Disordered Systems, Phase Transitions, and Emergent Localization

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(Dated: May 19, 2023)

Disordered systems have garnished significant attention over the last 50 years, as explorations of systems with sufficient disorder have lead to the discovery of new phases of matter, such as the spin-glass phase. Indeed, Parisi's work on understanding the emergence of the glassy phase lead to a Nobel prize. In a more modern context, quantum systems with sufficiently strong disorder have recently become quite popular to study. Such systems can enter into a dynamical many-body localized (MBL) phase, in which a system out-of-equilibrium fails to thermalize even at long times. These disordered quantum systems display similar behavior to the phenomenon of Anderson localization. Here, we provide a brief review of disordered systems, both classical and quantum, with an emphasis on the simplest and most easily digestible results.

I. INTRODUCTION

The emergence of order in chaotic systems is an interesting problem, and discussed at length in most treatments of statistical mechanics. One finds the emergence of phase transitions from a disordered phase (gas, paramagnets, etc.) to an ordered phase (liquids, ferromagnets, etc.), accompanied with a rich and interesting behaviours near the transition point. However, many systems can have coupling strengths or symmetry breaking fields which are irregular, namely these bond and/or field variables are allowed to be distributed as random variables. In such settings, even determining the proper order parameter to adequately capture the thermodynamic properties of the disordered is non-trivial [1, 2]. It is perhaps quite surprising that sufficiently random systems can still undergo a phase transition, at finite temperature, into what is known as the "glassy phase" [1].

For this work, we will focus on magnetic systems, which can be described using lattice models, like the Ising model. However, unlike the Ising model, we will relax the regularity of the bond variables, and allow for the coupling strength to be random across sites. Notably,

$$\mathcal{H} = J \sum_{<i,j>} \sigma_i \sigma_j \longrightarrow \sum_{<i,j>} J_{ij} \sigma_i \sigma_j, \tag{1}$$

where $\{J_{ij}\}$ is now a collection of random variables. Physically, if each σ_i corresponds to a single spin, then such randomness would be caused by random lattice deformations, either from random crystal defects, strain fields, or other sources. Alternatively, we can imagine that the bond strength as a function of distance is given by a function, $J(\boldsymbol{r})$. But now, we allow our material to be an alloy of two species, one magnetic and the other non-magnetic. Then, the model for such a system is to randomly place spins at lattice sites $\boldsymbol{x}_i$, leading to a random coupling strength $J_{ij} = J(\boldsymbol{x}_i - \boldsymbol{x}_j)$.

For the case of quantum spins, it is more common to take the symmetry breaking field as random, so that

$$h \sum_i \sigma_i \longrightarrow \sum_i h_i \sigma_i. \tag{2}$$

In such systems, the state variables σ_i are promoted to operators, as is standard in quantum mechanics. In this work, we will review some results on the quantum XXZ model (sometimes called the Heisenberg-Ising model [3]) with disorder,

$$\mathcal{H} = \frac{J_t}{2} \sum_i \left(\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(i+1)} + \hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(i+1)} \right) + \frac{J_z}{2} \sum_i \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(i+1)} + \sum_i h_i \hat{\sigma}_z^{(i)}. \tag{3}$$

Namely, we will outline numerical studies which provide evidence for a transition at finite disorder strength between a "thermal" phase and a MBL phase [4].

Finally, we conclude by briefly analyzing the double quantum model with disorder,

$$\mathcal{H} = J \sum_i \left(\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(i+1)} - \hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(i+1)} \right) + \sum_i h_i \hat{\sigma}_z^{(i)}. \tag{4}$$

This model is non-interacting integrable, and more importantly, dynamically accessible via Floquet engineering on our analog quantum simulator. In principle, the XXZ model is also accessible, but due to system constraints we cannot explore the full phase space, namely we must have $J_z/J_t = -0.5$. Thus, will will focus on reviewing previous work which explores the entire parameter space.

