Quantum kinetic Ising models

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\textbf{Abstract.} In this paper, we introduce a quantum generalization of classical kinetic Ising models (KIM), described by a certain class of quantum many-body master equations. Similarly to KIMs with detailed balance that are equivalent to certain Hamiltonian systems, our models reduce to a set of Hamiltonian systems determining the dynamics of the elements of the many-body density matrix. The ground states of these Hamiltonians are well described by the matrix product, or pair entangled projected states. We discuss critical properties of such Hamiltonians, as well as entanglement properties of their low-energy states.

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1. Introduction

This paper, prepared for the special issue of the *New Journal of Physics* on ‘Quantum information and many-body theory’, has two apparently independent motivations. Firstly, it is motivated by recent interest in many-body quantum master equations and the design of open systems for quantum state engineering and quantum simulations. Secondly, it is about the entanglement properties of quantum many-body states corresponding to classical kinetic models with detailed balance and their generalizations to quantum master equations.

1.1. Quantum master equations

The quantum master equation (QME) is the basic theoretical tool used to describe the evolution of open systems that undergo Markovian dynamics [1, 2]. While the initial studies of QMEs dealt with many-body applications, over the last few decades most research has focused on systems of few degrees of freedom, mainly because of the unquestionable complexity of the many-body QMEs. In the last 15 years, however, there have been two waves of renewed interest in many-body QMEs, related to the unprecedented progress of experimental control and engineering of ultracold atomic and molecular systems. On the one hand, there has been a wealth of interest in the studies of various kinds of cooling processes using QMEs. Zoller, Gardiner and collaborators [3] studied in a series of papers the growth of a Bose–Einstein condensate in a trapped bosonic gas. One of us (ML), together with Cirac, Zoller, Castin and others, developed the theory of laser cooling of Bose gases [4], in particular in the so-called festina lente limit [5]. Similar ideas were applied to the processes of laser cooling of Fermi gases [6] and sympathetic cooling [7]–[9].

On the other hand, several authors proposed to make use of the capabilities of modern quantum optics and atomic physics experimental methods to design and realize experimentally QMEs that allow us to engineer interesting quantum many-body pure states [10]–[12]. These
pure states range from simple Bose–Einstein condensates to the stabilizer states, matrix product states (MPS)/pair entangled projected states (PEPS) states, or states with topological order. The first experiment realizing these ideas was conducted by the group of Rempe [13], who were able to prepare a one-dimensional (1D) bosonic Tonks–Girardeau [14] gas employing three-body losses. So far most of these new proposals concern ultracold atoms, molecules—in particular polar molecules—or ions, but recently they have started to involve Rydberg atoms, which are particularly suitable for the design and realization of three-body, four-body, etc interactions, thanks to the Rydberg blockade mechanism. Weimer et al [15] proposed to use many-body quantum gates stroboscopically, employing the Rydberg blockade effect to engineer the topologically ordered ground state of the famous Kitaev toric code, the color code [16] and even to realize a quantum simulator of the U(1) lattice gauge theory.

Motivated by these developments, we propose in this paper a new class of many-body QMEs generalizing classical kinetic models (in particular kinetic Ising models (KIMs); for a review see [17]). Our QMEs have as stationary states thermal Boltzmann–Gibbs states of the underlying classical model. Note that these thermal states might correspond to very complex quantum states, for instance if the underlying classical model concerns kinetics of commuting stabilizer operators for the cluster states [18], as we discuss in section 5. The diagonal elements of the density matrix in our models undergo dynamics equivalent to that of the underlying classical model. The off-diagonal elements of the density matrix exhibit complex evolution, but fortunately can be grouped into independently evolving blocks. Similarly to KIMs with detailed balance, which are equivalent to certain Hamiltonian systems, our models reduce to a set of Hamiltonian systems determining the dynamics of the elements of the many-body density matrix. In 1D, we identify classes of these models that are exactly soluble. In general, the ground states of these Hamiltonians are well described by the MPS or PEPS [19, 20].

It should be noted that previous efforts in the above direction exist: for example, in [18] and [21] a general master equation for the kinetic Ising model with an environment was derived. Under some assumptions, the diagonal elements of these formulations also reproduce Glauber’s kinetic model, although no full solution of the equation was attempted.

1.2. Entanglement in many-body systems

Studies of the role of entanglement in many-body systems were initiated by the seminal work [22], but they go back to the early works on area laws in quantum systems [23] (for a review see [20, 24, 25]). We recall that ground states of (non-critical) many-body systems with local Hamiltonians exhibit the area law. This means that if we divide the whole system into subsystems $A$ and $B$ where the size $|A|$ is large, but much smaller than $|B|$, and calculate the von Neumann entropy of the reduced density matrix of $A$, the latter will scale as the size of the boundary (‘area’) of $A$, $S_A \propto |\partial A|$. The area law expresses the fact that away from criticality, correlations—and in particular quantum correlations responsible for entanglement—decay on short length scales.

The situation is different at criticality, although so far only 1D systems are fully understood. In one dimension, the area law at criticality may get logarithmic corrections so that the entropy of the block of size $L$ scales as $S_L \propto c \log(L)$, where the constant $c$ can be related to the charge of the conformal field theory describing the corresponding critical behavior. In higher dimensions the situation is much less clear, and no universal laws at criticality are known [20]. Very recently, Masanes [26] proved that under quite general conditions, for the ground states of systems with local Hamiltonians, the entropy of a block $A$ is bounded from above by $|A| \log A$. 

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There is a class of quantum states that always fulfill the area law in any dimension, despite the fact that they exhibit criticality for certain values of parameters [20]. These states are related to thermal states of classical Hamiltonians, such as the Ising or the Potts models. In fact, any set of local quantum mechanical commuting operators can be used to build such models. For example, one can take stabilizer operators for cluster states [18], or star and plaquette operators of the Kitaev model [16]. In the following, we will mainly focus on Ising models, leaving the discussion of more complicated cases to further publications.

For Ising models, the states in question have the form

$$|\Psi_1\rangle = \frac{1}{\sqrt{Z_N}} \sum_\sigma \exp[-\beta H(\sigma)/2]|\sigma\rangle,$$

(1)

where $\sigma = (\sigma_1, \ldots, \sigma_N)$ denotes a configuration of $N$ Ising spins, $|\sigma\rangle$ stands for a vector representing $\sigma$ in the corresponding Hilbert space, $H(\sigma)$ is the corresponding classical Hamiltonian and $Z_N = \text{Tr} \exp[-\beta H(\sigma)]$ is the partition function. As pointed out in [19, 20] and references therein, these states have the following properties.

- They are associated with a family of classical KIMs that describe the approach to the classical thermal equilibrium state $\exp[-\beta H(\sigma)/2]/Z_N$ and obey detailed balance.
- The KIMs in question can be transformed by an appropriate ansatz into an equivalent problem of Hamiltonian dynamics in imaginary time (i.e. describing decay in time), with a certain quantum Hamiltonian $\hat{H}$ parametrically depending on $\beta$.
- The Hamiltonian $\hat{H}$ is non-negative and has one eigenvector given by expression (1) corresponding to the eigenvalue zero. Away from criticality $\hat{H}$ is gapped, i.e. excited states have strictly positive energies. As $\beta \to \beta_c$ the gap vanishes, and at $\beta_c$ the Hamiltonian is gapless. The way the gap vanishes determines the dynamical critical exponent $z$ of the associated KIM.
- The ground state (1) fulfills the area law and does not exhibit any special behavior at criticality. It can be exactly represented as an MPS in 1D, or as a PEPS in higher dimensions [19].

