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Indirect Hamiltonian identification through a small gateway

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Abstract. Identifying the many-body Hamiltonian of a large quantum system is essential in understanding many physical phenomena, yet extremely difficult in general. We show that coupling strengths in networks of spin-1/2 particles can be estimated indirectly through a gateway, provided that the coupling topology is known. The criterion for the feasibility of identification is described only by a simple topological property concerning how the gateway is connected to the entire network. We also address the issues of process efficiency and how degeneracies of the system can be lifted.

Contents

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1. Introduction

When studying any quantum mechanical system, precise knowledge of its nature is crucially important. In quantum mechanics, any observable phenomena can be explained rigorously, in principle, if we have complete knowledge of the system. More specifically, we need to identify the states of the system and the Hamiltonian that governs their dynamics.

The full information acquisition is, however, in general very hard from an operational as well as from a computational and mathematical points of view, even for small systems [1]–[5]. For large many-body systems spectroscopy reveals only little information about the Hamiltonian, and generally local addressing of its components is required in order to obtain details about the system. Instead, we may access and manipulate the system by operating individual spins in a small subsystem, as a *gateway*. Such situations, in which only a subsystem is accessible, arise for example in networks of 'dark spins' in diamond and solid state quantum devices [6]–[8].

Yet, a common dilemma is that such a gateway not only allows us to interact with the system but also introduces noise to it (see figure 1). From a Hamiltonian identification perspective, it is therefore crucial to find minimal gateways that suffice to obtain full knowledge on the system. While this is impossible to answer in general, bounds can be derived if the topology of the system is known. In this context, some positive results have been presented for the case of one-dimensional (1D) chains of spin-1/2 particles [9, 10]. That is, the coupling strengths between neighbouring spins can be estimated by accessing only the spin at the end of the chain. Since schemes to initialize the state of spins as $|\downarrow\downarrow\ldots\downarrow\rangle$ by operating on the chain end are known [11], such identification of the Hamiltonian is sufficient to determine the dynamics of the system completely. These results are of interest in their own right, yet they were limited to the simplest of networks, i.e. 1D chains.

Here, we present an estimation scheme for general graphs of spins (for an example see figure 2). As well as the details of the Hamiltonian identification procedure, we give a precise condition for the 'gateway' (accessible region) that suffices to make the identification possible. For the important cases of finite 2D/3D lattices such a gateway is given by tone edge or one face of the lattice, respectively. This is remarkable because the ratio between the gateway size and the unknown parameters is higher than in the 1D case. We will also show that while in the 1D case the decay properties of the state in the gateway can identify the Hamiltonian, in the 2D case we need its decay properties as well as the transport properties within the gateway. Interestingly, our general condition turns out to coincide with the criterion for the controllability of spin networks [12].

We will study a network with Heisenberg-type interaction. This allows us to describe an estimation procedure that is numerically stable, mathematically simple and efficient (given that we consider arbitrary and large systems). What we attempt to estimate are the coupling strengths between interacting spins and the strengths of local magnetic fields. Such inhomogeneous fields are very common in experiments, and can cause much trouble through dephasing. Hence it is worth estimating them (such analysis was lacking in [9, 10]). Another interesting new aspect we introduce in this paper is how to lift degeneracies on the system by applying extra fields on the gateway. We show that this is always possible, a result which might be relevant beyond the scope of estimation.

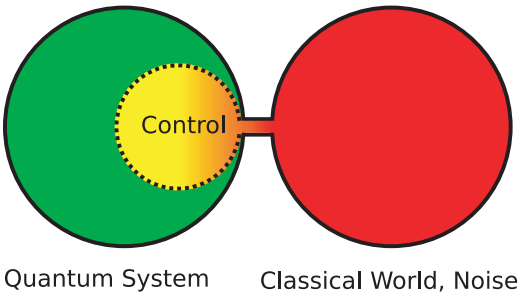

Figure 1. In classical mechanics, restricted estimation becomes important when access to the whole system is not possible. In quantum mechanics, restricted estimation is useful even if in principle the whole system could be accessed. This is because the control required for the estimation opens up a gateway to the classical world, introducing noise.