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II. THE GLASSY PHASE

To illustrate some of the basic physics, and deep challenges, of disordered systems we focus on the Edwards–Anderson Model, first proposed in 1975 [5]. For a regular d-dimensional "square" lattice, the Hamiltonian is written,

$$-\beta\mathcal{H} = \sum_{<i,j>} J_{ij}\sigma_i\sigma_j, \tag{5}$$

where J_{ij} are normal i.i.d. random variables, such that

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi J^2}} \exp\Big(-d\frac{J_{ij}^2}{J^2}\Big). \tag{6}$$

Here, we will follow the work of Thouless, Anderson, and Palmer who scale the interaction strength by the number of nearest neighbors, $2d$, to "ensure a sensible thermodynamic limit" [6].

Now, we treat this system as having a "quenched" disorder. Namely, we compute the partition function for a fixed set of randomly sampled $\{J_{ij}\}$, and then average physical quantities over the probability distributions for these coupling constants [1, 2, 5]. This procedure reflects that while the specific coupling strengths are random, they are fixed in a given system over any reasonable experimental timescale [1]. Thus, averaging of quenched disorder is a akin to averaging over many experimental instances, or perhaps equivalently over many identical subsystems.

Then, for a given set of coupling strengths, we can make a high temperature expansions in the bond variables, using the usual identity

$$e^{J_{ij}\sigma_i\sigma_j} = \cosh(J_{ij})\big(1 + \sigma_i\sigma_j t_{ij}\big), \tag{7}$$

where

$$t_{ij} = \tanh J_{ij}. \tag{8}$$

This allows us to write down an expression for the configuration specific free energy,

$$-\beta F = \log \prod_{<i,j>} \cosh(J_{ij}) + \log \mathrm{tr} \prod_{<i,j>} (1 + t_{ij}\sigma_i\sigma_j), \tag{9}$$

which can be diagrammatically expanded and averaged over all possible configurations [6]. Importantly, we bring attention to the fact that this computation results in a singular contribution to the quench disorder averaged free energy,

$$-\beta\overline{F}_{singular} = \frac{N}{4}\log(1 - J^2). \tag{10}$$

Thus, we have predicted that when $J = \beta\tilde{J} = 1$, there is a phase transition!

This simple approach has confirmed that a phase transition is possible, where the disorder strength (disorder standard deviation scaled by temperature as usual), plays the role of the tunable system knob leading to a phase transition. However, many questions remain. Namely, this procedure does not fully elucidate the low temperature behavior. More importantly, it is still unclear what the meaningful order parameter is for this system. To this end, we will introduce the Sherrington-Kirkpatrick model and the technique of replica averaging, with an emphasis on its successes and shortcomings.

A. Replica Symmetry and Negative Entropy

For this section, we will focus on an infinite range (all-to-all connected) version of the Edwards–Anderson Model, known as the Sherrington-Kirkpatrick model [7]:

$$-\beta\mathcal{H} = \sum_{i<j} J_{ij}\sigma_i\sigma_j + h\sum_i \sigma_i. \tag{11}$$

Notice that we have also included a symmetry breaking magnetic field term, which will help us explore a two dimensional phase space akin to the Ising ferromagnet. Further, each J_{ij} is randomly distributed as a Gaussian, now with non-zero mean, such that

$$P(J_{ij}) = \sqrt{\frac{N}{2\pi J^2}} \exp\Big(-\frac{N}{2J^2}\big(J_{ij} - J_0/N\big)^2\Big). \tag{12}$$

Above, we have re-scaled the interaction strengths by the system size (which is equivalent to the number of nearest neighbors) so that extensive quantities still scale as expected with system size [7], and is analogous to the d-dimensional rescalling taken by Thouless, Anderson, and Palmer in the limit where $d = N$ [6].

For a given instance of quenched disorder, $\{J_{ij}\}$, the free energy is

$$-\beta F = \log Z, \tag{13}$$

as usual. However, the disorder averaged free energy leads to an extensive number of intractably difficult integrations:

$$-\beta\overline{F} = \int \prod_{i<j} \mathrm{d}J_{ij} P(J_{ij}) \log Z. \tag{14}$$

To solve this dilemma, we introduce the "replica method", which was first introduced in part by Edwards and Anderson, and slowly formalized leading up to the Sherrington and

Kirkpatrick solution [5, 7]. The trick underlying this method is to use the identity

$$\log Z = \lim_{n \longrightarrow 0} \frac{Z^n - 1}{n}. \tag{15}$$

Thanks to the nature of the Gaussian probability distribution, disorder averaging of Z^n is quite tractable for integer n. From such an expression, we then take the limit as $n \longrightarrow 0$, under the assumption that the analytic continuation to non-integer n will be well defined. Hence the replica method – we will average over the product of many instances of the partition function, all with the same disordered configuration, aptly called replicas of the original system.