Intrigued by the fact that the states (1) always fulfill the area law, we have attempted to look more closely into their properties, and the properties of their parent Hamiltonians $\hat{H}$. One possible way is to study the entanglement properties of the excited states of $\hat{H}$, but we have chosen another approach. We have generalized the KIMs to quantum models by defining a new class of QMEs, as explained in the previous subsection. These QMEs define new classes of parent Hamiltonians, and the ground states of these Hamiltonians are expected to be again well described by matrix product or PEPS. This paper is devoted to the discussion of the critical properties of such Hamiltonians, as well as entanglement properties of their low-energy states.

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5 We would like to warn our readers against a possible misunderstanding: at issue are irreversible processes whose quantum behavior in general involves mixed states described by density operators. The generators in the pertinent master equations are non-Hermitian operators, precisely due to the irreversible dynamics. However, given detailed balance a master equation can be rewritten such that the generator becomes Hermitian and is then called a ‘Hamiltonian’. Following widespread practice, we shall call a thus-transformed master equation a ‘Schrödinger equation in imaginary time’ and write about eigenstates of the ‘Hamiltonian’; the resulting formalism then even allows one to deal with superposition states, equation (1) being the first example. Nevertheless, this paper is about density operators and damped motion. The ‘state’ in equation (1) represents the canonical density operator.

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1.3. Plan of the paper

The paper is organized as follows. In section 2, we remind the readers of the basics of KIMs with detailed balance, associated Hamiltonians and such like. In section 3, we present the main result of this paper: we describe the generalization of KIMs to QMEs, and we discuss the properties of the QMEs. In particular, we show how the equations for \(2^N \times 2^N\) matrix elements of the density matrix split into \(2^N\) equations of the KIM type for functions of \(2^N\) spin configurations. Detailed balance allows one to transform these quasi-KIM equations to a Hamiltonian form, and we derive here the new classes of Hamiltonians. The properties of these Hamiltonians and their low-energy states are discussed in section 4. Here we show that Hamiltonians describing the evolution of the off-diagonal density matrix elements (coherences) are strictly positive\(^6\), which implies that the corresponding coherences decay to zero. At criticality, we observe the effects of critical slowing down of coherences; the Hamiltonians become gapless, implying that at criticality the decay is of the form of an exponential decay times algebraic tails. In some cases, criticality may even lead to survival of coherences for infinite times. In section 4, we also discuss entanglement properties of the ground and excited states of the corresponding Hamiltonians. Our conclusions and outlook are contained in section 5.

2. Basics of kinetic Ising models

As discussed in section 4, the methods developed in this paper can be straightforwardly generalized and applied to models other than Ising models: Potts models, classical clock models or models employing commuting stabilizer operators. For simplicity and concreteness, we will limit the discussion to Ising models, with Ising variables \(\sigma_i = \pm 1\), described quantum mechanically by the commuting Pauli matrices \(\sigma_i^Z\). We will consider systems with a classical Hamiltonian \(H(\sigma)\) following Markovian dynamics toward the thermal equilibrium state.

The dynamics for a Markovian stochastic process is most conveniently formulated for the conditional probability \(P(\sigma, t|\sigma_0, 0)\) for the configuration \(\sigma\) at time \(t\), provided the initial configuration was \(\sigma_0\) at \(t = 0\). This conditional probability allows one to calculate all multi-time correlation functions of the process. Note that \(P(\sigma, 0|\sigma_0, 0) = \delta_{\sigma \sigma_0}\), i.e. at the initial time conditional probability is obviously given by the Kronecker delta of the configurations \(\sigma\) and \(\sigma_0\). In the following, in order to avoid too many arguments we will consider the dynamics of probability of configurations \(P(\sigma, t)\), which fulfills the same equation as \(P(\sigma, t|\sigma_0, 0)\), but with a more general initial condition.

2.1. Kinetic Ising models with detailed balance

Here, we define in a more detailed way the classical KIMs and recall some of the literature results concerning particular examples of such models. In general, KIMs are defined by specifying the so-called kinetic (master) equation for probability \(P(\sigma, t)\) of the form

\[
P(\sigma, t) = \sum_{\sigma'} \left[ w(\sigma' \rightarrow \sigma) P(\sigma', t) - w(\sigma \rightarrow \sigma') P(\sigma, t) \right],
\]

\(^6\) An operator \(O \in B(H)\) for some Hilbert space \(H\) is said to be positive if \(\langle \psi | O | \psi \rangle \geq 0\) for any \(|\psi\rangle \in H\). Then we say that \(O\) is strictly positive if \(\langle \psi | O | \psi \rangle > 0\) for any \(|\psi\rangle \in H\). For a Hermitian operator \(O\) acting on finite-dimensional Hilbert space, both conditions are equivalent to non-negativity and strict positivity of eigenvalues of \(O\).
where the sum runs over all possible configurations $\sigma$. The function $w(\sigma \to \sigma')$, hereafter also called transition probability, stands for the probability per unit time that the system changes its configuration from $\sigma$ to $\sigma'$.

Usually, one imposes the so-called detailed balance condition (DBC) that says that at equilibrium the probability per unit time of a transition from $\sigma$ to $\sigma'$ is the same as the probability of transition in the opposite direction, $\sigma' \to \sigma$. Mathematically, it reads

$$w(\sigma' \to \sigma)P_{eq}(\sigma') = w(\sigma \to \sigma')P_{eq}(\sigma),$$

where $P_{eq}(\sigma)$ is the equilibrium probability distribution $P_{eq}(\sigma) = P(\sigma, t \to \infty)$.

To support the above general remarks with some more detailed investigations, let us now discuss some previously studied examples of such kinetic models. At the beginning, let us focus on the 1D Ising spin system, i.e. a chain of $N$ spins uniformly distributed on a line. In this case, $\sigma$ denotes one of the $2^N$ possible configurations of $N$ spins and can be represented as an $N$-dimensional vector $(\sigma_1, \ldots, \sigma_N)$ with $\sigma_i = \pm 1$ ($i = 1, \ldots, N$).

We restrict our attention to the case in which the behavior of the $i$th spin is local, i.e. depends only on the nearest neighbors (generalizations to local models with next-nearest neighbors are straightforward). We also assume that the probability distribution at equilibrium is

$$P_{eq}(\sigma) = \frac{1}{Z_N} e^{-\beta H(\sigma)}$$

with $H$ denoting the classical (local) Ising Hamiltonian. In particular, we consider here the ferromagnetic Ising model, which in 1D corresponds to

$$H(\sigma) = -J \sum_i \sigma_i \sigma_{i+1} \quad (J > 0).$$

In this case, the partition function has the explicit form $Z_N = 2^N (\cosh^N \beta J + \sinh^N \beta J)$. The simplest possible process that may occur here is a single flip of the $i$th spin. Schematically, this process can be stated as $\sigma \to D_i \sigma$, where $D_i$ denotes the flip at the $i$th position, $D_i \sigma = (\sigma_1, \ldots, -\sigma_i, \ldots, \sigma_N)$. Also, let $w(\sigma \to D_i \sigma)$ denote the transition probability for that process.

