Relaxation for an Open System of Interacting Spins

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I want to thank a few people.

ABSTRACT

The preface pretty much says it all.

TABLE OF CONTENTS

List of Figures

Introduction

Introductory content.

Note on Notation

The mathematical formalism for quantum mechanics requires three levels of linear algebra: vectors, operators (maps between vectors), and superoperators (maps between operators). We will write each object with slightly differerent notation so that the type of an expression may be inferred if the reader is confused.

Vector	$\lvert v \rangle$		Real numbers	$\mathbb{R}$
$\lvert v \rangle$ in coordinates	$\boldsymbol{v}$		Complex numbers	$\mathbb{C}$
Tuple	$\boldsymbol{n}$		Integers modulo n	$\mathbb{Z}_n$
Operator	A		Hilbert space	$\mathcal{H}$
Vector operator	$\boldsymbol{B}$		Bounded operators	$\mathcal{B}(\mathcal{H})$
A in coordinates	$\boldsymbol{A}$		Liouville space	$\mathcal{L}(\mathcal{H})$
Superoperator	$\mathcal{A}$		Hamiltonian operator	H
One	1		Density operator	ρ
Identity operator	1		Pauli operators	σ_i
Identity superoperator	$\mathbb{1}$		Spin operators	$S_i = \hbar \sigma_i / 2$
Zero	0		Inner product on $\mathcal{L}$	$\langle A \vert B \rangle$
Zero operator	0		Transpose of $\boldsymbol{A}$	$\boldsymbol{A}^{\mathsf{T}}$
Zero superoperator	$\mathbb{0}$		Adjoint of A	$A^{\dagger}$
			Trace of A	$\operatorname{tr} A$
Sign of x	$\operatorname{sgn} x$		Partial trace over S	tr_S
Sinc function	$\operatorname{sinc} x = \dfrac{\sin x}{x}$		Expected value of A	$\langle A \rangle = \operatorname{tr}(\rho A)$
			Hermitian part of A	$\operatorname{He} A = \dfrac{A + A^{\dagger}}{2}$

The text uses **natural units** where $\hbar = c = \varepsilon_0 = m_e = 1$.

This is the color version of the document. Plots, code, and links are colored. Example: continue to chapter 1.

CHAPTER 1

OPEN QUANTUM SYSTEMS

YOU, a novice baker, mix ingredients to make cake batter. You know everything about this cake batter: after all, you made it. However, you are unsure about how the cake will turn out in your dodgy oven. You bake the cake and let it cool. You try to cut a slice of cake, but instead you get a slice of disaster: the inside is goopy. As consolation for your experience, take pride in the fact that you just performed a quantum measurement.

The setup in quantum theory is just like the cake. One starts with a **quantum state**, which encodes the probabilities one assigns to each outcome of an operation. These operations could be anything, and the outcomes are often not mutually exclusive. When we do consider operations with exclusive outcomes, like the operation of checking if the cake is baked or not, there is sometimes an upper bound on the number of outcomes we may see. For the cake system there are two outcomes. This property of a quantum system is its **dimension**.

1.1 THE MATHEMATICAL FORMALISM

Different mathematical formalisms for quantum mechanics differ in how they represent states and operations, but they agree on the assignment of probabilities to outcomes. We will now review postulates for quantum theory based on Hilbert spaces.

Postulate 1. A quantum system is described by a separable complex Hilbert space $\mathcal{H}$.[1]

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[1] Since a quantum system is identified only by its dimension d, we may wonder which d-dimensional Hilbert space to assign. However, all finite d-dimensional (separable) complex Hilbert spaces are isometrically isomorphic to $\mathbb{C}^d$, and all infinite-dimensional separable Hilbert spaces are isometrically isomorphic to ℓ^2 (square-summable sequences) and to L^2 (square-integrable functions).

Postulate 2. An outcome corresponds to an **effect** E, which is a self-adjoint operator on $\mathcal{H}$ such that $0 \leqslant E \leqslant 1$.[2]

Postulate 3. A state corresponds to a **probability measure** P on effects. That is:

    1. $0 \leqslant P(E) \leqslant 1$ for all effects E,

    2. $P(1) = 1$,

    3. $P(E_1 + E_2 + \cdots) = P(E_1) + P(E_2) + \cdots$ for any sequence of events with $E_1 + E_2 + \cdots \leqslant 1$.

Postulate 4. States form a convex set. If $\sum_i p_i = 1$, the convex sum of states $\{P_i\}$ is defined by

$$\left(\sum_i p_i P_i \right)(E) = \sum_i p_i P_i(E). \tag{1.1}$$

Such a combination is known as an **ensemble**.

Note that the convex structure of the set of quantum states is necessary for consistency. One must obtain the same results when one makes two state assignments, predicts outcomes for each, and averages the results, as when one assigns the average state first and then predicts outcomes.

It is simple to prove that any probability measure P on an effect E may be represented by the **Born rule**

$$P(E) = \mathrm{tr}(\rho E), \tag{1.2}$$

where $\rho \geqslant 0$ is a self-adjoint operator known as a **density operator** [1, 2].[3] Equation (1.2) implies that $\mathrm{tr}\,\rho = 1$ and that a convex sum of states is represented by the same sum of density operators. The Born rule uniquely identifies density operators with states, so we will use the term state to refer to density operators from now on.

An **observable** result of an operation is described by an assignment of each outcome m to an effect E_m, where $\sum_m E_m = 1$. Since effects are positive operators that determine the probabilities of each outcome, such an observable is called a **positive operator valued measure** (POVM). The special case where the effects are projectors is called a **projection**

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[2]The notation $A \leqslant B$ means that $\langle v|A|v\rangle \leqslant \langle v|B|v\rangle$ for all $v \in \mathcal{H}$.

[3]The more specific case where effects are restricted to be projections $|v\rangle\langle v|$ for $v \in \mathcal{H}$ is significantly harder, and is known as Gleason's theorem [3].

valued measure (PVM). A PVM with the maximum number of outcomes may be conveniently represented by the self-adjoint operator

$$M = \sum_m m |v_m\rangle\langle v_m| . \tag{1.3}$$

By virtue of this definition, the expected value of the PVM is

$$\langle M \rangle = \sum_m m P(m) \tag{1.4}$$

$$= \sum_m m \, \text{tr}(\rho |v_m\rangle\langle v_m|) \tag{1.5}$$

$$= \text{tr}\left(\rho \left(\sum_m m |v_m\rangle\langle v_m| \right) \right) \tag{1.6}$$

$$= \text{tr}(\rho M). \tag{1.7}$$

From here on, most observables will be PVMs represented by self-adjoint operators.