Then, we can write down an expression for Z^n, by introducing a "replica index", and using the usual tr notation to indication a summation over all spin configurations:

$$Z^n = \mathrm{tr} \exp\left(\sum_{i<j} \sum_{\alpha=1}^{n} J_{ij} \sigma_i^\alpha \sigma_j^\alpha + h \sum_i \sum_\alpha S_i^\alpha \right). \tag{16}$$

In this form, the integration over each J_{ij} can be performed, and in the limit of large N, we are left with the following [1, 2, 7]:

$$\overline{Z}^n = e^{NJ^2 n/4} \,\mathrm{tr} \exp\left(\frac{J^2}{2N} \sum_{\alpha<\beta} \sum_{i,j} \sigma_i^\alpha \sigma_i^\beta \sigma_j^\alpha \sigma_j^\beta + \frac{J_0}{2N} \sum_\alpha \sum_{i,j} \sigma_i^\alpha \sigma_j^\alpha + h \sum_\alpha \sum_\alpha \sigma_i^\alpha \right). \tag{17}$$

Equation (17) is a significant improvement to be sure, but still it is not clear how to proceed further in the derivation. To that end, we will define more macroscopically minded order parameters for the system, and then perform Gaussian integration[8]. Namely,

$$m_\alpha = \left(\sum_i \sigma_i^\alpha \right)^2 = \sum_{i,j} \sigma_i^\alpha \sigma_j^\alpha \tag{18}$$

$$q_{\alpha\beta} = \left(\sum_i \sigma_i^\alpha \sigma_i^\beta \right)^2 = \sum_{i,j} \sigma_i^\alpha \sigma_i^\beta \sigma_j^\alpha \sigma_j^\beta. \tag{19}$$

Following this chain of logic, one can proceed to show that $\overline{Z}^n$ is dominated by the exponential of complicated term, and importantly, this term is extensive (scales with N). Hence in the thermodynamic limit, we are able to take the saddle point approximation and find an expression for the free energy. Since each replica is seemingly indistinguishable, we find that

$$q_{\alpha\beta} \longrightarrow q = \overline{\langle \sigma_i \rangle^2}, \tag{20}$$

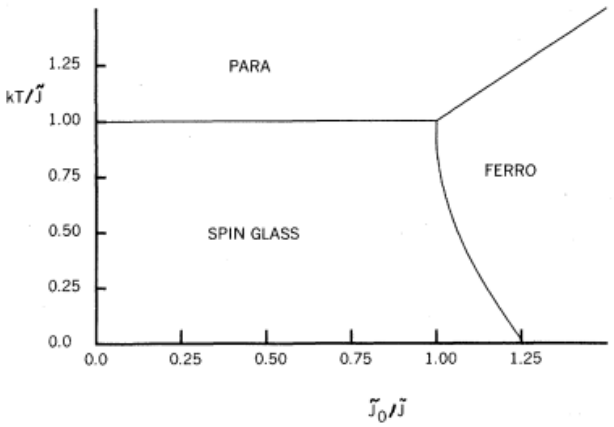

FIG. 1. Phase diagram of the Sherrington-Kirkpatrick model, taken from their original paper [7].

is the spin glass order parameter, and

$$m_\alpha \longrightarrow m = \overline{\langle \sigma_i \rangle} \tag{21}$$

is the usual magnetization, albeit averaged over disorder [7].

Within the thermodynamic limit, we extremize the order parameters, and find conditions on m and q. It is reassuring that we find a novel phase of matter, dubbed the spin glass phase, which has $m = 0$ and $q > 0$. Further, the phase transition occurs at $J = 1$, as predicted by the high temperature expansion in the closely related Edwards–Anderson model. By increasing the mean of the disorder distribution, we eventually arrive to a region which exhibits $m > 0$ ferromagnetic order. This phase diagram is shown in figure 1.