The only processes that lead to the configuration $\sigma$, appearing on the left-hand side of equation (2), are spin flips $D_i \sigma \to \sigma$ for any $i = 1, \ldots, N$. The inverse type of processes can drag the system away from $\sigma$. This means that the general kinetic equation (2) can be reduced in this case to a much simpler form

$$\dot{P}(\sigma, t) = \sum_{i=1}^N \left[ w(D_i \sigma \to \sigma)P(D_i \sigma, t) - w(\sigma \to D_i \sigma)P(\sigma, t) \right].$$

The most general form of $w(\sigma \to D_i \sigma)$ in the case where the interaction with both nearest neighbors is symmetric and leads the system to the equilibrium state (4) was shown to be [27]

$$w(\sigma \to D_i \sigma) = \Gamma (1 + \delta \sigma_{i-1} \sigma_{i+1}) \left[ 1 - \frac{1}{2} \gamma \sigma_i (\sigma_{i-1} + \sigma_{i+1}) \right],$$

where $\gamma = \tanh 2\beta J$ (note that the value $\gamma = 0$ corresponds to infinite temperature, whereas $\gamma = 1$ corresponds to zero temperature), $|\delta| \leq 1$ and $0 < \Gamma < \infty$.

The case of $\delta = 0$ was thoroughly investigated by Glauber, and was shown to be solvable in the sense that all the relevant physical quantities can be computed analytically. In particular, the non-equilibrium expectation values and equilibrium correlation functions were determined.
Moreover, this model was shown to have the dynamical exponent$^7$ $z = 2$. Later on, the above model was treated in a series of papers [28, 31, 32] for nonzero $\delta$. In particular, it was shown in [31, 32] that the choice $\delta = \gamma / (2 - \gamma)$ entails the dynamical exponent $z \neq 2$.

KIMs have also been studied in two and higher dimensions, although in these cases there is no known analytical solution. However, by using efficient techniques precise numerical results have been obtained for relevant quantities such as the critical dynamical exponent [33].

2.2. Associated quantum Hamiltonians

Interestingly, as was shown in e.g. [27, 29, 30] the DBC (3) allows one to rewrite the master equation (2) as a Schrödinger equation. In order to see that, let us introduce the function $\phi(\sigma, t)$ related to the probability $P(\sigma, t)$ through $P(\sigma, t) = \sqrt{P_{\text{eq}}(\sigma)} \phi(\sigma, t)$, where as above $P_{\text{eq}}$ is the equilibrium distribution. Inserting the latter in the master equation (2) and reorganizing slightly some terms, we arrive at

$$
\dot{\phi}(\sigma, t) = \sum_{\sigma'} \left[ P_{\text{eq}}^{-1/2}(\sigma) w(\sigma' \rightarrow \sigma) P_{\text{eq}}^{1/2}(\sigma') - P_{\text{eq}}^{-1/2}(\sigma') w(\sigma' \rightarrow \sigma) P_{\text{eq}}^{1/2}(\sigma') \right] \delta_{\sigma\sigma'} \phi(\sigma', t)
$$

$$
\equiv - \sum_{\sigma'} H_{\sigma\sigma'} \phi(\sigma', t)
$$

(8)

with $H$ denoting the real matrix with elements given by

$$
H_{\sigma\sigma'} = \sum_{\sigma''} w(\sigma' \rightarrow \sigma'') \delta_{\sigma\sigma'} - P_{\text{eq}}^{-1/2}(\sigma) w(\sigma' \rightarrow \sigma) P_{\text{eq}}^{1/2}(\sigma').
$$

(9)

Due to the DBC (3), one sees that $H$ is symmetric and hence equation (8) gives the aforementioned Schrödinger equation.

Diagonalization of the Hamiltonian $H$ is equivalent to the full solution of the corresponding master equation (2). Many of the previously discussed systems were investigated from this point of view. Below we recall some of the known results for the 1D Glauber model. The Hamiltonian associated with Glauber’s master equation (8) with spin rates given by (7) has the form

$$
H(\gamma, \delta) = -\Gamma \sum_i \left\{ [A(\gamma, \delta) - B(\gamma, \delta)\sigma_i^z \sigma_{i+1}^z] \sigma_i^z - (1 + \delta \sigma_i^z \sigma_{i+1}^z) [1 - \frac{\gamma}{2} \sigma_i^z (\sigma_{i+1}^z + \sigma_{i-1}^z)] \right\},
$$

(10)

where $\gamma$, $\delta$ and $\Gamma$ are specified as previously; $\sigma^z$ and $\sigma^x$ are the standard Pauli matrices and

$$
A(\gamma, \delta) = \frac{(1 + \delta) \gamma^2}{2(1 - \sqrt{1 - \gamma^2})} - \delta, \quad B(\gamma, \delta) = 1 - A(\gamma, \delta).
$$

(11)

For $\delta = 0$, it was shown in [29] (see also [35] for another approach) that the standard procedure consisting of the Jordan–Wigner transformation [36] followed by Fourier and Bogoliubov–Valatin transformations [37, 38] brings the Hamiltonian $H(\gamma, 0)$ to its diagonal form with non-interacting fermions. The eigenvalues are given by

$$
\Lambda(q_k) = \sum_{i=1}^k \lambda_{q_i}, \quad \lambda_{q} = 1 - \gamma \cos q,
$$

(12)

$^7$ This means that the time-dependent spin–spin correlation function decay on time scale as $t_{\text{dec}} \propto \xi^z$, where $z$ is the dynamical critical exponent, and $\xi$ denotes the correlation length; $\xi$ scales as $(1 - \gamma)^{-1/2}$ when $\gamma \rightarrow 1$. 

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where $q_k$ denotes the ordered chain ($q_1 < q_2 < \ldots < q_k$) with each $q_i$ from $\{\pm \pi/N, \pm 3\pi/N, \ldots, \pm (N-1)\pi/N\}$ for even $N$ and $\{0, \pm 2\pi/N, \pm 4\pi/N, \ldots, \pi\}$ for odd $N$. The ground state, which is here the zero-energy state, is the one given by equation (1). Moreover, the first nonzero eigenvalue is $1 - \gamma$ and goes to zero for $\gamma \to 1$ (zero temperature limit).

The fermionic representation allows one to go beyond Glauber’s seminal work and solve exactly a whole class of master equations that are associated with the Hamiltonians given by equation (10). The inverse approach has also been explored. Given a quantum Hamiltonian that can be solved (at least partially), what are the corresponding classical master equations, and do they represent interesting physical systems [39]?

3. Quantum kinetic Ising models

Now we are in a position to proceed with the quantum generalization of the classical kinetic equations (2). Here, we only discuss such a generalization for the Glauber master equation (6) with single-spin flips. However, further generalizations are obviously possible and are left for future work (see also section 5). We start by defining our notation. Naturally, as the computational basis in $(\mathbb{C}^2)^\otimes N$ we take the eigenstates of $N$-fold tensor product of $\sigma^z$. The basis consists of $2^N$ vectors hereafter denoted by $|\sigma\rangle \equiv |\sigma_1, \ldots, \sigma_N\rangle$ ($\sigma = 0, \ldots, 2^N - 1$) with $\sigma_i$ denoting an eigenvalue of $\sigma_i^z$. After appropriate rescaling, we may look at $(\sigma_1, \ldots, \sigma_N)$ as the binary representation of the decimal number $\sigma$.

