chains of spins and conclude in section 5.

2. Notation and diagonalization

The most general quadratic Hamiltonian of $N$ indistinguishable particles is written as

$$H = \sum_{n,m=1}^{N} A_{nm} a_n^\dagger a_m + \frac{1}{2} \sum_{n,m=1}^{N} (B_{nm} a_n^\dagger a_m^\dagger + B_{nm}^* a_m a_n),$$

(1)

where $a_n^\dagger$ and $a_m$ are creation and annihilation operators and $A$ and $B$ are matrices describing the parameters we would like to estimate. For $H$ to be Hermitian, we must have $A = A^\dagger$ and $B^T = -\epsilon B$, where we introduced the parameter $\epsilon = 1$ for fermions and $\epsilon = -1$ for bosons. We will mostly follow the notation of [14], although we shall write all vectors in Dirac notation. At first, we put all Hamiltonian parameters into the Hermitian $2N \times 2N$ matrix

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

(2)

and introduce the column vector operator

$$\alpha \equiv \begin{pmatrix} a_1 \\ \vdots \\ a_N \\ a_1^\dagger \\ \vdots \\ a_N^\dagger \end{pmatrix},$$

so that equation (1) can be expressed up to a constant as

$$H = (1/2) \alpha^\dagger M \alpha.$$

Throughout this paper, we make the following technical assumptions. Firstly, all coupling strengths are real and their sign is assumed to be known. Although some phases of these matrix elements are easy to determine and others are physically insignificant, this requires complicated studies of gauge invariance that do not seem to be worthwhile. In many practical cases all elements are real and positive. Secondly, the ratio $B_{n,n+1}/A_{n,n+1} = \gamma$ (anisotropy) is assumed to be constant and known. This means, similar to the models in [2, 3], that the type of interaction is known from the underlying physics, and what remains to be estimated are the interaction strengths. Finally, for the bosonic case we assume that the matrix $M$ is positive definite. Again, in principle this can be generalized, but this way we avoid difficulties of symplectic transformations [14].

As in [3], the efficiency of our method depends on how many entries of $M$ are a priori known to be zero, that is, on knowledge of the coupling graph. If such knowledge is not available, we have to carry out measurements on all but one of the qubits. If the graph is known to be highly sparse (for instance a chain) we only need to access a single qubit. But before
going into the details of Hamiltonian identification, let us briefly review the diagonalization of the Hamiltonian equation (1) and thus the dynamics, introducing some notation. For more detailed descriptions on the diagonalization procedure, see e.g. [14].

For quadratic Hamiltonians of the form in equation (1), there exist quasi-particle creation and annihilation operators \( b_k^\dagger \) and \( b_k \), with which the Hamiltonian can be represented by the simple form of non-interacting modes,

\[
H = \sum_{k=1}^{N} E_k b_k^\dagger b_k + \text{const.} \tag{3}
\]

For this reason, quadratic Hamiltonians are also referred to as ‘quasi-free’ interactions. We need to know the transformation \( T \) that maps the operators \( a \) and \( a^\dagger \) for particles to \( b \) and \( b^\dagger \) for quasi-particles, i.e. \( \beta = T\alpha \), where \( \beta \) is defined by

\[
\beta \equiv \begin{pmatrix}
 b_1 \\
 \vdots \\
 b_N \\
 b_N^\dagger \\
 \vdots \\
 b_1^\dagger
\end{pmatrix}.
\]

In order to ensure the canonical commutation relations for the operators \( b_k \) and \( b_k^\dagger \), \( T \) must satisfy \( T^{-1} = \eta T^\dagger \eta \), where

\[
\eta = \begin{pmatrix}
 1 & 0 \\
 0 & \epsilon \mathbb{1}
\end{pmatrix}.
\]

The Hamiltonian is now written as

\[
H = \frac{1}{2} \beta^\dagger \eta (T \eta M T^{-1}) \beta + \text{const.}
\]

It can then be shown that \( \eta M \) is diagonalized by \( T \) as

\[
T \eta M T^{-1} = \begin{pmatrix}
 E & 0 \\
 0 & -E
\end{pmatrix},
\]

where \( E = \text{diag}(E_1, \ldots, E_N) \), to have the desired form of equation (3). Note that the energy eigenvalues appear in pairs of positive \( E_k \) and negative \( E_{k+N} \equiv -E_k \) values (\( k = 1, \ldots, N \)).