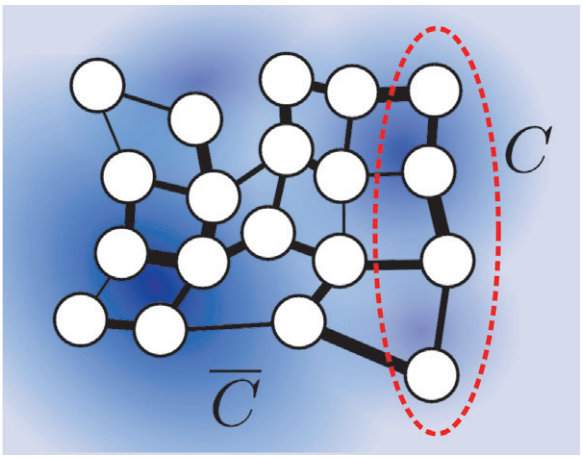

Figure 2. All coupling strengths (black lines) and local magnetic fields (blue background) of a 2D network $G = (V, E)$ of spins (white circles) can be estimated indirectly by quantum state tomography on a gateway C (enclosed by the dashed red line). The coupling strengths and field intensities are represented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

2. Setup and main result

Suppose that we have a network of spin-1/2 particles, such as the one in figure 2. We assume that we have knowledge of the graph $G = (V, E)$, which describes the network: nodes V of the graph correspond to spins and edges E connect spins that are interacting with each other. The pairwise interaction between spins is Heisenberg type with a known anisotropy Δ, and there is an inhomogeneous magnetic field applied on the spins. Then, the Hamiltonian we consider has the form

$$H = \sum_{(m,n)\in E} c_{mn}\left(\sigma_m^x\sigma_n^x + \sigma_m^y\sigma_n^y + \Delta\sigma_m^z\sigma_n^z\right) + \sum_{n\in V} b_n\sigma_n^z,$$

where c_{mn} represent the unknown coupling strengths between spins m and n, and b_n the unknown intensity of the magnetic field at n, respectively. Here, we also assume $c_{mn} < 0$ for all m

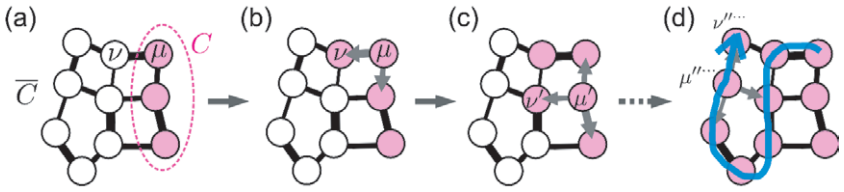

Figure 3. An example of graph infection. (a) Initially, three coloured nodes in the region C are 'infected'. As the node ν is the only one uninfected node among the neighbours of μ, it becomes infected as in (b). (c) Similarly, ν' becomes infected by μ'. (d) Eventually all nodes will be infected one by one.

and n, i.e. ferromagnetic interactions, though the setup is readily generalized to other cases. In the above, $\sigma_n^i (i = x, y, z)$ are the standard Pauli matrices. The purpose of the following will be to estimate c_{mn} and b_n over the entire set V of spins by only accessing a small gateway, described by a subset $C \subset V$ (see figure 2). For almost all practical cases of the Hamiltonian identification problem, analysing the dynamics in the *single excitation sector* $\mathcal{H}_1$ turns out to be sufficient. We will thus denote a single excitation state as $|\mathbf{n}\rangle \in \mathcal{H}_1$ when the spin $n \in V$ is in the state $|\uparrow\rangle$ and all others are in $|\downarrow\rangle$ for clarity. The state with all spins in $|\downarrow\rangle$ will be written as $|\mathbf{0}\rangle$.

Naturally, the challenge here is to obtain information about the inaccessible spins $\bar{C} \equiv V \backslash C$, which could be the large majority of the set. The question is however how small can C be such that we can (in principle) still learn all the couplings and fields in V?

This can be answered by using a graph property, known as 'infecting,' of a subset $C \subset V$ of the nodes [12]–[14]. In many-body quantum mechanics this property has many interesting consequences on the controllability and on relaxation properties of the system [12, 13]. 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'. The graphs in figures 2 and 3 are examples in which C infects V (we encourage the reader to confirm this by colouring the nodes in region C and applying the above propagation rule—this will make the following proof much more intuitive). With this definition, the main result of the paper is the following: *if C infects V, then all c_{nm} and b_n can be obtained by acting on C only*. Thus, we provide an upper bound on the smallest number of spins we need to access in order to perform Hamiltonian tomography, i.e. given by the cardinality $|C|$ of the smallest set C that infects V. To prove the above statement, let us assume that C infects V and that all eigenvalues E_j $(j = 1, \ldots, |V|)$ 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 first show that these assumptions lead to full Hamiltonian identification, and then show how the data for the assumptions can be obtained by simple tomography experiments.