Let us consider the following master equation:

$$\frac{d\rho(t)}{dt} = \sum_i \left\{ \sigma_i^z [w_i(\sigma^z)]^{1/2} \rho(t) [w_i(\sigma^z)]^{1/2} \sigma_i^z - \frac{1}{2} \{w_i(\sigma^z), \rho(t)\} \right\}. \quad (13)$$

Here $\{,\}$ denotes the anticommutator and $w_i(\sigma^z)$ are quantum mechanical generalizations of spin rates introduced already in the preceding sections\(^8\) (the Ising variables $\sigma = \pm 1$ are replaced by the Pauli matrix $\sigma^z$). Thus, all the spin rates $w_i(\sigma)$ ($i = 1, \ldots, N$) are diagonal in the computational basis $|\sigma\rangle$. It is then clear that the diagonal part of equation (13) reproduces the kinetic equations (2) for all configurations $\sigma$. Notice that equation (13) can be written as

$$\frac{d\rho(t)}{dt} = \sum_i \left( L_i \rho(t) L_i^\dagger - \frac{1}{2} (L_i^\dagger L_i, \rho(t)) \right) \quad (14)$$

with the Lindblad operators given by $L_i = \sigma_i^z [w_i(\sigma^z)]^{1/2}$. It is then clear that we deal only with the dissipative part of the general master equation describing Markov processes.

Nevertheless, further generalizations to the full master equation are possible (e.g. [17] and [21]) as, for instance, for the Ising Hamiltonian, the part governed by the Hamiltonian vanishes and such an equation would also reproduce the kinetic equations (2).

In what follows, we consider only the spin rates that satisfy detailed balance, i.e.

$$w_i(\sigma^z) = w_i(D_i \sigma^z) \exp[-2\beta J \sigma_i^z (\sigma_{i-1}^z + \sigma_{i+1}^z)]. \quad (15)$$

Let us now proceed with solving the above master equation. As we will see below, our method relies—as in the case of classical kinetic equations—on the observation that the whole equation can be brought to a set of $2^N$ Schrödinger equations. For this purpose, it is convenient to use the

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\(^8\) For the sake of clarity and simplicity in the case of quantum spin rates, we change the notation slightly from $w(\sigma \to D_i \sigma)$ to $w_i(\sigma^z)$. According to this convention, $w(D_i \sigma \to \sigma)$ is replaced with $w_i(D_i \sigma^z)$.
isomorphism between matrices from $M_d(C)$ and vectors from $C^d \otimes C^d$. More precisely, we can represent the density matrix $\varrho(t)$ as

$$\varrho(t) = \sum_{\sigma, \tilde{\sigma}} [\varrho(t)]_{\sigma, \tilde{\sigma}} |\sigma\rangle \langle \tilde{\sigma}| \quad \longleftrightarrow \quad |\varrho(t)\rangle = \sum_{\sigma, \tilde{\sigma}} [\varrho(t)]_{\sigma, \tilde{\sigma}} |\sigma\rangle \langle \tilde{\sigma}|. \quad (16)$$

This form of $\varrho(t)$ allows one to rewrite the master equation (13) as the following matrix equation:

$$|\dot{\varrho}(t)\rangle = \sum_{i} \left\{ \sigma_i^z \tilde{\sigma}_i^z \sqrt{w_i(\sigma^z)w_i(\tilde{\sigma}^z)} - \frac{1}{2} \left[ w_i(\sigma^z) + w_i(\tilde{\sigma}^z) \right] \right\} |\varrho(t)\rangle. \quad (17)$$

It should be emphasized that operators corresponding to the ‘tilded’ and ‘non-tilded’ spins act on the ‘tilded’ and ‘non-tilded’ kets in the vector representation of the density matrix $\varrho(t)$ (16) (for instance $\sigma_i^z \tilde{\sigma}_i^z |s\rangle \langle \tilde{s}| = \sigma_i |s\rangle \langle \tilde{s}|$).

It is evident that the matrix appearing on the right-hand side of equation (17) is not Hermitian. In order to bring it to Hermitian form, we can use the DBC (15). This suggests the following transformation (see e.g. [29]):

$$|\varrho(t)\rangle = \exp\{-(\beta/4)[\mathcal{H}(\sigma) + \mathcal{H}(\tilde{\sigma})]\} |\psi(t)\rangle, \quad (18)$$

with $\mathcal{H}$ denoting the quantum generalization of the Ising Hamiltonian given by equation (5). Application of the above to equation (17) leads us to

$$|\psi(t)\rangle = \sum_{i} \left\{ \sigma_i^z \tilde{\sigma}_i^z [v_i(\sigma^z)]^{1/2} [v_i(\tilde{\sigma}^z)]^{1/2} - \frac{1}{2} \left[ w_i(\sigma^z) + w_i(\tilde{\sigma}^z) \right] \right\} |\psi(t)\rangle, \quad (19)$$

where $v_i(\sigma^z) = w_i(\sigma^z) \exp \left[ -(\beta J) \sigma_i^z (\sigma_{i-1}^z + \sigma_{i+1}^z) \right]$. Now, due to the DBC, it is clear that $\sigma_i^z$ and $v_i(\sigma^z)$ commute, and consequently we have a Schrödinger equation $|\dot{\psi}(t)\rangle = -\mathcal{H} |\psi(t)\rangle$ with Hermitian $\mathcal{H}$. Let us note that the above procedure, being just a ‘quantum’ generalization of the procedure described in section 2.2, replaces the problem of solving the master equation for $N$ spins with the problem of solving the corresponding Schrödinger equation for $2N$ spins.

As we will see below, the above equation can be further simplified. Namely, identifying operators that commute with $\mathcal{H}$ we can split the equation into a group of $2^N$ Schrödinger equations. For this purpose, let us note that $\mathcal{H}$ commutes with $\sigma_i^z \tilde{\sigma}_i^z$ ($i = 1, \ldots, N$). We can therefore introduce new variables $\tau_i = \sigma_i^z \tilde{\sigma}_i^z$ ($i = 1, \ldots, N$), which are constants of the motion. Then, one sees that the tilded variables can be expressed by $\tau = (\tau_1, \ldots, \tau_N)$ and $\sigma$ variables as $\tilde{\sigma}_i^z = \tau_i \sigma_i^z$ for any $i$. In other words, we have replaced $\sigma$ and $\tilde{\sigma}$ by $\tau$ and $\sigma$, of which $\tau$ is conserved. The Hamiltonian $H_\tau$ then takes the form

$$H_\tau = -\sum_{i} \left\{ \sigma_i^z [v_i(\tau \sigma^z)]^{1/2} [v_i(\tau \sigma^z)]^{1/2} - \frac{1}{2} \left[ w_i(\tau \sigma^z) + w_i(\tau \sigma^z) \right] \right\}, \quad (20)$$

where $\tau \sigma^z$ denotes $\tau_i \sigma_i^z$ ($i = 1, \ldots, N$). Let us make a comment on the notation. One sees that there are $2^N$ different configurations of $\tau$-spins. We label them by the natural numbers $0, \ldots, 2^N - 1$; because we will have to repeatedly refer to the two fully homogeneous configurations, we simply denote these as $\tau = 0$ (all $\tau$-spins up) and $\tau = 2^N - 1$ (all $\tau$-spins down), without further specifying the association of naturals with configurations.

By definition, the $\tau = 0$ configuration represents the equal values of $\sigma$ and $\tilde{\sigma}$ spins. Consequently, via equation (16), the corresponding Schrödinger equation describes the diagonal
elements of the master equation (13) and thus recovers the classical kinetic equations (6). In the remaining cases of \( \tau \) configurations, the \( \sigma \) and \( \tilde{\sigma} \) variables have to differ on at least one position implying that the Schrödinger equation related to any \( \tau \neq 0 \) describes the set of \( 2^N \) off-diagonal elements of \( \varphi(t) \).