We conclude this section by noting that the spin-glass models are highly successful in predicting the emergence of the glassy phase, however, there is a serious issue hiding in the equations of state. Namely, the low temperature spin-glass phase eventually reaches a negative entropy [1]. There are many mathematically suspect steps taken during the derivation, and it was originally believed that the exchange of the replica limit $n \longrightarrow 0$ and the thermodynamic limit $N \longrightarrow \infty$ was responsible for this apparent violation of thermodynamic stability. However, it was later shown that the assumption of replica symmetry (wherein the indices of q were discarded) was to blame [9]. It was finally Parisi who discovered that the replica symmetry must be broken (infinitely many times) [10, 11]. Intuitively, systems which can enter into a spin glass phase are not just disordered, but also frustrated. Thus, the simple thermodynamic limit argument failed to account for all possible, but not ergodically connected, glassy states [9]. By replacing q with a probability distribution $q(x)$, Parisi connected spin glasses to percola-

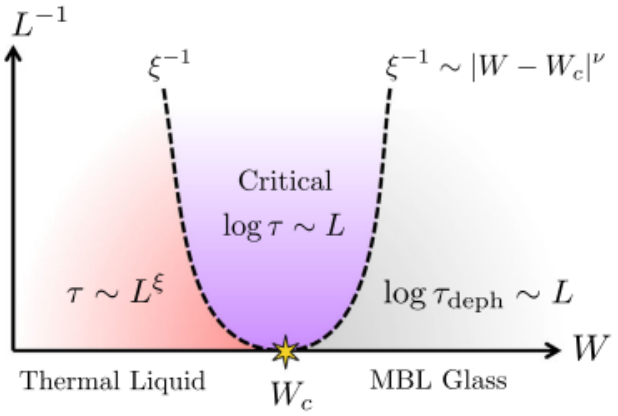

FIG. 2. Dynamical phase diagram of the MBL phase transition in the one dimensional disordered XXZ chain, taken from Potter, Vasseur, Parameswaran [13]. L denotes the system size, which is on the order of 500 spins, and W denotes the strength of the disordered field, such that h_i is uniformly random on the interval $(0, W)$. The pseudo-order parameter is given by τ, which is describes the timescale of thermalization of the system under its own dynamics. The critical exponent here is $\nu \sim 3.5$.

tion theory, and found solutions which were well behaved and matched simulations at all temperatures [8, 10]. This discovery, among others, led to Parisi receiving the Nobel prize in 2021.

III. MANY BODY LOCALIZATION

For this section, we turn our attention to dynamics of large interacting disordered systems. As it currently stands, the spin-glass Hamiltonians presented do not intrinsically allow for dynamical evolution [2]. However, spin glass evolution has been studied theoretically, computationally, and experimentally, even within the context of the Edwards–Anderson model [1, 2, 12]. However, for this discussion we wish to highlight some results in quantum spin chains.

The model of interest is the disordered XXZ chain, which is an interacting integrable model, meaning it can be mapped onto a Hamiltonian describing spin-less fermions. Namely,

$$\mathcal{H} = \frac{J_t}{2} \sum_i \left(\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(i+1)} + \hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(i+1)} \right) + \frac{J_z}{2} \sum_i \hat{\sigma}_z^{(i)} \hat{\sigma}_z^{(i+1)} + \sum_i h_i \hat{\sigma}_z^{(i)}, \tag{22}$$

where h_i is a random variable which describes a random local field. The Jordan–Wigner mapping leads to a collection of N fermionic ladder operators $\hat{a}_i$, and occupation operators $\hat{n}_i = \hat{a}_i^\dagger \hat{a}_i$. In this basis,

$$\mathcal{H} \sim \sum_i \left(\epsilon_i \hat{n}_i + J_t \big(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_i \hat{a}_{i+1}^\dagger \big) + J_z \hat{n}_i \hat{n}_{i+1} \right), \tag{23}$$

wherein the random field h_i has become a random on-site energy ϵ_i [13]. Since this model is integrable, it is computationally tractable to numerically estimate dynamics and correlation lengths numerically. By doing so, one can estimate a phase diagram, and compute critical exponents of the phase transition, shown in figure 2. Notably, the transition into the melted phase is a second order phase transition in which the correlation length ξ is diverging [13].