The matrix \( T \) consists of the right eigenvectors \( \langle E_k \rangle \) of \( \eta M \) as

\[
T \equiv \eta \begin{pmatrix}
 \langle E_1 \rangle \\
 \vdots \\
 \langle E_{2N} \rangle
\end{pmatrix} \eta,
\]
and the inverse of $T$ is given by
\[
T^{-1} = (|E_1 \rangle \cdots |E_{2N} \rangle).
\]

For bosons, the matrix $\eta M$ is not Hermitian and making a distinction between right and left eigenvectors is necessary. This gives rise to a few further peculiarities, such as the modified normalization and completeness relationship (see below). Fortunately, in this paper we are solving an inverse problem and do not have to discuss how to find these vectors and how numerically stable the corresponding algorithms are.

It is worth pointing out that the $|E_k \rangle$ are not representing physical states but are just introduced here as a part of solving the Heisenberg equation of motion for the creation and annihilation operators. The completeness relationship is given by
\[
\sum_{k=1}^{N} |E_k \rangle \langle E_k| + \epsilon |E_{k+N} \rangle \langle E_{k+N}| = \mathbb{1}_{2N \times 2N},
\]

and the vectors $|E_k \rangle$ are chosen to fulfil the normalization relationship
\[
\langle E_k | \eta | E_{k'} \rangle = \eta_{kk'}.
\]

For convenience, let us also introduce vectors $|n \rangle$ as the canonical basis vectors:
\[
|n \rangle \equiv \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 1 \\ \vdots \\ 0 \end{pmatrix} \quad \text{← n th row.}
\]

Due to the structure of the matrix $M$, the upper and lower eigenvectors of $\eta M$ are related as
\[
|n \rangle |E_k \rangle = |n \oplus N \rangle |E_k \rangle^*.
\]

where $\oplus$ is the addition modulo $2N$. The dynamics of the original operators $\alpha$ can be found from $\beta_n(t) = e^{-iE_n t} \beta_n(0)$ as
\[
\alpha_n(t) = \sum_{m,k} s(m, k) e^{-iE_k t} T^{-1}_{nk} (T^{-1})^*_{km} \alpha_m(0),
\]

where we have introduced a sign function $s(m, k)$ through
\[
\begin{align*}
s(m, k) &= 1 \quad (m = 1, \ldots N; \ k = 1, \ldots N), \\
s(m, k) &= \epsilon \quad (m = 1, \ldots N; \ k = N + 1, \ldots 2N), \\
s(m, k) &= \epsilon \quad (m = N + 1, \ldots 2N; \ k = 1, \ldots N), \\
s(m, k) &= 1 \quad (m = N + 1, \ldots 2N; \ k = N + 1, \ldots 2N).
\end{align*}
\]
3. Estimation method

3.1. Experimental requirements

Let us first consider a 1D chain of interacting particles, meaning that $A$ and $B$ are tridiagonal. Also assume that we can initialize the chain in a fixed state $\rho_0$. This state could, for instance, be a thermal state, but we do not require to have the exact form of $\rho_0$: we just have to be able to repeatedly initialize the chain to the same state $\rho_0$. As before [2, 5], we perform initializations followed by measurements at the first site. The quantity we need to measure at the first site is $a_1 \pm a_1^\dagger$ for different times up to $N^2$ [2]. In order to eradicate the dependence on the initial state $\rho_0$, we measure two sequences of $\langle a_1(t) \rangle$ after preparing the first site to give two different initial values, i.e. $\langle a_1(0) \rangle = c_1$ and $\langle a_1(0) \rangle = c_2$. Using $\langle a_n \rangle = \overline{\langle a_n \rangle}$, and thus $\langle a_n(0) \rangle = c_n^*$, and subtracting the measurement results, we obtain a quantity that only depends on $\Delta c \equiv c_1 - c_2$. It is given through equation (6) by

$$
\langle a_1(t) \rangle_{c_1} - \langle a_1(t) \rangle_{c_2} = \left[ \sum_{m,k=1}^{N} s(m, k) e^{-iE_k t} T_{1k}^{-1}(T^{-1})_{km} \langle a_m(0) \rangle \right]_1 - \left[ \sum_{m,k=1}^{N} \ldots \right]_2
$$

$$
= \Delta c \sum_{k=1}^{2N} s(k, k) e^{-iE_k t} |T_{1k}^{-1}|^2 + \Delta c^* e \sum_{k=1}^{2N} s(N + 1, k) e^{-iE_k t} T_{1k}^{-1}(T^{-1})_{k,N+1}^\dagger.
$$