Thus, by identifying \( N \) operators commuting with \( H \) we brought the solution of the general master equation (13) to the problem of diagonalization of \( 2^N \) Hamiltonians, each of dimension \( 2^N \times 2^N \).

Let us now concentrate on a particular choice for the transition probabilities \( w_i(\sigma^z) \). In what follows, we investigate the quantum version of the rates given by (7) (\( \sigma_i \) are replaced with \( \sigma_i^z \)), that is,

\[
w_i(\sigma^z) = \Gamma(1 + \delta \sigma_{i-1}^z \sigma_{i+1}^z)[1 - \frac{\gamma}{2} \sigma_i^z (\sigma_{i-1}^z + \sigma_{i+1}^z)]
\]

with \( \Gamma, \delta \) and \( \gamma \) defined as before. Putting this into equation (20) and after some algebra, we obtain

\[
H_\tau(\gamma, \delta) = -\Gamma \sum_i \left\{ \tilde{A}_i(\gamma, \delta) - \tilde{B}_i(\gamma, \delta) \sigma_{i-1}^z \sigma_{i+1}^z \right\} \sigma_i^x - 1
\]

\[
+ \frac{\gamma}{2} (1 + \delta) \sigma_i^z \left[ f(\tau_{i-1} \tau_i) \sigma_{i-1}^z + f(\tau_i \tau_{i+1}) \sigma_{i+1}^z \right]
\]

\[
- \delta f(\tau_{i-1} \tau_{i+1}) \sigma_{i-1}^z \sigma_{i+1}^z \right\},
\]

where

\[
\tilde{A}_i(\gamma, \delta) = \begin{cases} A(\gamma, \delta), & \tau_{i-1} = \tau_{i+1}, \\ \sqrt{1 - \delta^2 \sqrt{1 - \gamma^2}}, & \tau_{i-1} = -\tau_{i+1} \end{cases}
\]

and

\[
\tilde{B}_i(\gamma, \delta) = \begin{cases} B(\gamma, \delta), & \tau_{i-1} = \tau_{i+1}, \\ 0, & \tau_{i-1} = -\tau_{i+1} \end{cases}
\]

with \( A(\gamma, \delta) \) and \( B(\gamma, \delta) \) defined as in equation (11) and \( f(x) = (1/2)(1 + x) \). One sees that for \( \tau = 0 \) or \( \tau = 2^N - 1 \) the function \( f \) equals 1 for \( i = 1, \ldots, N \) and therefore we obtain the Hamiltonian given in equation (10). Let us stress again that the Schrödinger equation corresponding to \( \tau = 0 \) describes the diagonal elements of the master equation (13) and thus gives the classical kinetic equations (6). All the remaining \( \tau \)s correspond to the off-diagonal elements of \( \varphi(t) \).

For the interesting special case \( \delta = 0 \), all Hamiltonians \( H_\tau \) can be diagonalized using the results of [41]. This is because for any \( \tau = 0, \ldots, 2^N - 1 \), the Jordan–Wigner transformation [36] brings \( H_\tau(\gamma, 0) \) to Hamiltonians, which are quadratic in the fermion operators

\[
c_i = -i \left( \prod_{j=1}^{i-1} \sigma_j^x \right) \sigma_i^+, \quad \sigma_i^+ = \frac{1}{2} (\sigma_i^x + i \sigma_i^z).
\]

This, by virtue of the results of [41], means that diagonalization of any of \( H_\tau(\gamma, 0) \) reduces to the diagonalization of an \( N \times N \) matrix. Because, in principle, the latter can be performed numerically efficiently, the Hamiltonians (22) are diagonalizable.
For the case of \( \delta \neq 0 \), the Jordan–Wigner transformation gives us Hamiltonians containing terms that are quartic in \( c_i \). In this case, we can try the transformation proposed by Siggia [35]. For this purpose, we introduce new bond variables \( Z_i = \sigma_i^z \sigma_{i-1}^z \), \( \sigma_i^z = X_{i-1} X_i \) and \( Y_i = -iZ_i X_i \). They commute when their indices are different (different bonds), whereas for coinciding indices (the same bond) they obey the algebra of Pauli matrices \( (X_i^2 = 1, X_i Y_i = iZ_i, \text{ etc}) \). The bond variables allow one to rewrite the Hamiltonian from equation (22) as

\[
H_\tau(\gamma, \delta) = -\Gamma \sum_i \left\{ \tilde{A}_i(\gamma, \delta) X_{i-1} X_i + \tilde{B}_i(\gamma, \delta) Y_{i-1} Y_i - \delta f(\tau_{i-1} \tau_i) Z_{i-1} Z_i \right\} - \left[ 1 - \gamma (1 + \delta f(\tau_{i-1} \tau_i) Z_i) \right].
\] (26)

Generally, this is the anisotropic Heisenberg Hamiltonian with some external field. In some particular cases, such Hamiltonians are analytically diagonalizable (for a pedagogical review of the Heisenberg model and the Bethe ansatz that is used to solve it, see [42]). It seems that the general case \( \delta \neq 0 \) defies exact diagonalization. However, in the following subsection, we show that for \( \delta = -1 \), \( H_\tau(\gamma, \delta) \) can be diagonalized analytically for all values of \( \tau \).

4. Properties of the Hamiltonians associated with the quantum master equation

Here we study some of the properties of the Hamiltonians \( H_\tau \). First, we show that all of them are positive and in a majority of cases even strictly positive. We also discuss the cases in which \( H_\tau \) have zero eigenvalues and thus identify possible stationary states of the master equation (13). Then we study the fully soluble case of the so-called energy conserving spin flips, where all Hamiltonians \( H_\tau, \tau = 0, \ldots, 2^N - 1 \), are diagonalizable. Finally, we numerically investigate the properties of entropy of ground states of our Hamiltonians.

4.1. Zero eigenvalues of \( H_\tau \)—stationary states of the evolution

It is interesting to ask which states survive the evolution, that is, which of the off-diagonal elements of \( \rho(t) \) do not decay to zero with \( t \to \infty \). This can be done by studying the positivity properties of \( H_\tau \) and in particular their eigenstates corresponding to zero eigenvalues. Generically, as we will see below, for any \( \tau \) except for \( \tau = 0 \) and \( 2^N - 1 \), the Hamiltonians \( H_\tau \) are strictly positive except for two different \( (\gamma, \delta) \) points, namely, \( \delta = \gamma = 0 \) and \( \delta = \gamma = 1 \). On the other hand, for \( \tau = 0 \) or \( 2^N - 1 \), it is known [28, 29] that the corresponding Hamiltonian has zero eigenvalues (twofold degenerate) for any value of \( \gamma \) and \( \delta \).