We can attempt to simulate our own disordered system by choosing a non-interacting integrable model. One such model is the one dimensional double quantum Hamiltonian,

$$\mathcal{H} = J \sum_i \left(\hat{\sigma}_x^{(i)} \hat{\sigma}_x^{(i+1)} - \hat{\sigma}_y^{(i)} \hat{\sigma}_y^{(i+1)} \right) + \sum_i h_i \hat{\sigma}_z^{(i)}. \tag{24}$$

This model maps to spin-less fermions with hopping, but no interactions, giving

$$\mathcal{H} \sim \sum_i \left(\epsilon_i \hat{n}_i + J \big(\hat{a}_i^\dagger \hat{a}_{i+1} + \hat{a}_i \hat{a}_{i+1}^\dagger \big) \right). \tag{25}$$

While the interacting integrable model is tractable numerically using Bethe ansatz techniques, the non-interacting model is much easier to simulate directly, as time evolution is simply an automorphism on the space of quadratic fermionic operators. This model is especially of interest, as our group is able to simulate this system in a solid state NMR device, albeit fixed in the $T \longrightarrow \infty$ limit [14, 15]. In figure 3, we show what appears to be localization at increased disorder magnitude under 10,000 averages over randomly sampled $h_i \sim N(0, h^2)$, with $L = 50$ spins. For more information on how the simulation is carried out, see the appendix.

IV. CONCLUSION

In this work we have shown that disorder systems present a unique mathematical challenge. However, disordered systems are ever present in nature, and are becomingly increasingly interesting to study. Spin glasses, which began to be fully understood in the 1970s and 1980s demonstrated unique challenges and required clever observations to overcome the difficulties. Better understanding of advanced probability theory, percolation theory, and analysis are needed for a complete treatment of classic disordered systems.

Looking beyond fundamental interest of exploring new physics, understanding solutions of these systems is growing

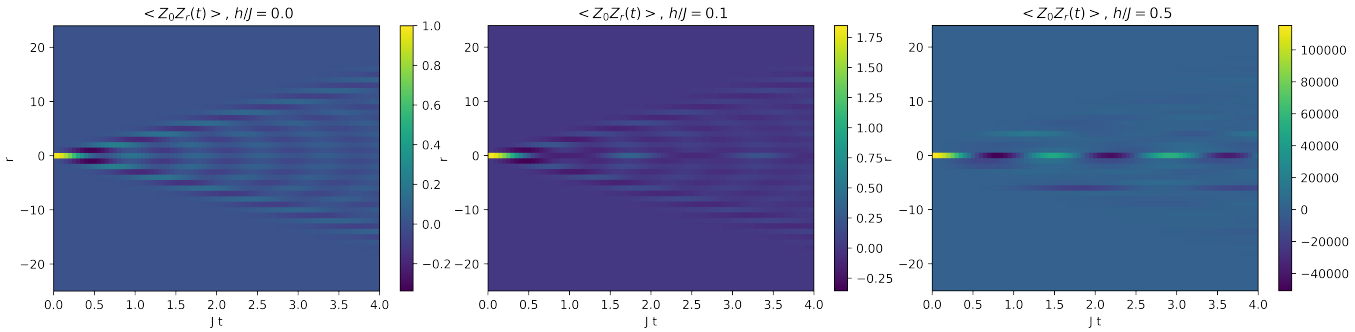

FIG. 3. Two point correlation as a function of time in an infinite temperature $L = 5$ spin chain. We notice that when the disorder standard deviation h is small, the dynamics looks similar to the ordered case. However, for strong disorder, $h/J = .5$, we see what looks like strong evidence of highly local confinement. However, these is some evidence of numerical instability or diverging correlations due to the abnormally increased scales present.

increasingly relevant in quantum technologies. For instance, many computationally intractable problems (NP-complete problems) can be mapped onto an Ising spin network [16]. Solving such problems is of great interest for optimization, and has spurred on fascinating work in Rydberg arrays [17] and superconducting quantum annealers [18]. Very recent work at D-Wave has lead to analog simulation of spin-glass dynamics in a three dimensional system, and has broad implications to the field of quantum annealing [19].