We now describe how operations change states.

Postulate 5. An **operation** with outcome m is described by a map $\mathcal{O}_m$. The state ρ after the operation becomes

$$\rho'_m = P(m)^{-1} \mathcal{O}_m(\rho). \tag{1.8}$$

Since ρ'_m must be a density operator, postulate 5 implies that $\mathcal{O}_m\rho \geqslant 0$ and

$$\text{tr} \, \mathcal{O}_m(\rho) = P(m) = \text{tr}(\rho E_m). \tag{1.9}$$

If an operation is performed but the outcome is unknown, we may assign the state

$$\rho' = \sum_m P(m)\rho'_m = \sum_m \mathcal{O}_m(\rho), \tag{1.10}$$

so that an effect E has the expected probability $\text{tr}(\rho' E) = \langle \text{tr}(\rho'_m E)\rangle_m$.

The state of the ensemble $\rho = \sum_i p_i \rho_i$ after an operation with outcome m is

$$\frac{\mathcal{O}_m(\rho)}{\text{tr} \, \mathcal{O}_m(\rho)} = \sum_i P(i|m) \frac{\mathcal{O}_m(\rho_i)}{\text{tr} \, \mathcal{O}_m(\rho_i)} \tag{1.11}$$

By Bayes' theorem,

$$P(i|m) = \frac{P(i)P(m|i)}{P(m)} = \frac{p_i \, \text{tr} \, \mathcal{O}_m(\rho_i)}{\text{tr} \, \mathcal{O}_m(\rho)}. \tag{1.12}$$

Now eq. (1.11) becomes

$$\mathcal{O}_m\left(\sum_i p_i \rho_i \right) = \sum_i p_i \mathcal{O}_m(\rho_i). \tag{1.13}$$

Thus operations are convex linear.

1.2   COMPOSITE SYSTEMS

The success of physics lies in the apparent lack of causal connections between phenomena separated in space and time. Different things are different, and the actions of someone on the other side of the world have no immediate effect on an experiment performed now. We then expect that some physical systems are composed of a number of subsystems. The whole system may be affected as different parts that each respond the same way as if nothing else was there. [4]

Given a quantum system with Hilbert space $\mathcal{H}$, a decomposition into **subsystems** is de-scribed by Hilbert spaces $\mathcal{H}_i$ with $\prod_i \dim \mathcal{H}_i = \dim \mathcal{H}$ and maps f_i, g_i such that

$$\operatorname{tr}(\rho f_i(E_i)) = \operatorname{tr}(g_i(\rho)E_i) \tag{1.14}$$

for any state ρ on $\mathcal{H}$ and effect E_i on $\mathcal{H}_i$. The maps f_i lift an effect from the subsystem to the composite system, while the g_i reduce a composite state to a subsystem state.

What are f_i and g_i? We will first consider their action on states of definite composition. Consider states ρ_A and ρ_B on $\mathcal{H}_A$ and $\mathcal{H}_B$ where $\dim \mathcal{H}_A \dim \mathcal{H}_B = \dim \mathcal{H}$. How do we represent the **product state** ρ, which satisfies $g_A(\rho) = \rho_A$ and $g_B(\rho) = \rho_B$? Perhaps ρ is just the pair (ρ_A, ρ_B). By postulate 4, a convex combination of such pairs is also a composite state. However, suppose that $\rho_A = \sum_i \alpha_i \rho_i^A$ and $\rho_B = \sum_j \beta_j \rho_j^B$. We mean the same state when we consider either an ensemble of composites or a composite of ensembles, which is the equivalence

$$\left(\sum_i \alpha_i \rho_i^A, \sum_j \beta_j \rho_j^B \right) \sim \sum_{ij} \alpha_i \beta_j \left(\rho_i^A, \rho_j^B \right) \tag{1.15}$$

on the composite states. Thus the product state is not a pair, but an equivalence class $[(\rho_A, \rho_B)]$ of $(\mathcal{B}(\mathcal{H}_A) \times \mathcal{B}(\mathcal{H}_B))/\sim$. These classes are called **tensors**. The product state equivalence class is written with the **tensor product** as $\rho_A \otimes \rho_B$, and the whole space is called $\mathcal{B}(\mathcal{H}_A) \otimes \mathcal{B}(\mathcal{H}_B) \cong \mathcal{B}(\mathcal{H})$. [5] The same argument gives the **product effect** $E_A \otimes E_B$. Yet the same could be said for the operator $\rho_A E_A$, which leads us to define $(\rho_A \otimes \rho_B)(E_A \otimes E_B) = \rho_A E_A \otimes \rho_B E_B$.

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[4] For example, we will later consider each spin in a spin chain to be a subsystem, since each spin may be separately affected. However, each of two electrons would not be a subsystem, since removal of one electron changes where the other electron is likely to be found.

[5] Is this Hilbert space separable as required by postulate 1? Yes, but later we will consider a bath described by an infinite tensor product of harmonic oscillators. Such a Hilbert space is not separable, but the subspace that is physically relevant is separable. Since we will neglect high-frequency modes anyway, it also suffices to truncate the product once the energies are sufficiently high. For more discussion, see [4, pp. 84–87].

What is $\operatorname{tr}(A \otimes B)$? Product effects represent independent events. For the probabilities to multiply, we must have

$$\operatorname{tr}(A \otimes B) = \operatorname{tr} A \operatorname{tr} B. \tag{1.16}$$

Thus an effect E_A is lifted as $f_A(E_A) = E_A \otimes 1$.

We now extend to non-product states, which are called **entangled** states. Consider a map f of the f_i and the countable sum of events $E = \sum_a E_a$. By eq. (1.14),

$$\operatorname{tr}\left(\rho \sum_a f(E_a)\right) = \sum_a \operatorname{tr}\left(\rho f(E_a)\right) \tag{1.17}$$

$$= \sum_a \operatorname{tr}\left(g(\rho) E_a\right) \tag{1.18}$$

$$= \operatorname{tr}\left(g(\rho) \sum_a E_a\right) \tag{1.19}$$

$$= \operatorname{tr}\left(\rho f\left(\sum_a E_a\right)\right) \tag{1.20}$$

for all ρ. Thus f is countably additive. If $E_1 \leqslant E_2$, then

$$0 \leqslant \operatorname{tr}(g(\rho)(E_2 - E_1)) \tag{1.21}$$

$$= \operatorname{tr}(\rho f(E_2 - E_1)), \tag{1.22}$$

so $f(E_1) \leqslant f(E_2)$. It then follows that the f_i are convex.[6] By symmetry, the same argument shows that the g_i are convex.