Let us treat the two cases \( \tau \neq 0 \) and \( \tau \neq 2^N - 1 \) in a more detailed way. For this purpose, let us note that we may write \( H_\tau(\gamma, \delta) \) as \( H_\tau(\gamma, \delta) = \sum_i H_\tau^{(i)}(\gamma, \delta) \) and study positivity of each \( H_\tau^{(i)}(\gamma, \delta) \). On the other hand, for any \( \tau \neq 0 \), \( 2^N - 1 \) we may divide all such terms into two groups, one consisting of \( H_\tau^{(i)}(\gamma, \delta) \) for which \( \tau_{i-1} = \tau_{i+1} \) and one for which \( \tau_{i-1} = -\tau_{i+1} \). More precisely, we can write \( H_\tau(\gamma, \delta) \) as

\[
H_\tau(\gamma, \delta) = \sum_{|i| \tau_{i-1} = \tau_{i+1}} H_\tau^{(i,=)}(\gamma, \delta) + \sum_{|i| \tau_{i-1} = -\tau_{i+1}} H_\tau^{(i,\neq)}(\gamma, \delta). \] (27)
In the first case of equal \( \tau s \), we have
\[
H^{(i,=)}_\tau(\gamma, \delta) = \Gamma \left[ 1 - \frac{\gamma}{2} (1 + \delta) f(\tau_{i-1} \tau_i) \sigma^z \left( \sigma^z_{i-1} + \sigma^z_{i+1} \right) + \delta \sigma^z_{i-1} \sigma^z_{i+1} \right. \\
- \left[ A_i(\gamma, \delta) - B_i(\gamma, \delta) \sigma^z_{i-1} \sigma^z_{i+1} \right] \sigma^z_i \right].
\] (28)

One finds that \( H^{(i)}_\tau(\gamma, \delta) \) has four different eigenvalues, each twofold degenerate. For \(-1 \leq \delta \leq 1\) their explicit forms are \( \lambda_1 = 0 \), \( \lambda_2 = 2\Gamma(1-\gamma) \),
\[
\lambda^{(=)}_{3,4} = \Gamma (1 + \delta) \left[ 1 \pm \sqrt{1 - \gamma + \left( \frac{1 - \tau_{i-1} \tau_i}{2} \right)^2 \gamma^2} \right].
\] (29)

For the chosen parameter region \( \lambda^{(=)}_2 \geq 0 \), while \( \lambda^{(=)}_3 \) is manifestly positive. On the other hand, to prove non-negativity of \( \lambda^{(=)}_4 \) it suffices to note that \( 1 - \gamma + [(1 - \tau_{i-1} \tau_i)/2]^2 \gamma^2 \leq 1 - \gamma + \gamma^2 \leq 1 \) for \( \gamma \leq 1 \).

In the case of \( \tau_{i-1} = -\tau_{i+1} \), we have
\[
H^{(i,\neq)}_\tau(\gamma, \delta) = \Gamma \left[ 1 - \frac{\gamma}{2} (1 + \delta) \sigma^z \left( f(\tau_{i-1} \tau_i) \sigma^z_{i-1} + f(\tau_{i} \tau_{i+1}) \sigma^z_{i+1} \right) - \sqrt{1 - \delta^2} \sqrt{1 - \gamma^2} \sigma^z_i \right].
\] (30)

Here one finds that because \( \tau_{i-1} = -\tau_{i+1} \), one of the factors \( f(\tau_{i-1} \tau_i) \) or \( f(\tau_{i} \tau_{i+1}) \) vanishes. Without any loss of generality, let us assume that \( f(\tau_{i-1} \tau_i) = 0 \). Then, obviously \( f(\tau_{i-1} \tau_i) = 1 \) and the above Hamiltonian can be brought to
\[
H^{(i,\neq)}_\tau(\gamma, \delta) = 1 - \frac{\gamma}{2} (1 + \delta) \sigma^z \left( \sqrt{1 - \delta^2} \sqrt{1 - \gamma^2} \right) + \frac{1}{2} \sqrt{\gamma^2 (1 + \delta)^2 + 4 \sqrt{1 - \gamma^2} (1 - \delta^2)}. \]
\] (32)

One sees that obviously \( \lambda^{(\neq)}_2 \geq 0 \). To see that also \( \lambda^{(\neq)}_3 \) is non-negative it suffices to note that for \( 0 \leq \gamma \leq 1 \) and \( |\delta| \leq 1 \) the maximal value of the function of \( \gamma \) and \( \delta \) appearing under the sign of square root is four and it is this value that is attained for \( \gamma = \delta = 0 \) and \( \delta = \gamma = 1 \). This also means that \( \gamma = \delta = 0 \) and \( \gamma = \delta = 1 \) are the only points for which \( H^{(i,\neq)}_\tau(\gamma, \delta) \) can have zero eigenvalues.

In conclusion, it follows from the above analysis that all \( H^{(i)}_\tau(\gamma, \delta)s \) are positive and therefore the Hamiltonian \( H_\tau(\gamma, \delta) \) is positive for any \( \tau = 0, \ldots, 2^N - 1 \), and the parameter region specified by the conditions \(-1 \leq \delta \leq 1, 0 \leq \gamma \leq 1 \) and \( \Gamma > 0 \). Moreover, it follows that for all \( \tau \neq 0, 2^N - 1 \), the Hamiltonians \( H_\tau(\gamma, \delta) \) are in general strictly positive except the points \( \delta = \gamma = 0 \) and \( \delta = \gamma = 1 \). Thus these two points together with two values of \( \tau = 0, 2^N - 1 \) are the only possible cases when \( H_\tau(\gamma, \delta) \) can have zero eigenvalues. Let us briefly discuss each of these cases.

For \( \tau = 0 \) and \( 2^N - 1 \), as previously noted, the corresponding Hamiltonian (10) has a zero-eigenvalue eigenstate given by equation (1). The case \( \tau = 0 \) (\( \tau = 2^N - 1 \)) corresponds to the diagonal (anti-diagonal) elements of \( \varrho(t) \), which as it follows from equations (1) and (18) are of the form (taking into account the normalization)
\[
|\varrho(t)\rangle = \frac{1}{Z_N} e^{-\beta H(\sigma)} \sum_\sigma |\sigma\rangle \quad (\tau = 0, 2^N - 1). \] (33)
For the zero temperature limit ($\beta \to \infty$), the above becomes the well-known $N$-partite Schrödinger cat state (or Greenberger–Horne–Zeilinger state)

$$|\psi^{(N)}_+\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\rangle^{\otimes N} + |\downarrow\rangle^{\otimes N} \right)$$

(34)

with $|\uparrow\rangle$ and $|\downarrow\rangle$ denoting the eigenvectors of $\sigma^z$ corresponding to the positive and negative eigenvalues, respectively. Moreover, for $\gamma = 1$ the twofold degeneracy appears in the ground state of $H_1(1, \delta)$ and the second zero-energy eigenstate is

$$|\psi^{(N)}_-\rangle = \frac{1}{\sqrt{2}} \left( |\uparrow\rangle^{\otimes N} - |\downarrow\rangle^{\otimes N} \right).$$

(35)

Because generically the remaining off-diagonal elements of $\varrho(t)$ vanish in the $t \to \infty$ limit (except for the already mentioned values of $\gamma$ and $\delta$), we have an example of a state that is a stationary state of the master equation and becomes a genuine multipartite entangled state in the limit of zero temperature.