This initialization can be performed by a von Neumann measurement or, as long as the reduced density matrix at site one is not maximally mixed, by applying different single qubit rotations (in some experiments von Neumann measurements are hard). As we see in equation (7), the dependence on the initial state is completely removed. This is thanks to the absence of the interactions between particles: they (almost) do not see each other, so the information on the ‘injected’ particle can be extracted by subtracting the influence from others.

For the spin chain case the eigenfrequencies are non-degenerate and $T_{1k}^{-1} = |1E_k\rangle \neq 0 \quad (\forall k)$ [2, 3]. For the present case of quadratic Hamiltonians, we were unable to prove this, but could confirm it numerically. Hence, a Fourier analysis provides us with the frequencies $E_k$ and the amplitudes $\Delta c |T_{1k}^{-1}|^2 + \Delta c^* e T_{1k}^{-1}(T^{-1})_{k,N+1}^\dagger$. Summing these amplitudes gives the value of $\Delta c$,

$$
\sum_{k=1}^{N} \left( \Delta c |T_{1k}^{-1}|^2 + \Delta c^* e T_{1k}^{-1}(T^{-1})_{k,N+1}^\dagger \right) + \epsilon \sum_{k=N+1}^{2N} \left( \Delta c |T_{1k}^{-1}|^2 + \Delta c^* e T_{1k}^{-1}(T^{-1})_{k,N+1}^\dagger \right)
$$

$$
= \Delta c \langle 1|1 \rangle + \Delta c^* e \langle 1|N + 1 \rangle = \Delta c,
$$

where we used the completeness relationship equation (4). Equation (7) still contains mixtures of the coefficients $|T_{1k}^{-1}|$ and $T_{1k}^{-1}(T^{-1})_{k,N+1}^\dagger$. We can separate them by measuring another pair of initializations $c'_n$; as long as $\Delta c' \neq r \Delta c$, we can solve the linear equation for $|T_{1k}^{-1}|$. Without loss of generality, we choose $|\langle 1|E_k \rangle| = |T_{1k}^{-1}| = T_{1k}^{-1} = |1E_k\rangle \quad (\forall k)$ by arranging the global phase of each eigenstate $|E_k\rangle$. In conclusion, a few random rotations or initializations of the first qubit, followed by measurements, provide us with $E_k$ and $|\langle 1|E_k\rangle|$, as well as $|\langle N+1|E_k\rangle|$. 

Figure 3. The coupling graph that represents $M$ for a 1D chain as an adjacency matrix.

Let us now describe how to obtain the parameters of $M$ from these observed data. We have to distinguish between the generic case where the off-diagonal couplings $A_{n,n+1}$ and $B_{n,n+1}$ are distinct and the special case where they are equal.

3.2. Different off-diagonal couplings

As we have seen above, what we diagonalized is the $2N \times 2N$ matrix $\eta M$, so it is helpful to regard $M$ as a representation of a graph consisting of $2N$ nodes (see figure 3). Its off-diagonal entries correspond to the coupling strengths between nodes, whereas the diagonal elements represent the intensity of the 'field' at each node. We can then start with a recursive algorithm similar to [1]–[3] by applying $M$ to the local states at sites 1 and $N+1$. To do this, let us introduce the following notation:

$$|n^\pm\rangle \equiv \frac{1}{\sqrt{2}} (|n\rangle \pm |n+N\rangle), \quad n = 1, \ldots, N.$$

Because the elements $\langle 1^\pm | E_k \rangle$ are already known from the procedure in the previous subsection, we learn $A_{11}$ and $B_{11}$, as

$$\langle 1^\mp | \eta M | 1^\pm \rangle = A_{11} \pm B_{11},$$

where the lhs can be evaluated by inserting equation (4). Noting that $B_{nn} \neq 0$ only for bosons ($\epsilon = -1$), we have

$$M \eta |n^\pm\rangle = (A_{n-1,n} \pm \epsilon B_{n-1,n}) |n-1^\mp\rangle + (A_{nn} \mp B_{nn}) |n^\mp\rangle + (A_{n+1,n} \pm \epsilon B_{n+1,n}) |n+1^\mp\rangle$$