The map g_A is known as a **partial trace**. The partial trace over B of $\rho_A \otimes \rho_B$ is

$$g_A(\rho) = \operatorname{tr}_B(\rho_A \otimes \rho_B) \equiv \rho_A \operatorname{tr} \rho_B = \rho_A, \tag{1.23}$$

and is extended linearly to combinations of product states.

1.3   Closed dynamics

Now that we have described the composition of quantum systems, how do they change in time? We are often interested in the case where the information held by the quantum state does not change. This is called a **closed** quantum system. While all isolated physical systems are thought to correspond to closed quantum systems, the converse is not true. For example, atomic spins subject to external control from lasers are still closed systems.

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[6]The argument is the same as that for the real linearity of a probability measure on effects given in [2].

The change in a closed system is the result of an operation $\mathcal{O}$ with a single, definite outcome. The operation $\mathcal{O}$ is convex by eq. (1.13). Since the information in the state ρ cannot change, $\mathcal{O}$ must be invertible. Kadison's theorem [7] states that all such operations have the form

$$\mathcal{O}\rho = U\rho U^\dagger, \tag{1.24}$$

where the operator U is either **unitary** ($U^\dagger U = 1$) or **antiunitary** ($U^\dagger U = -1$) [5, 8].

In contexts like quantum computation or control, all that matters is the state before and after the operation. To consider the notion of an isolated physical system, we must relate the quantum state to the physical time. We then have an operator $U(t)$ which gives the state

$$\rho(t) = U(t)\rho(0)U^\dagger(t) \tag{1.25}$$

as a function of time. We expect that $U(t)$ changes continuously [8] and satisfies

$$U(t + t') = U(t)U(t') \tag{1.26}$$

for real t, t'. Then since $U(0) = 1$ is unitary, $U(t)$ is unitary. We would like a description of $U(t)$ that does not depend on time. This is provided by Stone's theorem [10], which states that there is a self-adjoint operator H such that

$$U(t) = e^{-iHt}. \tag{1.27}$$

This allows us to differentiate eq. (1.25) to find

$$\dot{\rho} = \dot{U}(t)\rho(0)U^\dagger(t) + U(t)\rho(0)\dot{U}^\dagger(t) \tag{1.28}$$

$$= -iH\big(U(t)\rho(0)U^\dagger(t)\big) + \big(U(t)\rho(0)U^\dagger(t)\big)iH \tag{1.29}$$

$$= -i[H, \rho], \tag{1.30}$$

which is known as the **Liouville** or **von Neumann equation**. [9]

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[7] Wigner's theorem on symmetries of pure states is a special case [5, p. 77]. Many similar results hold, such as that only unitary transformations preserve the entropy (relative or not) [6, 7].

[8] More precisely, $U(t)$ is **strongly continuous** if $\lim_{t \to t_0} U(t)|v\rangle = U(t_0)|v\rangle$ for all real t_0 and $|v\rangle \in \mathcal{H}$. Stone's theorem is novel since it allows us to consider the time derivative of $U(t)$, even though we only assume that the map $t \mapsto U(t)$ is strongly continuous. Von Neumann showed that the strong continuity requirement may be relaxed to only being weakly measurable [9].

[9] Equation (1.30) is given in **natural units** where $\hbar = c = \varepsilon_0 = m_e = 1$. Otherwise $\dot{\rho} = -i[H, \rho]/\hbar$.

Given an observable A, its expected value over time is

$$\langle A \rangle = \text{tr}(\rho(t)A) \tag{1.31}$$

$$= \text{tr}\left(U(t)\rho(0)U^\dagger(t)A\right) \tag{1.32}$$

$$= \text{tr}\left(\rho(0)U^\dagger(t)AU(t)\right). \tag{1.33}$$

This suggests that the state may be regarded as constant, while an observable changes in time as

$$A_H(t) = U^\dagger(t)AU(t). \tag{1.34}$$

This perspective is known as the **Heisenberg picture**, and leads to the analogous **Heisenberg equation of motion**

$$\dot{A}_H = -i[A_H, H] \tag{1.35}$$

for observables. For reference, the usual perspective where the state changes in time is known as the **Schrödinger picture**.

1.4 CANONICAL QUANTIZATION

The discussion of quantum theory thus far has been fully general. The Liouville equation (eq. (1.30)) specifies how a state ρ changes in time, given the Hilbert space for the system, the operator H, and the initial state $\rho(0)$. How does one determine these quantities for a particular physical system? We will only consider physical systems that can be modeled by nonrelativistic classical mechanics. Consider a classical system with generalized coordinates q_i and momenta p_i. If the system has classical Hamiltonian $H(\boldsymbol{q}, \boldsymbol{p})$, then Hamilton's equations of motion are

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = \{q_i, H\} \tag{1.36}$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = \{p_i, H\}, \tag{1.37}$$

in terms of the **Poisson bracket**

$$\{f, g\} = \sum_i \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i} \right). \tag{1.38}$$

We notice that Hamilton's equations are similar to the Heisenberg equations of motion

$$\dot{q}_i = -i[q_i, H] \tag{1.39}$$

$$\dot{p}_i = -i[p_i, H], \tag{1.40}$$

where the time-evolution operator H takes the place of the Hamiltonian. This suggests the idea of a quantization map Q that maps functions f and g on phase space to operators. We expect that $Q(1) = 1$, $Q(q_i) = q_i$ and $Q(p_i) = p_i$. Then to obtain the Heisenberg equations of motion we must require that

$$Q(\{f, g\}) = -i[Q(f), Q(g)]. \tag{1.41}$$

In particular, since $\{q_i, p_j\} = \delta_{ij}$, Q must yield the **canonical commutation relations** (CCRs)

$$[q_i, p_j] = i\delta_{ij}. \tag{1.42}$$

For the moment, consider a classical system with only one degree of freedom. [10] One can show that the only possible quantization for polynomials in q and p with degree less than four is the **Weyl quantization**. This simply averages over all possible operator orders. [11] For example,

$$Q(3qp^2) = qp^2 + pqp + p^2q. \tag{1.44}$$

What about a degree four polynomial like q^2p^2? One may compute that

$$q^2p^2 = \frac{1}{9}\{q^3, p^3\} = \frac{1}{3}\{q^2p, qp^2\}, \tag{1.45}$$

yet

$$\frac{1}{9}[Q(q^3), Q(p^3)] \neq \frac{1}{3}[Q(q^2p), Q(qp^2)], \tag{1.46}$$

so there is no quantization of q^2p^2. This result on the nonexistence of a general quantization map is known as Groenewold's theorem [12, p. 272]. Luckily, we will only consider systems where the Weyl quantization satisfies eq. (1.41), and we may put the issue of quantization aside.