Finally, we discussed many-body localization, which is related to spin glasses, but is distinctly dynamical in nature. In the simplest of models we reviewed formulations which found the emergence of MBL using simulations of hundreds of spins. Since MBL is characterized by non-thermalizing behavior, is is difficult to formulate a proper order parameter, but the thermalization time-scale, and the speed of energy transport, seem to the leading candidates. Within the MBL phase, these systems fail to thermalize by trapping information and energy locally, resulting in a emergent integrability through the context of dynamically induced local integrals of motion [15]. Others have used renormalization group approaches to attempt to better understand the MBL phase [20]. In a simple non-interacting system, we demonstrate what appears to be emergent localization through the dynamics of the two point correlator of a double quantum spin chain with disorder. However, the scale of the correlations appears to be misbehaving, and may be indicative of numerical instability, or a phase transition accompanied by a non-negligible contribution from a non-analytic term in the partition function/free energy.

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V. APPENDIX: JORDAN–WIGNER TRANSFORMATION

Consider the following integrable spin-1/2 Hamiltonian in an infinite temperature system:

$$\mathcal{H} = h\sum_{i=1}^{N}\sigma_z^{(i)} - J\sum_{i=1}^{N-1}\left(\sigma_x^{(i)}\sigma_x^{(i+1)} - \sigma_y^{(i)}\sigma_y^{(i+1)}\right). \tag{26}$$

This can be mapped to a system of N spin-less fermions via the following Jordan–Wigner transformation:

$$\sigma_z^{(i)} \longrightarrow a_i a_i^\dagger - a_i^\dagger a_i = \mathbb{1} - 2a_i^\dagger a_i \tag{27}$$

$$\sigma_x^{(i)} \longrightarrow -\left(\prod_{j<i}\sigma_z^{(j)}\right)(a_i + a_i^\dagger) \tag{28}$$

$$\sigma_y^{(i)} \longrightarrow \mathrm{i}\left(\prod_{j<i}\sigma_z^{(j)}\right)(a_i^\dagger - a_i). \tag{29}$$

These fermionic operators are chosen such that they satisfy the canonical anti–commutation relations

$$\{\hat{a}_i, \hat{a}_j\} = 0 \tag{30}$$

$$\{\hat{a}_i^\dagger, \hat{a}_j\} = \delta_{ij}\mathbb{1}. \tag{31}$$

We rewrite the Hamiltonian in terms of fermionic operators under this mapping, and throw out the term proportional to the identity. The resulting Hamiltonian is a quadratic form over the basis of fermionic operators, and we write it in a way that emphasises this fact:

$$\mathcal{H} = \sum_{i,j}\left(a_i^\dagger A_{ij} a_j + \frac{1}{2}\left(a_i^\dagger B_{ij} a_j^\dagger + a_i B_{ji}^* a_j\right)\right). \tag{32}$$

Above, we have defined the $N \times N$ matrices A and B such that A is self–adjoint, and B is anti self–adjoint.

Any quadratic fermionic Hamiltonian of this form can be exactly diagonalized via a Bogolioubov transformation. Generally, we are free to requantize the Hamiltonian via a linear combination of fermionic operators, such that

$$f_k = \sum_i G_{ki} a_i + H_{ki} a_i^\dagger. \tag{33}$$

G and H can be chosen to be real orthogonal matrices, and we desire that this transformation diagonalizes the Hamiltonian. That is, we need to find G and H such that

$$\mathcal{H} = \sum_i \lambda_i f_i^\dagger f_i. \tag{34}$$

We must further impose that this transformation is consistent with the canonical anti–commutation relations to preserve the essential structure of the algebra. It can be shown that these constraints can be recast as the following matrix equations:

$$GG^\dagger + HH^\dagger = \mathbb{1}$$
$$GH^\dagger + HG^\dagger = 0.$$

This desired transformation induces a unique set of eigenvalue problems for the rows of the sum and difference of G and H. Generally, an induced eigenvalue problem for G and H is non-unique unless we also impose the above constraints [21]. Then, the solution of this set of N eigenvalue problems diagonalizes the Hamiltonian. That is, we have fully determined an operator T, which diagonalizes the Hamiltonian. This operator can be conveniently written as a $2N \times 2N$ block matrix acting on symbolic vectors of the creation and annihilation operators,

$$\begin{bmatrix} \boldsymbol{f} \\ \boldsymbol{f}^\dagger \end{bmatrix} = \begin{bmatrix} G & H \\ H^* & G^* \end{bmatrix} \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{a}^\dagger \end{bmatrix} = T \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{a}^\dagger \end{bmatrix}. \tag{35}$$