$$= (1 \pm \epsilon \gamma) A_{n-1,n} |n-1^\mp\rangle + (A_{nn} \mp B_{nn}) |n^\mp\rangle + (1 \mp \gamma) A_{n+1,n} |n+1^\mp\rangle, \quad n = 1, \ldots, N,$$

where we set $A_{01} = A_{N,(N+1)} = 0$. In some sense, this equation is very similar to a 1D chain case. Then, for $n = 1$, we obtain

$$E_k \langle 1^\pm | E_k \rangle = \langle 1^\pm | \eta M | E_k \rangle$$

$$= (A_{11} \mp B_{11}) \langle 1^\mp | E_k \rangle + (1 \mp \gamma) A_{21} \langle 2^\mp | E_k \rangle.$$

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Therefore, the only unknown in equation (9) is $A_{21} \langle 2^±|E_k⟩$, from which we obtain $A_{21} \langle 2|E_k⟩$,

$$A_{21}^2 = \sum_{k=1}^{N} |A_{21} \langle 2|E_k⟩|^2 + \epsilon |A_{21} \langle 2|E_{k+N}⟩|^2 = \text{known.}$$

In order to separate them, we use the completeness relation (4). Since $A_{21}$ is assumed to be real with known sign, we determine $A_{21}$. Then, from equation (9), we acquire the values of $\langle 2^±|E_k⟩$.

Now that we have $\langle 1^±|E_k⟩$, $\langle 2^±|E_k⟩$, $E_k$ and all $A_{mn}$, $B_{mn}$ for $m, n = 1, 2$, we can proceed to a similar set of equations for the next site $\langle 2^±|\eta M|E_k⟩$. By induction, all matrix elements of $A$ and $B$ can be obtained, as desired. We will now look at the cases with equal off-diagonal couplings in more detail, because such physical systems are often encountered, for example transverse Ising for fermions and coupled harmonic oscillators for bosons.

3.3. Equal off-diagonal couplings

When $\gamma = 1$, the above method fails, because the term $(1 - \gamma)A_{21} \langle 2^-|E_k⟩$ in equation (9) vanishes and we cannot estimate $\langle 2^-|E_k⟩$. This is the case for interacting harmonic oscillators without the rotating wave approximation [15] and for quantum Ising models, and is therefore of interest in a number of practical situations. The diagonal elements $A_{nn}$ and $B_{nn}$ are always different if there is a transverse field (fermions) or if the masses are finite (bosons). The necessity of a non-zero transverse field for the Ising model is also a result of the physical property that excitations do not propagate along the chain without the field.

Equation (8) above now becomes

$$M_{\eta} |n^±⟩ = (1 ± \epsilon)A_{n-1,n} |n − 1^±⟩ + (A_{nn} ± B_{nn}) |n^±⟩ + (1 ± 1)A_{n+1,n} |n + 1^±⟩, \quad n = 1, \ldots, N,$$

where $A_{01} = A_{N,(N+1)} = 0$ again. As before, we learn $A_{11}$ and $B_{11}$ from $\langle 1^±|\eta M|1^±⟩ = A_{11} ± B_{11}$, and $A_{21}$ and $\langle 2^±|E_k⟩$ from $\langle 1^-|\eta M|E_k⟩$ through normalization. For bosons, we obtain $A_{22} − B_{22} = \langle 2^±|\eta M|2^-⟩$ through the completeness relation, followed by $\langle 2^-|E_k⟩$ through

$$E_k \langle n^+|E_k⟩ = \langle n^+|\eta M|E_k⟩ = (A_{nn} − B_{nn}) \langle n^-|E_k⟩.$$

For $A_{22}$ and $B_{22}$, equation (4) can be used again for

$$A_{22} + B_{22} = (2^-|\eta M|2^+).$$

On the other hand, for fermions, the information on $A_{22}$ and $\langle 2^-|E_k⟩$ is attained from

$$E_k \langle 2^+|E_k⟩ = \langle 2^+|\eta M|E_k⟩ = 2A_{12}(1^-|E_k⟩ + A_{22}(2^-|E_k⟩),$$

as above. Knowing all parameters at site 2, we can then proceed through induction.