Let us now treat the cases of $\gamma = \delta = 0$ and $\delta = \gamma = 1$. In the first one, the Hamiltonians $H_t(\gamma, \delta)$ simplify significantly and are of the form

$$H_t(0, 0) = \Gamma \sum_i (1 - \sigma_i^z) \quad (\tau = 0, \ldots, 2^N - 1),$$

(36)

meaning that the only zero energy state is $|\longrightarrow\rangle^{\otimes N}$ where $|\longrightarrow\rangle$ and $|\leftarrow\rangle$ stand for the normalized eigenstates of $\sigma^z$ corresponding to positive and negative eigenvalues, respectively. As it follows from equation (18), for $\gamma = 1$ it holds that $|\varrho(t)\rangle = |\psi(t)\rangle$ for any $\tau$, therefore $|\varrho(t)\rangle = (1/\sqrt{2^N})|\longrightarrow\rangle^{\otimes N}$ for $\tau = 0, \ldots, 2^N - 1$. Consequently, the stationary state is fully separable and is given by $\varrho_{st}(t) = P|\longrightarrow\rangle^{\otimes N} P_{|\leftarrow\rangle}$ with $P_{|\leftarrow\rangle}$ denoting a projector onto $|\longrightarrow\rangle$.

The case of $\delta = \gamma = 1$ is a little bit more difficult. Now, from equation (22) it follows that

$$H_t(1, 1) = \Gamma \sum_i \left\{ 1 - \sigma_i^z \left[ f(\tau_{i-1} \tau_{i}) \sigma_{i-1}^z + f(\tau_{i} \tau_{i+1}) \sigma_{i+1}^z \right] + f(\tau_{i-1} \tau_{i+1}) \sigma_{i-1}^z \sigma_{i+1}^z \right\}.$$ 

(37)

It is clear that this Hamiltonian is diagonal in the standard basis $|\sigma\rangle$ in $(\mathbb{C}^2)^{\otimes N}$ and thus we can look for the eigenstates among the standard basis in $(\mathbb{C}^2)^{\otimes N}$. Interestingly, using the previously introduced bond variables $Z_i = \sigma_{i-1}^z \sigma_i^z$, in the case of periodic boundary conditions this Hamiltonian can be brought to the antiferromagnetic Ising Hamiltonian with magnetic field

$$H_t(1, 1) = \Gamma N + \sum_i f(\tau_{i-1} \tau_{i+1}) Z_{i-1} Z_i - 2\Gamma \sum_i f(\tau_{i-1} \tau_{i}) Z_i.$$ 

(38)

Let us concentrate on the zero-energy eigenstates of $H_t(1, 1)$. The latter can be found by solving the corresponding equation for eigenvalues of $\sigma^z$. This, however, due to the fact that in this equation each term under the sum is positive, means solving the following set of equations:

$$f(\tau_{i-1} \tau_{i}) \sigma_{i-1}^z \sigma_i^z + f(\tau_{i} \tau_{i+1}) \sigma_i \sigma_{i+1}^z - f(\tau_{i-1} \tau_{i+1}) \sigma_{i-1}^z \sigma_{i+1}^z = 1,$$ 

(39)

where $i = 1, \ldots, N$ and $\sigma_i$ stands for the eigenvalue of $\sigma_i^z$. For instance, for all configurations of $\tau$ that consist of blocks of length greater or equal to two separated by the domain walls, one of the possible solutions is given by $\sigma_i = \tau_i$. This is because in such a case the above set becomes $f(\tau_{i-1} \tau_{i}) + f(\tau_{i} \tau_{i+1}) - f(\tau_{i-1} \tau_{i+1}) = 1$ ($i = 1, \ldots, N$). The only possible triples

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(τ_{i-1}, τ_{i}, τ_{i+1}) that can appear in the discussed case are ↑↑↑, ↓↓↓, ↑↓↓, ↓↑↑, ↑↑↑ and ↓↓↑. It is clear that for all of them these equations are satisfied. One may also easily check that generically the zero-energy eigenstates are degenerate. As a result, it seems that in the case of γ = δ = 1 there is a variety of states ρ(t) that are stationary states of our master equation.

4.2. The case of energy-conserving spin flips

Here we consider the case of energy-conserving spin flips, that is, when δ = −1. One sees now that the Hamiltonians H_{\tau} simplify significantly and read

\[ H_{\tau}(\gamma, -1) = \Gamma N - \Gamma \sum_i f^\tau_i (X_{i-1}X_i + Y_{i-1}Y_i + Z_{i-1}Z_i), \]  

(40)

where f^\tau_i = f(τ_{i-1}τ_{i+1}). For τ = 0 and 2^N − 1, this is the isotropic ferromagnetic Heisenberg model with spectrum shifted by \( \Gamma N \). In the general case, however, \( H_{\tau}(\gamma, -1) \) depends on the numbers \( f_i \), which are either zero or one depending on the configuration τ. To deal with this, it suffices to note that for any configuration of τ ≠ 0, 2^N − 1 some set of indices \{i_1, \ldots, i_k\} exists for which \( f_{i_k} = 0 \) and between these zeros the \( f_i \) are constant and equal to one. It is clear from equation (40) that such zeros divide the Hamiltonian into a sum of ‘smaller’ commuting Hamiltonians. More precisely, if \( f_{i_j} = 0 \) for \( j = 1, \ldots, k \), then

\[ H_{\tau}(\gamma, -1) = \Gamma N - \Gamma \sum_{n=1}^{i_1-1} S_{n-1} \cdot S_n - \Gamma \sum_{n=i_k+1}^{i_2-1} S_{n-1} \cdot S_n - \cdots - \Gamma \sum_{n=i_{k-1}+1}^{i_k-1} S_{n-1} \cdot S_n, \]  

(41)

where \( S_n = [X_n, Y_n, Z_n] \). It follows that \( S_{n-1} \cdot S_n \) commutes with \( S_{m-1} \cdot S_m \) whenever |n − m| ≥ 2.

This means that for a given configuration of τ we can split \( H_{\tau}(\gamma, -1) \) into a group of commuting isotropic ferromagnetic Heisenberg Hamiltonians with free ends. Such Hamiltonians can be treated using the so-called Bethe ansatz [43]. To visualize what we have just said let us consider the following illustrative example. Let us assume the periodic boundary conditions in equation (40) and let the τ configuration together with the corresponding chain \( f^\tau_i \) be given by

\[
\begin{array}{c|cccccccccccc}
\tau & \uparrow & \uparrow & \uparrow & \downarrow & \downarrow & \uparrow & \uparrow & \downarrow & \downarrow & \uparrow & \uparrow & \uparrow & \\
f_i & 1 & 1 & 0 & 0 & 0 & 1 & 0 & 1 & 1 & 1 & 0 & 1 & 1
\end{array}
\]  

(42)

and then the Hamiltonian becomes (forgetting about the constant part and putting \( \Gamma = 1 \))

\[ H_{\tau}(\gamma, -1) = -(\sum_{i=1}^{12} S_{i-1} \cdot S_i + S_6 \cdot S_7 + \sum_{i=9}^{11} S_{i-1} \cdot S_i + \sum_{i=13}^{14} S_{i-1} \cdot S_i). \]

4.3. Entropy of the ground state of the off-diagonal Hamiltonians

Here we take a brief detour and study the entanglement between parts of the ground state of the Hamiltonians \( H_{\tau}(\gamma, \delta) \) that control the dynamics of the off-diagonal terms of the QME. In order to study our system for arbitrary values of \( \delta \), we take advantage of the matrix product state structure that the ground state of these Hamiltonians has. For this, we extend the time-evolving block decimation (TEBD) algorithm of Vidal [44] to include next-nearest neighbor
Our goal is to compute the bipartite entropy $S = \text{tr} \rho_L \log_2 \rho_L$, where $\rho_L$ is the reduced density matrix obtained after tracing out $N - L$ contiguous spins of the chain. For this, instead of obtaining and diagonalizing $\rho_L$, we make use of the Schmidt coefficients that appear explicitly in the TEBD representation of the state. We study two representative cases of $\tau$ configurations, one in which only two $\tau$'s are different from the rest, and one where half of the neighboring $\tau$'s are equal between them and different from the other half—a case that we call a ‘domain wall’. We also concentrate on two relevant values of $\delta$, firstly, $\delta = 0$ (the Glauber model), shown in figures 1 and 2, and secondly, the temperature-dependent $\delta = \gamma / (2 - \gamma)$ (the Haake–Thol model that gives the dynamical critical exponent $z = 4$), shown in figures 3 and 4. For comparison, we also compute the bipartite entropy of the diagonal component of the QME, i.e. the classical KIM.