We observe that the coupling strengths between spins *within* C are easily obtained because of the relation

$$c_{mn} = \langle \mathbf{m}|H|\mathbf{n}\rangle = \sum E_k \langle \mathbf{m}|E_k\rangle\langle E_k|\mathbf{n}\rangle, \tag{1}$$

Figure 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).

where we defined $c_{mm} \equiv \langle \mathbf{m}|H|\mathbf{m}\rangle$ for the diagonal terms. Since C infects V there is a $\mu \in C$ and a $\nu \in \bar{C} \equiv V \backslash C$ such that ν is the only neighbour of μ outside of C, i.e.

$$\langle \mathbf{n}|H|\boldsymbol{\mu}\rangle = 0 \ \ \forall n \in \bar{C}\backslash\{\nu\}. \tag{2}$$

For an example see figure 3. Using the eigenequation, we obtain for all j

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

Multiplying with $\langle\boldsymbol{\mu}|$ and using equation (2), we obtain

$$E_j\langle\boldsymbol{\mu}|E_j\rangle - \sum_{m\in C} c_{\mu m}\langle \mathbf{m}|E_j\rangle = c_{\mu\nu}\langle\boldsymbol{\nu}|E_j\rangle.$$

By assumption and by equation (1), the left-hand side (LHS) is known for all j. This means that up to an unknown constant $c_{\mu\nu} < 0$ the expansion of $|\boldsymbol{\nu}\rangle$ in the basis $|E_j\rangle$ is known. Through normalization of $|\boldsymbol{\nu}\rangle$, we then obtain $c_{\mu\nu}$ and hence $\langle\boldsymbol{\nu}|E_j\rangle$. Redefining $C \Rightarrow C \cup \{\mu\}$, it follows by induction that all c_{mn} are known. Finally, we have

$$c_{mm} = \langle \mathbf{m}|H|\mathbf{m}\rangle = E_0 - \Delta \sum_{n\in N(m)} c_{mn} + 2b_m, \tag{3}$$

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

$$E_0 = \frac{1}{2}\Delta \sum_{(m,n)\in V} c_{mn} - \sum_{n\in V} b_n \tag{4}$$

is the energy of the ground state $|\mathbf{0}\rangle$. Summing equation (3) over all $m \in V$ and using equation (4), 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 equation (3).

An interesting application of the above scheme is a 1D spin chain with non-nearest neighbour interactions [15]. 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 figure 4. Similarly, if spins interact with up to kth nearest neighbours, all coupling strengths can be estimated by including the k end spins in C.

3. Tomography

Here, we describe how to obtain the information that is assumed to be known in the above proof. That is, 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. Let us consider the case where the eigenvalues in $\mathcal{H}_1$ are non-degenerate. The general case is discussed in section 4. To start the estimation, we initialize the system as $\frac{1}{\sqrt{2}}(|\mathbf{0}\rangle + |\mathbf{1}\rangle)$. As discussed in [11], this can be done efficiently by acting on the region C only. Then, we perform quantum state tomography on the spin $n \in C$ after a time lapse t. By repeating the preparation and tomographic measurements on spin n for various times t, we obtain the following matrix elements of the time evolution operator as a function of t:

$$e^{iE_0 t}\langle \mathbf{n}|U(t)|\mathbf{1}\rangle = \sum_j \langle \mathbf{n}|E_j\rangle\langle E_j|\mathbf{1}\rangle e^{-i(E_j-E_0)t}. \tag{5}$$

If we take $n = 1$ and Fourier transform equation (5) we can get information on the energy spectrum of the Hamiltonian in $\mathcal{H}_1$. Up to an unknown constant E_0, which will turn out to be irrelevant later, we learn the values of all E_j corresponding to eigenstates that have nonzero overlap with $|\mathbf{1}\rangle$. We also obtain the values of $|\langle \mathbf{1}|E_j\rangle|^2$ for all eigenstates. Due to the freedom in determining the overall phase of a state, we can assume that the coefficients for $|\mathbf{1}\rangle$ of all $|E_j\rangle$ are real and positive, $\langle \mathbf{1}|E_j\rangle > 0$. Hence observing the decay/revival of an excitation at $n = 1$, we can already learn some E_j and all the $\langle \mathbf{1}|E_j\rangle$. This is analogous to the $1D$ case, where this knowledge would suffice to obtain the full Hamiltonian [9].