3.4. Estimation of general graphs

We now briefly describe how the linear case is generalized to arbitrary graphs. This is almost identical to [3], so we will not repeat the details. Similar to the spin case, in the general graph
setting, measurements on a single spin do not suffice: we need to consider transport in the network. Depending on the network topology, we choose a set $C$ of ‘infecting’ nodes, which are the ones we will perform initializations and measurements on. For clarity, let us recall the definition of graph ‘infection’. Suppose that a subset $C$ of nodes of the graph is ‘infected’ with some property, e.g. the flu. 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’.

Similar to the measurements described in section 3.1, initializing the site $m \in C$ and measuring the $\ell$th node after some time, we can obtain

$$\langle a_{\ell}(t) \rangle = \sum_{n=1}^{N} \sum_{k=1}^{2N} \left[ s(n,k) e^{-iE_k T_{lk}^{-1}} T_{kk}^{-1} (T^{-1})_{kn} a_n(0) \rangle + s(N+n,k) e^{-iE_k T_{lk}^{-1}} T_{kk}^{-1} (T^{-1})_{kn} a_n(0) \rangle \right].$$

(11)

Again, the dependence on the initial state $\rho_0$ may be removed by subtracting data for different initial conditions on the site $m$. Starting from some element in $C$, say $m = \ell = 1$, we can get $T_{kk}^{-1}$, as described in section 3.1. Then we initialize in $m$ and measure at a different site $\ell \in C$, obtaining $T_{kk}^{-1}$ including its phase from equation (11). Hence, all $T_{kl}$ with $k, \ell \in C$ can be learnt from simple experiments on the set $C$. The 1D estimation and infection are then used to infer the remaining parameters, as described in more detail in [3].

4. Application to one-dimensional spin chains

Naturally, the above scheme can be applied directly to many cases of Hamiltonian identification for systems of spin-1/2 particles. A typical example is the XY chain of spin-1/2 particles, as it can be transformed into quasi-free fermions by means of the Jordan–Wigner transformation. As has been noted already in [5], the estimation for this model can be done without initialization of the entire chain. In the Jordan–Wigner picture, this becomes very clear. That is, after locally measuring an eigenstate of $X_1 = a_1 + a_1^\dagger$, thus making $\langle Z_1 \rangle = 0$, the initial expectation values of the $a_n$ and $a_n^\dagger$ for $n > 1$ are all zero. This is because the Jordan–Wigner transformation of $a_n$ for $n > 1$, i.e. $a_n = \sigma_n^+ \prod_{m<n} Z_m$, always contains $Z_1$ in the product. One might say that the local initialization in the spin picture corresponds to a global initialization in the fermionic picture. Combined with the weak dependence of local observables on the initial condition that comes from the quasi-free interaction, the state dependence of the measurements at the first site is completely removed. Hence, our scheme is a proper generalization of [5] to include magnetic field and the transverse Ising case, which is important in various physical systems, for example superconducting (flux) qubits [16], NMR, etc. Such models have also attracted attention in the context of indirect quantum control recently [17, 18], where our estimation scheme is crucial.
5. Conclusions

We found a simple and efficient method to identify the Hamiltonian of a system of coupled bosons or fermions. While the methods are completely analogous to the spin case [2, 3], it is surprising that the higher number of parameters in the Hamiltonian that arises from the non-conservation of excitations can still be estimated using the same resources. Similarly to [5], we can deal with very weak system initialization, such as thermal states. Therefore, our methods can drastically reduce the required resources for system identification. As for the effect of errors in the procedure, such as the state preparation, the measurements, and decoherence, thanks to the linearity of the equations we need, eventual errors in the estimated parameters are also bounded linearly. This is one of the notable advantages of our protocol over other methods that rely on ad hoc algorithms, such as fitting. Also, to grasp a more intuitive picture, see [2] for an example of numerical simulations in which the method is applied to a spin chain with random coupling strengths. Although the simulation in [2] is for an excitation-preserving chain, the necessary numerical calculations here for quadratic Hamiltonians are essentially the same.

From the theory side, the present study once more confirmed a type of ‘holographic principle’ for estimation: looking only at the surface of short-range interacting systems can help us to determine their Hamiltonian completely. It would be interesting to see whether this has direct connections with area laws of entanglement [19]. While the efficiency of our method relied on the quadratic form of the Hamiltonian, we conjecture that even for models with true interaction terms, for example quartic terms in the Hamiltonian, all system parameters remain discoverable on the surface in principle.

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