Now we know that q and p must satisfy the CCR. But what are they? Weyl showed that q and p must be operators on an infinite-dimensional Hilbert space [13]. The usual assignment for square-integrable functions f is $qf(q) = qf(q)$ and $pf(q) = -if'(q)$, which

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[10] All the considerations to follow generalize naturally to many degrees of freedom.

[11] In general, the Weyl quantization of f is

$$Q(f) = \exp\left(\frac{1}{2i} \sum_i \frac{\partial^2}{\partial q_i \partial p_i}\right) \hat{f}(\boldsymbol{q}, \boldsymbol{p}), \tag{1.43}$$

where $\hat{f}$ is f in the normal form where q_i always precedes p_i [11].

satisfies the CCR. How do we know that this is the right assignment? What if one should assign a different Hilbert space $\mathcal{H}$ with other position and momentum operators q' and p'? By Stone's theorem, there are unitary operators $U(t) = e^{itq'}$ and $V(s) = e^{isp'}$. Then a formal application of the Baker-Campbell-Hausdorff (BCH) formula [12] gives that

$$U(t)V(s) = e^{-ist}V(s)U(t), \tag{1.48}$$

which is known as the Weyl relation [12, p. 281].[13] The Stone-von Neumann theorem[14] is that there is a unitary operator $T : L^2(\mathbb{R}) \to \mathcal{H}$ such that

$$T^{\dagger}U(t)T = e^{itq} \tag{1.49}$$

$$T^{\dagger}V(s)T = e^{isp}. \tag{1.50}$$

Differentiating and setting $t = s = 0$ then gives that

$$T^{\dagger}q'T = q \tag{1.51}$$

$$T^{\dagger}p'T = p. \tag{1.52}$$

Given a density operator ρ on $L^2(\mathbb{R})$, we may assign a density operator on $\mathcal{H}$ by $\rho' = T\rho T^{\dagger}$, which satisfies that

$$\text{tr}(\rho'q') = \text{tr}(\rho q) \tag{1.53}$$

$$\text{tr}(\rho'p') = \text{tr}(\rho p), \tag{1.54}$$

and similar for polynomials in p and q. Thus the predictions of quantum theory do not depend on the representation of a system's canonical coordinates, and we are justified in making the usual assignment for q and p.

1.5   Open dynamics

An **open system** is a quantum system where the information held by the quantum state may change. We will consider only open quantum systems that model interacting physical

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[12]Namely that if $[A, [A, B]] = [B, [A, B]] = 0$, then

$$e^A e^B = e^{A+B+[A,B]/2}. \tag{1.47}$$

[13]Since the Weyl relation was derived through a merely formal procedure, not all operators satisfying the CCR satisfy the Weyl relation. The usual q and p do satisfy the Weyl relation, so we may as well stipulate that any putative operators q' and p' must satisfy it as well.

[14]The Stone-von Neumann theorem was also used to prove the equivalence between the Schrödinger equation and Heisenberg's matrix mechanics.

systems. First, a larger closed system $\mathcal{H}$ is identified and separated into two subsystems: the open system $\mathcal{H}_S$ of interest and the environment or bath $\mathcal{H}_B$ that the open system interacts with. We know that the initial state of the open system is ρ_0. The system is said to follow **open dynamics** if the state at time t is determined by the following procedure.

1. The state ρ_0 is promoted to a state of the composite system according to an **assignment map** $\mathcal{A}(\rho_0)$. A consistent assignment map should have the following intuitive properties: [14]

    (a) $\mathcal{A}$ is convex,

    (b) $\text{tr}_B \mathcal{A}(\rho_0) = \rho_0$,

    (c) $\mathcal{A}(\rho_0)$ is a density operator.

2. The assigned composite state becomes $\rho(t) = U(t)\mathcal{A}(\rho_0)U^\dagger(t)$ as usual for a closed system.

3. The state $\rho(t)$ is reduced to give the open system state $\rho_S(t) = \text{tr}_B \rho(t)$.

In summary, the state at time t is

$$\rho_S(t) = \text{tr}_B(U(t)\mathcal{A}(\rho_0)U^\dagger(t)), \tag{1.55}$$

which we may express as the **dynamical map** $\mathcal{V}(t)\rho_S(0) = \rho_S(t)$. Note that property (b) of $\mathcal{A}$ ensures that $\rho_S(0) = \rho_0$, which is consistent.

One can show that the only consistent assignment maps for a two-dimensional system are of the form $\mathcal{A}(\rho_0) = \rho_0 \otimes \rho_B$, where ρ_B is a constant density operator on $\mathcal{H}_B$ [15]. We will consider ρ_B to be a stationary state of the bath, such as a thermal state at some temperature. Why do we not require that the composite state $\rho(t)$ is always assignable, remaining within the image of $\mathcal{A}$? This would make $\mathcal{V}$ satisfy that

$$\mathcal{V}(t+s) = \mathcal{V}(t)\mathcal{V}(s). \tag{1.56}$$

Since ρ_B does not change in time, this requires that the system does not interact with the bath. The only allowed open systems would be closed systems! What is wrong with requiring the composite state to be assignable? The issue is that interactions will inevitably entangle the system with the bath, causing one to be unable to consider the composite as the two subsystems in the product assignment.

However, we are interested in the reduced dynamics of the system, and what happens on the timescale τ_R where the system changes appreciably. If the timescale of the correlations in the bath is τ_C, then from the perspective of a system with $\tau_C \ll \tau_R$, the bath is

effectively stationary. Thus $\rho(t)$ is approximately assignable if we only aim to consider the coarse-grained system dynamics. The notion of reduced dynamics only makes sense on system timescales, and requires several conditions on eq. (1.55) for the coarse-graining to be possible. Since the system must be weakly coupled to the bath for the bath to remain approximately stationary, these simplifications are collectively called the **weak-coupling limit**.