In arbitrary graphs, however, this is no longer the case. In fact, even if we observed the decay/revival at each $n \in C$, we would only obtain the $|\langle \mathbf{n}|E_j\rangle|^2$, but could not determine their phase freely anymore. To obtain the required knowledge about E_j and $\langle \mathbf{n}|E_j\rangle$ for the Hamiltonian identification, we need to observe the *transport* within C. This is represented by Fourier transforming equation (5) for $n \neq 1$, allowing us to extract the coefficient $\langle \mathbf{n}|E_j\rangle$ correctly, including their relative phase with respect to $\langle \mathbf{1}|E_j\rangle$. We also obtain those eigenvalues E_j, for which $\langle \mathbf{n}|E_j\rangle \neq 0$. Continuing this analysis over all elements of C, we learn all eigenvalues which have overlap with some $n \in C$. Could there be eigenstates in $\mathcal{H}_1$ that have no overlap with any $n \in C$? The answer is no, as it is shown in [13]. 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).

4. Efficiency and degeneracy

The efficiency analysis of the Hamiltonian tomography is roughly the same as in [9]. Due to the conservation of excitations, the sampling can be restricted to an effective $|V|$-dimensional Hilbert space, and the speed is some polynomial in $|V|$, provided localization is negligible. Also decoherence could lower the accuracy of the estimation practically, but our scheme is rather stable. That is, since the couplings are obtained from a linear system of equations, errors in the tomography or effects of noise degrade the estimation only linearly.

In the above, the spectrum in $\mathcal{H}_1$ was assumed to be non-degenerate. While this is always true in the 1D case, [17], the assumption may break down in general spin networks. Of course

'exact degeneracy' is highly unlikely; however, approximate degeneracy could make the scheme less efficient.

Here, we suggest to lift degeneracies by applying extra fields on the gateway C. Since C is only a small subset of the graph, it is not obvious at all that this is possible. We prove a perhaps startling consequence of the infection property: there *always* exists an operator B_C on C that lifts all degeneracies of H in the single excitation subspace. 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 the degeneracy-lifting B_C has a finite volume, thus even by choosing B_C randomly the probability of lifiting the degeneracies converges exponentially fast to one. Once all degeneracies are lifted, we can estimate the full Hamiltonian $H + \lambda B_C$ and subtracting the known part λB_C completes our identification task.

Let us denote the eigenvalues of H as E_k and the eigenstates as $|E_k^d\rangle$, where $d = 1, \ldots, D(k)$ is a label for the $D(k)$-fold degenerate states. Let us first concentrate on one specific eigenspace $\{|E_k^d\rangle, d = 1, \ldots, D(k)\}$ corresponding to an eigenvalue E_k. Since the eigenstates considered here are in the single excitation subspace $\mathcal{H}_1$, we can always decompose them as $|E_k^d\rangle_{C\bar{C}} = |\boldsymbol{\phi}_k^d\rangle_C \otimes |\mathbf{0}\rangle_{\bar{C}} + |\mathbf{0}\rangle_C \otimes |\boldsymbol{\psi}_k^d\rangle_{\bar{C}}$, where the unnormalized states $|\boldsymbol{\phi}_k^d\rangle_C$ and $|\boldsymbol{\psi}_k^d\rangle_{\bar{C}}$ are in the single excitation subspace of C and $\bar{C}$, respectively. As shown in [13] we know that $|\boldsymbol{\phi}_k^d\rangle_C \neq 0\, \forall d$, because if there was an eigenstate in the form of $|\mathbf{0}\rangle_C \otimes |\boldsymbol{\psi}_k^d\rangle_{\bar{C}}$ then applying H repeatedly on it will necessarily introduce an excitation to the region C, in contradiction to being an eigenstate. Furthermore, the set $\{|\boldsymbol{\phi}_k^d\rangle_C,\ d = 1, \ldots, D(k)\}$ must be linearly independent: for, if it was linearly dependent, there would be complex numbers α_{kd} such that $\sum_d \alpha_{kd}|\boldsymbol{\phi}_k^d\rangle_C = 0$, and because the eigenstates are degenerate, $\sum_d \alpha_{kd}|E_k^d\rangle_{C\bar{C}} = \sum_d \alpha_{kd}|\mathbf{0}\rangle_C \otimes |\boldsymbol{\psi}_k^d\rangle_{\bar{C}}$ would be an eigenstate with no excitation in C, again contradicting [13]. 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 the single excitation sector 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 we consider a Hermitian perturbation $\lambda_k B_{kC} \otimes \mathbb{1}_{\bar{C}}$ (to be specified later) on the system and compute the shift in energies. We shall see that it suffices to assume that $B_{kC}|\mathbf{0}\rangle_C = 0$. In the first order, we need to compute the eigenvalues of the perturbation matrix ${}_{C\bar{C}}\langle E_k^d| B_{kC} \otimes \mathbb{1}_{\bar{C}}|E_k^{d'}\rangle_{C\bar{C}} = {}_C\langle\boldsymbol{\phi}_k^d|B_{kC}|\boldsymbol{\phi}_k^{d'}\rangle_C$. Can we find a B_{kC} such that all eigenvalues differ? For that, note that $\{|\boldsymbol{\phi}_k^d\rangle_{\bar{C}}\}$ are linearly independent, which means that there is a similarity transform S_k (not necessarily unitary, but invertible) such that the vectors $|\boldsymbol{\xi}_k^d\rangle_C \equiv S_k^{-1}|\boldsymbol{\phi}_k^d\rangle_C$ are orthonormal. The perturbation matrix can then be written as ${}_C\langle\boldsymbol{\xi}_k^d|S_k^\dagger B_{kC} S_k|\boldsymbol{\xi}_k^{d'}\rangle_C$. If we set $S_k^\dagger B_{kC} S_k = \sum_d \epsilon_{kd}|\boldsymbol{\xi}_k^d\rangle_C\langle\boldsymbol{\xi}_k^d|$ we can see that the Hermitian operator $B_{kC} \equiv \sum_d \epsilon_{kd}(S_k^\dagger)^{-1}|\boldsymbol{\xi}_k^d\rangle_C\langle\boldsymbol{\xi}_k^d|S_k^{-1}$ gives us energy shifts ϵ_{kd}. Therefore, as long as we choose the ϵ_{kd} mutually different from each other, the degeneracy in this eigenspace is lifted by B_{kC}. This happens for an arbitrarily small perturbation λ_k. We choose λ_k such that the lifting is large, but in a way such that *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. Note that by construction B_{kC} conserves the number of excitations in the system. Therefore, we can now consider the perturbed Hamiltonian $H' = H + \lambda_k B_{kC}$ and find its remaining degenerate eigenspaces in $\mathcal{H}_1$. Following the above procedure, we pick one degenerate eigenspace and find an operator $B_{k'C}$. We continue to add perturbations, until a sum