Any pure state $|\psi\rangle$ of a quantum system partitioned into two parts $A$ and $B$ can be written in its Schmidt decomposition form, $|\psi\rangle = \sum_{\alpha=1}^{\chi} \lambda_{\alpha}^{1/2} |\phi_{\alpha}^{(A)}\rangle |\phi_{\alpha}^{(B)}\rangle$, where $\{|\phi_{\alpha}^{(A)}\rangle\}$ and $\{|\phi_{\alpha}^{(B)}\rangle\}$ are two orthonormal bases of the Hilbert space of parts $A$ and $B$, respectively, $\lambda_{\alpha}$ are non-negative real numbers (the Schmidt coefficients) and $\chi$ is the smallest of the dimensions of the Hilbert spaces of $A$ and $B$. If part $B$ is then traced out, the reduced density matrix of part $A$ can be written as a diagonal matrix in the $\{|\phi_{\alpha}^{(A)}\rangle\}$ basis, with the Schmidt coefficients in the diagonal. Because the TEBD algorithm basically stores the Schmidt coefficients and the Schmidt bases for all possible bi-partitions of the system, computing the von-Neumann entropy of the reduced density matrix $\rho_L$ for any $L$-value is quite easy.

---

**Figure 1.** Bipartite entropy $S(L) = \text{tr} \rho_L \log_2 \rho_L$, where $\rho_L$ is the reduced density matrix obtained after tracing out $N - L$ contiguous spins of the chain, for the Hamiltonian (22) in the $\delta = 0$ case, and where $\tau$ is a configuration where all but two components are equal. The curves, in ascending order, are for $\gamma = 0.1, 0.3, 0.5, 0.7$ and 0.9. The entropy reaches 1 for criticality at $\gamma = 1$. The system is a chain of 90 spins. Note how at the point of the flipped $\tau$'s the bipartite entropy is reduced but does not go to zero. In thin lines, for comparison, is shown the same entropy but for a configuration with all $\tau$'s equal to one (the classical KIM, here the diagonal part of the QME).
Figure 2. The same as figure 1 but for a configuration of $\tau_i$s where half are 1 and the other half are $-1$. Note how the entropy goes to zero at the domain wall.

Figure 3. The same system as figure 1, but for $\delta = \gamma/(2 - \gamma)$, where the classical KIM shows an anomalous dynamical exponent $z = 4$. In this case, the flipped $\tau_i$ induces a spike in entropy near the domain wall, indicating some interesting quantum correlation existing between domain walls. Still the curves, in ascending order, are for $\gamma = 0.1, 0.3, 0.5, 0.7$ and 0.9. In thin lines, for comparison, is the same system but for a configuration with all $\tau_i$s equal to one (the classical KIM, here the diagonal part of the QME).

We observe that the maximum value of entropy grows with $\gamma$ and approaches unity for criticality ($\gamma = 1$). The block length $L$ at which the entropy saturates also appears to be rather small, about five sites, although we expect this to grow near the critical point.

In all cases of $\delta$, a domain wall appears to de-entangle the two parts of the chain, giving zero entropy for a partition right at the domain boundary. On the other hand, a single flipped $\tau_i$ shows some residual entropy. Therefore, the separation of the Hamiltonian into commuting parts shown above for $\delta = -1$ is not possible for general $\tau$ configurations.
The case with an anomalous dynamical exponent $z = 4$, $\delta = \gamma/(2 - \gamma)$, shows some interesting behavior of the entropy near the domain walls or the flipped $\tau_i$. In particular, we observe an entropy spike before the end of the domain. The effect is acutely pronounced near criticality.

5. Conclusions and outlook

We have presented here a novel class of QMEs that have the following properties. (cf e.g. [17] and [21]).

- The diagonal elements of the density matrix in the ‘computational’ basis follow the dynamics of a certain classical kinetic model.
- The dynamics of the off-diagonal matrix elements splits into blocks, described by ‘kinetic-like’ models.
- For models fulfilling DBC, the dynamics can be transformed into a Hamiltonian dynamics in imaginary time.
- The ground and low excited states of the resulting Hamiltonians fulfill area law, and can be well described by the MPS or PEPS methods.

Our results suggest several directions for future investigation, which we would like to follow.

- In the present paper we have focused on Ising spins, and on generalized QME associated with KIMs. Generalizations to models associated with kinetics of a more general set of commuting operators, such as stabilizer operators, are possible and interesting.
- Several presented models admit exact solutions via the Wigner–Jordan transformation or Bethe ansatz in the manner of [29, 35] and/or approximate treatment using variational
methods in the manner of [28]. These methods should allow for more rigorous analysis of the novel types of Hamiltonians.

- Especially interesting are the two-spin-flip models such as those that conserve the magnetization [40] or energy [30]. In particular, for the energy conserving model in 1D, the generalized QME reads
  \[
  \frac{d\rho(t)}{dt} = \sum_{i=1}^{N} \left[ \sigma_{i}^{x} \sigma_{i+1}^{x} \sqrt{1 - \sigma_{i-1}^{z} \sigma_{i+1}^{z}} \rho(t) \sqrt{1 - \sigma_{i}^{z} \sigma_{i+2}^{z}} \sigma_{i}^{+} \sigma_{i+1}^{+} \sigma_{i+1}^{+} \sigma_{i}^{-} \sigma_{i+2}^{-} \rho(t) \right] - \frac{1}{2} \left\{ 1 - \sigma_{i-1}^{z} \sigma_{i+1}^{z} \sigma_{i+2}^{z}, \rho(t) \right\}.
  \]
  (43)

The high degeneracy of the ground state in this model allows one to expect the appearance of long-living coherences.

- Generalization to models that do not fulfill DBC, such as exclusion models (see [45, 46]), is possible. An example of somewhat ‘hidden’ DBC is the QME of the form
  \[
  \frac{d\rho(t)}{dt} = \sum_{i=1}^{N} \left[ \sigma_{i}^{x} \sigma_{i+1}^{x} \sqrt{1 - \alpha \sigma_{i+1}^{z}} \rho(t) \sqrt{1 - \alpha \sigma_{i}^{z} \sigma_{i+1}^{z}} \sigma_{i}^{+} \sigma_{i+1}^{+} \sigma_{i+1}^{+} \sigma_{i}^{-} \rho(t) \right] - \frac{1}{2} \left\{ 1 - \alpha \sigma_{i}^{z} \sigma_{i+1}^{z}, \rho(t) \right\},
  \]
  (44)

where \(-1 \leq \alpha \leq 1\) is a free parameter. This model corresponds to the 1D anisotropic Heisenberg model.

- Last, but not least, physical implementations of the considered models with ultracold atoms in optical lattices, or ions in trap arrays, or Rydberg atoms, are feasible, and will be studied.

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