This process will lead to a differential equation (eq. (1.83)) for ρ_S. It is worth mentioning that this equation, known as the Lindblad equation, is in the general form for any map $\mathcal{V}(t)$ on density matrices that satisfies eq. (1.56), with the technical condition that it is also completely positive.[15] On these grounds, it is often asserted that all reduced dynamics must be completely positive. This is not the case if the initial condition of the composite system is not a product state, and we have argued that the notion of reduced dynamics does not make sense outside of the weak-coupling limit. The debate concerning complete positivity remains a contentious issue [15, 17, 18].

1.6   The weak-coupling limit

We will now determine the conditions on the Hamiltonian of the composite system that give rise to reduced dynamics when the bath is in an equilibrium state ρ_B. We decompose the Hamiltonian as

$$H = H_0 + H_I \tag{1.57}$$
$$= H_S \otimes 1 + 1 \otimes H_B + H_I, \tag{1.58}$$

where H_S is the Hamiltonian of the system, H_B is the Hamiltonian of the bath, and H_I is the interaction Hamiltonian between the system and the bath. First, we will recast the dynamics of the composite system into a convenient form. Recall the Heisenberg picture from section 1.3. Given eq. (1.57), we may similarly decompose the expected value of an observable A for the composite system. If we let

$$U_0(t) = e^{-iH_0 t} \tag{1.59}$$
$$U_I(t) = U_0^\dagger(t)U(t), \tag{1.60}$$

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[15]For any Hilbert space $\mathcal{H}'$, define the combined operation $\mathcal{V}(t) \otimes \mathbb{1}$ by $(\mathcal{V}(t) \otimes \mathbb{1})(A \otimes B) = \mathcal{V}(t)A \otimes B$ and extending linearly. We say that $\mathcal{V}(t)$ is **completely positive** if $(\mathcal{V}(t) \otimes \mathbb{1})(C)$ is positive for every positive operator C on $\mathcal{H}_S \otimes \mathcal{H}'$ [16, p. 89].

then we may decompose the expected value as

$$\langle A \rangle = \text{tr}\Big(A U(t) \rho(0) U^\dagger(t) \Big) \tag{1.61}$$

$$= \text{tr}\Big(U_0^\dagger(t) A U_0(t) \, U_I(t) \rho(0) U_I^\dagger(t) \Big). \tag{1.62}$$

This suggests that we define the time-dependent operators

$$A_I(t) = U_0^\dagger(t) A U_0(t) \tag{1.63}$$

$$\rho_I(t) = U_I(t) \rho(0) U_I^\dagger(t). \tag{1.64}$$

This perspective is known as the **interaction picture**, and the associated equation of motion is

$$\dot\rho_I = -\mathrm{i}[H_I, \rho_I]. \tag{1.65}$$

We will use eq. (1.65) in its integral form

$$\rho_I(t) = \rho_I(0) - \mathrm{i} \int_0^t \mathrm{d}s \, [H_I(s), \rho_I(s)]. \tag{1.66}$$

It will also be helpful to relate the interaction Hamiltonian to transition frequencies of the system as follows. [16] First, we write a general interaction Hamiltonian as

$$H_I = \sum_\alpha A_\alpha \otimes B_\alpha. \tag{1.67}$$

If E is an eigenvalue of H_S, let $\Pi(E)$ denote the projector onto the eigenspace for E. Now we let

$$A_\alpha(\omega) = \sum_{E'-E=\omega} \Pi(E) A_\alpha \Pi(E'). \tag{1.68}$$

By the completeness of the energy projectors,

$$\sum_\omega A_\alpha(\omega) = \sum_\omega \sum_{E'-E=\omega} \Pi(E) A_\alpha \Pi(E') \tag{1.69}$$

$$= \sum_{E_1, E_2} \Pi(E_1) A_\alpha \Pi(E_2) \tag{1.70}$$

$$= A_\alpha. \tag{1.71}$$

The $A_\alpha(\omega)$ also satisfy that

$$[H_S, A_\alpha(\omega)] = -\omega A_\alpha(\omega). \tag{1.72}$$

---

[16]This decomposition requires that the spectrum of H_S is discrete.

Using eq. (1.72) to commute past the exponential in eq. (1.63) establishes that the corresponding interaction picture operators are

$$A_\alpha^I(\omega) = e^{-i\omega t} A_\alpha(\omega). \tag{1.73}$$

Thus the interaction Hamiltonian in the interaction picture is

$$H_I(t) = \sum_{\alpha\omega} e^{-i\omega t} A_\alpha(\omega) \otimes B_\alpha^I(t), \tag{1.74}$$

where by eq. (1.63)

$$B_\alpha^I(t) = e^{iH_B t} B_\alpha e^{-iH_B t}. \tag{1.75}$$

Since we are interested in how fluctuations in different environment modes are related, we will consider the **reservoir correlation functions**

$$\left\langle B_\alpha^\dagger(t) B_\beta(t-s) \right\rangle \tag{1.76}$$

and their one-sided Fourier transform

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty ds\, e^{i\omega s} \left\langle B_\alpha^\dagger(t) B_\beta(t-s) \right\rangle \tag{1.77}$$

$$\equiv i S_{\alpha\beta}(\omega) + \gamma_{\alpha\beta}(\omega)/2, \tag{1.78}$$

where the corresponding matrix $S = (\Gamma - \Gamma^\dagger)/2i$ is Hermitian and the matrix corresponding to the full Fourier transform

$$\gamma_{\alpha\beta}(\omega) \equiv \int_{-\infty}^\infty ds\, e^{i\omega s} \left\langle B_\alpha^\dagger(t) B_\beta(t-s) \right\rangle \tag{1.79}$$

is positive.

With this setup, we may now move to the main derivation. Applying eq. (1.65) to eq. (1.66) and tracing out the environment gives the closed equation

$$\dot{\rho}_S(t) = -\int_0^t ds\, \mathrm{tr}_B\left[H_I(t), [H_I(s), \rho_S(s) \otimes \rho_B] \right]$$

for the system density operator. In doing so we have made two assumptions: that

$$\mathrm{tr}_B\left[H_I(t), \rho(0) \right] = 0,$$

which is the **weak-coupling approximation**, and that

$$\rho(t) = \rho_S(t) \otimes \rho_B,$$

which is the **Born approximation**. It should be noted that weak-coupling follows if the reservoir averages of the interactions vanish: $\langle B_\alpha(t) \rangle = 0$.