Matrix exponentiation for diagonal operators is trivial. Thus by transforming back to the original fermionic operators a_i, we can write down time evolution in our physically motivated basis,

$$\begin{bmatrix} \boldsymbol{a}(t) \\ \boldsymbol{a}^\dagger(t) \end{bmatrix} = T^\dagger e^{-2itD} T \begin{bmatrix} \boldsymbol{a} \\ \boldsymbol{a}^\dagger \end{bmatrix}. \tag{36}$$

Explicitly, the time evolution of the set of fermionic operators is simply the following matrix equation,

$$\boldsymbol{a}(t) = U_1(t)\boldsymbol{a} + U_2(t)\boldsymbol{a}^\dagger, \tag{37}$$

where

$$U_1(t) = G^\dagger e^{-2itd} G + H^\dagger e^{2itd} H \tag{38}$$
$$U_2(t) = G^\dagger e^{-2itd} H + H^\dagger e^{2itd} G. \tag{39}$$

In principle, we have entirely "solved" the problem. However it is still unclear how to compute arbitrary observable spin quantities, especially those involving Pauli X and Y operators. As a proof of concept, we begin with the simplest case, a local two point NMR ZZ correlator.

$$\begin{aligned} 2^N \left\langle \sigma_z^{(i)}(t)\sigma_z^{(j)} \right\rangle &= \operatorname{tr}(\sigma_z^{(i)}(t)\sigma_z^{(j)}) \\ &= \operatorname{tr}\left(\mathbb{1} - 2(a_j^\dagger a_j + a_i^\dagger(t)a_i(t)) + 4a_i^\dagger(t)a_i(t)a_j^\dagger a_j\right) \\ &= 4\operatorname{tr}(a_i^\dagger(t)a_i(t)a_j^\dagger a_j) - 2\operatorname{tr}(a_i^\dagger(t)a_i(t)). \end{aligned}$$

We will need to expand the time evolved operators and compute a series of traces of quadratic and quartic fermion operators. Now, to compute the traces, we define $c_{ik}(t)$ and $d_{ik}(t)$ to be the kth element in the ith row of $U_1(t)$ and $U_2(t)$, respectively. In this language,

$$a_i(t) = \sum_k c_{ik}(t)a_k + d_{ik}(t)a_k^\dagger. \tag{40}$$

Then, the two body term is

$$\operatorname{tr}(a_i(t)^\dagger a_i(t)) = 2^{N-1} \sum_k \left(|c_{ik}(t)|^2 + |d_{ik}(t)|^2 \right) \tag{41}$$

The contributing summand terms of the four body trace can be analogously determined,

$$\mathrm{tr}(a_i^\dagger(t)a_i(t)a_j^\dagger a_j) = \sum_{k,l}\Big(c_{ik}(t)^* c_{il}(t)\,\mathrm{tr}(a_k^\dagger a_l a_j^\dagger a_j) + d_{ik}(t)^* d_{il}(t)\,\mathrm{tr}(a_k a_l^\dagger a_j^\dagger a_j)\Big). \tag{42}$$

Putting it all together, we are left with an elegant expression for the local TPC,

$$\left\langle \sigma_z^{(i)}(t)\sigma_z^{(j)}\right\rangle = |c_{ij}(t)|^2 - |d_{ij}(t)|^2\,. \tag{43}$$

Then, we have the ability to easily compute the global ZZ TPC, by writing

$$J_z = \sum_i \sigma_z^{(i)}, \tag{44}$$

such that

$$\langle J_z(t)J_z\rangle = \sum_{i,j=1}^{N}\left\langle \sigma_z^{(i)}(t)\sigma_z^{(j)}\right\rangle = \sum_{i,j=1}^{N}\left(\,|c_{ij}(t)|^2 - |d_{ij}(t)|^2\,\right) = \|U_1(t)\|_F^2 - \|U_2(t)\|_F^2\,, \tag{45}$$

where $\|\bullet\|_F$ is the Frobenius norm.