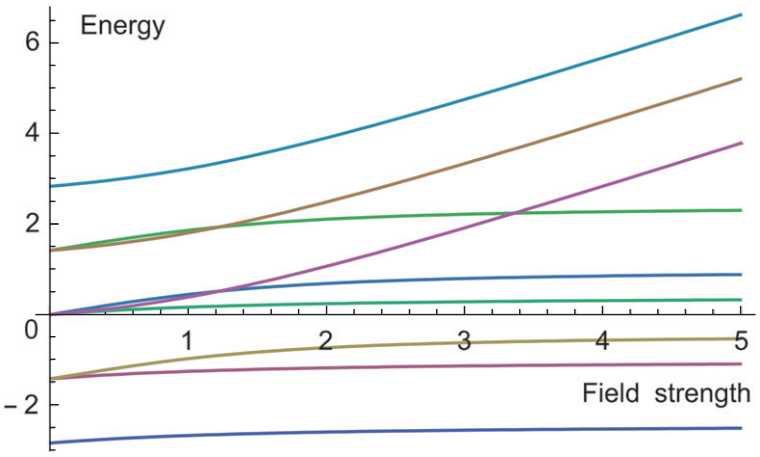

Figure 5. Numerical example for lifting degeneracies on a 3×3 lattice with homogeneous coupling strengths. A homogeneous magnetic field λB_C is applied to C, i.e. one lattice edge consisting of three spins, where B_C is of the same order of magnitude as the lattice coupling strength. Without field, there are two singlet, two doublet and one triplet levels. For most field strengths $\lambda > 0$ all nine levels are clearly visible.

of perturbations $B_C = \sum_k B_{kC}$ 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 (see figure 5 for an example).

5. Conclusions

We have shown how a small gateway can efficiently be used to estimate a many-body Heisenberg Hamiltonian, given that the topology of the system is known. It is surprising to see how a simple topological property of a network of coupled spins—infection—implies so many far-reaching properties, from control to relaxation, from the structure of eigenstates to possible degeneracies, and, as we have shown here, for Hamiltonian identification.

Our results can be seen as an example of inverse problems in quantum setting. Such problems have been actively studied in plenty of fields in science and engineering. It would be intriguing to explore a possible link between ours and similar problems in classical settings [17], such as 2D graphs of masses connected with springs. Further applications may include, for example, the indirect probing of open system dynamics [16] and Anderson localization.

Acknowledgments

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