We now make the **Markov approximation** that $\rho_S(s) = \rho_S(t)$, so that the time-evolution only depends on the present time, to obtain the **Redfield equation**. To simplify further, we make the substitution $s \mapsto t - s$ and set the upper limit of the integral to infinity:

$$\dot{\rho}_S = -\int_0^\infty ds \, \mathrm{tr}_B \left[H_I(t), [H_I(t - s), \rho_S(t) \otimes \rho_B] \right]. \tag{1.80}$$

This is justified when the reservoir correlation functions in eq. (1.77) vanish quickly over a time τ_C that is smaller than the relaxation time τ_R. Substituting eq. (1.74) into eq. (1.80) and using eq. (1.77) gives

$$\dot{\rho}_S = 2 \, \mathrm{He} \sum_{\alpha\beta\omega\omega'} e^{i(\omega' - \omega)t} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_S A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega') A_\beta(\omega) \rho_S \right), \tag{1.81}$$

where $\mathrm{He} \, C \equiv (C + C^\dagger)/2$. If the typical times

$$\tau_S = |\omega' - \omega|^{-1} \quad \text{for} \quad \omega' \neq \omega$$

for system evolution are small compared to the relaxation time τ_R, then the contribution from the fast-oscillating terms of eq. (1.81) where $\omega' \neq \omega$ may be neglected. This **rotating wave** or **secular approximation** is analogous to how we consider the high-energy position distribution in the infinite square well to be uniform, even though it is actually a fast-oscillating function. By coarse-graining in this sense, we obtain

$$\dot{\rho}_S = 2 \, \mathrm{He} \sum_{\alpha\beta\omega} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_S A_\alpha^\dagger(\omega) - A_\alpha^\dagger(\omega) A_\beta(\omega) \rho_S \right). \tag{1.82}$$

Now applying the decomposition eq. (1.78) gives the interaction picture **Lindblad equation**

$$\dot{\rho}_S = -i[H_{LS}, \rho_S] + \mathcal{D}(\rho_S), \tag{1.83}$$

where the **Lamb shift Hamiltonian** is

$$H_{LS} = \sum_{\alpha\beta\omega} S_{\alpha\beta}(\omega) A_\alpha^\dagger(\omega) A_\beta(\omega), \tag{1.84}$$

and the **dissipator** is

$$\mathcal{D}(\rho_S) = \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_S A_\alpha^\dagger(\omega) - \frac{1}{2} \left\{ A_\alpha^\dagger(\omega) A_\beta(\omega), \rho_S \right\} \right). \tag{1.85}$$

To transform back to the Schrödinger picture, one only needs to add the system Hamiltonian H_S to H_{LS}. One may then diagonalize $\gamma_{\alpha\beta}$ to put eq. (1.83) into the standard form of eq. (A.17). In our examples $\gamma_{\alpha\beta}$ will already be diagonal. In this case, we call the operators defined by eq. (1.72) in the dissipator the **jump operators** of the open system.

1.7 RELAXATION TO THERMAL EQUILIBRIUM

If the bath is in the **thermal state**

$$\rho_B = \frac{e^{-\beta H_B}}{\operatorname{tr} e^{-\beta H_B}}, \tag{1.86}$$

then we expect that the system will generally relax from any initial configuration to the thermal state

$$\rho_{\text{th}} = \frac{e^{-\beta H_S}}{\operatorname{tr} e^{-\beta H_S}}. \tag{1.87}$$

We will now prove that ρ_{th} is a stationary state. First, we see that the Lamb shift Hamiltonian commutes with the system Hamiltonian, since eq. (1.72) implies that

$$[H_S, A_\alpha^\dagger(\omega)A_\beta(\omega)] = 0. \tag{1.88}$$

Thus ρ_{th} is unchanged by the unitary part of $\mathcal{L}$, and may turn our attention towards showing that $\mathcal{D}(\rho_{\text{th}}) = 0$. We may also use eq. (1.72) to find that

$$\rho_{\text{th}}A_\alpha(\omega) = e^{\beta\omega}A_\alpha(\omega)\rho_{\text{th}} \tag{1.89}$$

$$\rho_{\text{th}}A_\alpha^\dagger(\omega) = e^{-\beta\omega}A_\alpha^\dagger(\omega)\rho_{\text{th}}. \tag{1.90}$$

The reservoir correlation functions obey the **KMS condition** [19, 20]

$$\left\langle B_\alpha^\dagger(t)B_\beta(0)\right\rangle = \left\langle B_\beta(0)B_\alpha^\dagger(t + i\beta)\right\rangle. \tag{1.91}$$

From eq. (1.91) it follows that

$$\gamma_{\alpha\beta}(-\omega) = e^{-\beta\omega}\gamma_{\beta\alpha}(\omega). \tag{1.92}$$

We may then use eqs. (1.89), (1.90) and (1.92) to compute that the dissipator is

$$\mathcal{D}(\rho_{\text{th}}) = \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega)\left(A_\beta(\omega)\rho_{\text{th}}A_\alpha^\dagger(\omega) - \frac{1}{2}\left\{A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_{\text{th}}\right\}\right) \tag{1.93}$$

$$= \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega)\left(e^{-\beta\omega}A_\beta(\omega)A_\alpha^\dagger(\omega) - \frac{1}{2}A_\alpha^\dagger(\omega)A_\beta(\omega) - \frac{1}{2}A_\alpha^\dagger(\omega)A_\beta(\omega)\right)\rho_{\text{th}} \tag{1.94}$$

$$= \left(\sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega)e^{-\beta\omega}A_\beta(\omega)A_\alpha^\dagger(\omega) - \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega)A_\alpha^\dagger(\omega)A_\beta(\omega)\right)\rho_{\text{th}} \tag{1.95}$$

$$= 0. \tag{1.96}$$

Thus $\dot{\rho}_{\text{th}} = 0$.

CHAPTER 2

APPLICATION TO INTERACTING SPINS

With the preceeding theory of open quantum systems in place, we are now in a position to consider the central problem of this thesis: How do interacting spins relax to thermal equilibrium? We will approach this question in stages, starting with a single spin.

2.1   THE CLOSED TWO-DIMENSIONAL SYSTEM

Our first task is to characterize the closed dynamics of the two-dimensional quantum system. An arbitrary two-dimensional density operator may be expressed in terms of the identity operator $1 \equiv \sigma^0$ and **Pauli operators** σ^a that satisfy the commutation relations

$$\left[\sigma^a, \sigma^b\right] = 2i\varepsilon_{abc}\sigma^c, \tag{2.1}$$

where ε_{abc} is the Levi-Civita symbol. These will be abbreviated as a single vector $\boldsymbol{\sigma}$. Then a **Bloch vector** $\boldsymbol{v}$ with $|\boldsymbol{v}| \leqslant 1$ determines the density operator

$$\rho = \frac{1}{2}(1 + \boldsymbol{v} \cdot \boldsymbol{\sigma}). \tag{2.2}$$

The expectation values of the Pauli operators are $\langle \boldsymbol{\sigma} \rangle = \boldsymbol{v}$, so it suffices to determine the time evolution of $\boldsymbol{v}$. A similar vector $\boldsymbol{\omega}$ determines the general Hamiltonian [1]

$$H = \frac{1}{2}\boldsymbol{\omega} \cdot \boldsymbol{\sigma}. \tag{2.3}$$

---

[1]If the Hamiltonian $H = E1 + H_0$ includes an energy shift E, the corresponding unitary operator is $U(t) = e^{-itE}U_0(t)$. Then $U(t)\rho U^\dagger(t) = U_0(t)\rho U_0^\dagger(t)$, so there is no difference.

The Liouville equation (eq. (1.30)) is then

$$\dot{\rho} = -\frac{i}{4}[\boldsymbol{\omega} \cdot \boldsymbol{\sigma}, \boldsymbol{v} \cdot \boldsymbol{\sigma}] \tag{2.4}$$

$$\frac{1}{2}\dot{\boldsymbol{v}} \cdot \boldsymbol{\sigma} = \frac{1}{2}(\boldsymbol{\omega} \times \boldsymbol{v}) \cdot \boldsymbol{\sigma}, \tag{2.5}$$

so the Bloch vector follows the differential equation

$$\dot{\boldsymbol{v}} = \boldsymbol{\omega} \times \boldsymbol{v}. \tag{2.6}$$

The solution of this equation is

$$\boldsymbol{v}(t) = e^{-t\boldsymbol{\omega} \cdot \boldsymbol{L}}\boldsymbol{v}(0), \tag{2.7}$$

where the components of $\boldsymbol{L}$ are generators of three-dimensional rotations which satisfy the commutation relations

$$\left[L^a, L^b\right] = \varepsilon_{abc}L^c. \tag{2.8}$$

Thus the most general time evolution for the two-dimensional system is precession of the Bloch vector around $\hat{\boldsymbol{\omega}}$ with angular frequency ω.

2.2   RELAXATION OF THE TWO-DIMENSIONAL SYSTEM

Now what happens when a two-dimensional system is coupled to a thermal bath? The most relevant application is the electronic states of an atom coupled to the electromagnetic field. We will approximate the atom as just two energy levels: a ground and first excited state. For simplicity we will consider the system Hamiltonian

$$H_S = \frac{\omega}{2}\sigma^z, \tag{2.9}$$

where ω is the frequency of light emitted from the transition. The weak-coupling limit for the electric dipole interaction with the bath is similar to that for the magnetic dipole interaction considered later in section 2.4, so will simply state the results here and focus on investigating the dynamics.[2] To focus on the relaxation of the system, we ignore the Lamb shift and consider only the effect of the dissipator. The jump operators are

$$\sigma^{\pm} = \frac{\sigma^x \pm i\sigma^y}{2} \tag{2.10}$$

---

[2]A full derivation is given in [16, pp. 141–149].

and the Lindblad equation is

$$\dot{\rho} = \gamma_0(N+1)\left(\sigma^-\rho\sigma^+ - \frac{1}{2}\{\sigma^+\sigma^-, \rho\}\right) + \gamma_0 N\left(\sigma^+\rho\sigma^- - \frac{1}{2}\{\sigma^-\sigma^+, \rho\}\right), \tag{2.11}$$

where

$$\gamma_0 = \frac{4}{3}\omega^3|\boldsymbol{d}|^2, \quad N = \frac{1}{e^{\beta\omega}-1}, \tag{2.12}$$

and $\boldsymbol{d}$ is the transition matrix element of the dipole operator from the excited to ground state. Equation (2.11) describes stimulated emission with rate $\gamma_0 N$, spontaneous emission with rate γ_0, and absorption with rate $\gamma_0 N$. Substituting the density operator in the form of eq. (2.2) into the Lindblad equation gives the differential equations

$$\dot{v}_x = -\frac{\gamma}{2}v_x, \tag{2.13}$$

$$\dot{v}_y = -\frac{\gamma}{2}v_y, \tag{2.14}$$

$$\dot{v}_z = -\frac{\gamma}{2}v_z - \gamma_0, \tag{2.15}$$

where the total transition rate is

$$\gamma = \gamma_0(2N+1). \tag{2.16}$$

The equilibrium solution is seen to be

$$v_x = v_y = 0 \quad \text{and} \quad v_z = -\frac{1}{2N+1}, \tag{2.17}$$

so the stationary population of the excited state is

$$n_e^{\text{th}} = \frac{1}{2}(1+v_z) = \frac{N}{2N+1}. \tag{2.18}$$

From the initial state $\boldsymbol{v}(0) = \hat{z}$, we see that the population explicitly approaches the thermal equilibrium value as

$$n_e(t) = n_e^{\text{th}}(1 - e^{-\gamma t}). \tag{2.19}$$

2.3 The transverse-field Ising chain

We now move to studying interacting spins. Of the many interacting spin models to study, the **transverse-field Ising model**[3]

$$H = -J\sum_{i\in\mathbb{Z}_N}\left(S_i^x S_{i+1}^x + \frac{g}{2}S_i^z\right) \tag{2.20}$$

---

[3]The translation to Pfeuty's constants is $g = \lambda^{-1} = J/2\Gamma$ [21].

is an interesting candidate because it undergoes a so-called quantum phase transition. The model is that N spins with an anisotropic nearest-neighbor interaction in the x-direction are subject to an external magnetic field in the z-direction. We impose periodic boundary conditions so that $\sigma_N^a = \sigma_0^a$. The parameter g characterizes the strength of the magnetic field relative to the interaction energy J. Taking iron for reference, [4] the interaction energy for two electron spins $a = 1\,\text{Å}$ apart is [22, p. 292]

$$J_e = \frac{\mu_e^2 \mu_0}{4\pi a^3} \approx 0.05\,\text{meV}, \tag{2.21}$$

while the corresponding exchange energy is around [23, p. 325]

$$J \approx \frac{1}{2} k_B T_c \approx 45\,\text{meV}. \tag{2.22}$$

The solution of this model is straightforward but somewhat involved, so it is given in appendix B. The idea is to formally transform the interacting spins into free fermions. Each of the N free fermion modes may be occupied or not, and is indexed by numbers k that are evenly spaced across the interval the first Brillouin zone $[-\pi, \pi]$ (according to eq. (B.30)). Each mode has energy

$$E_k = \sqrt{g^2 + 2g\cos k + 1} \tag{2.23}$$

relative to $J/2$, so the total energy in a given occupation state $|n\rangle\langle n|$ is

$$E = \sum_k n_k E_k, \tag{2.24}$$

where each $n_k \in \{0, 1\}$. Since setting only one $n_k = 1$ excites a single mode from the ground state, eq. (2.23) also gives the energies of elementary excitations from the ground state. It is plotted for different values of g in fig. 2.1.

```
isings = [1.5, 1.0, 0.5]'
plot([k → √(1 + g^2 + 2g*cos(π - k)) for g in isings], xlim=(-1.0π, 1.0π),
    legendtitle=L"g", label=[L"%$g" for g in isings], legend=:bottomright,
    xlabel=L"\pi - k", ylabel=L"E_k")
```

---

[4] α-Fe has $T_c = 1044\,\text{K}$.
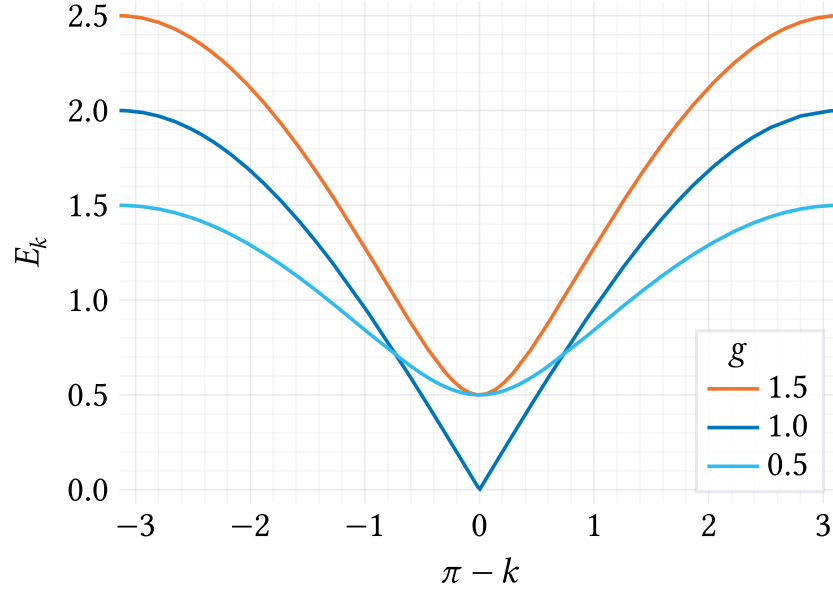
Figure 2.1: Elementary excitation spectra of the transverse-field Ising model across g.

From this, Pfeuty [21] has shown that the ground state in the continuum limit has

$$\langle \sigma_i^z \rangle = G(0) \tag{2.25}$$

$$\langle \sigma_i^z \sigma_{i+n}^z \rangle = -G(n)G(-n), \tag{2.26}$$

where

$$G(n) = L(n) + \frac{1}{g}L(n+1) \tag{2.27}$$

$$L(n) = \frac{1}{\pi} \int_0^\pi \mathrm{d}k \, \frac{\cos(kn)}{E_k}. \tag{2.28}$$

Pfeuty's $\langle \sigma_i^z \rangle$ is shown in fig. 2.2. Similar investigation of eq. (2.26) shows evidence of a quantum phase transition at zero temperature.

- For $0 \leqslant g < 1$, the system is in a ferromagnetic ordered phase. The exchange interaction dominates and in the extreme case when $g = 0$, all spins align along the x-axis, giving the ground state twofold degeneracy.

- For $g = 1$, the system is said to undergo a quantum phase transition. The energy gap for excitations in fig. 2.1 vanishes.

- For $g > 1$, the system is in a disordered phase. The transverse field dominates and in the extreme case where $g \to \infty$, all spins are aligned with the field along the z-axis.
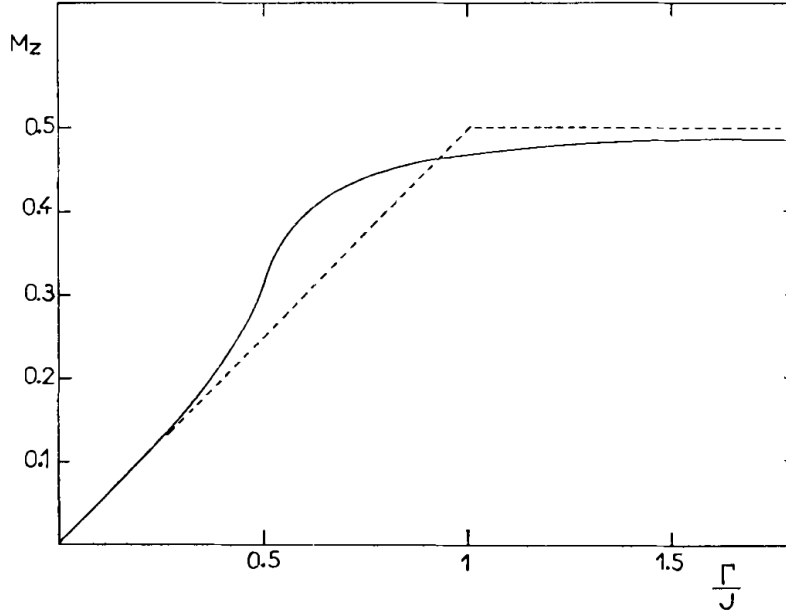
Figure 2.2: $M_z = \langle \sigma_i^z \rangle / 2$ as a function of $g/2 = \Gamma/J$ [21]. The dotted line is the result from mean-field theory. *Reprinted under STM guidelines [24].*

2.4   THE WEAK-COUPLING LIMIT FOR THE ISING CHAIN

Does the presence of a quantum critical point influence the relaxation of the Ising spin chain at finite temperature, where the phase transition vanishes? What about at zero temperature, where the system may still relax due to interactions with the electromagnetic vacuum? To approach these questions, we carry out the weak-coupling limit for magnetic dipole interactions with the electromagnetic field as the bath.

Before we begin, the system Hamiltonian eq. (2.20) requires modification. We would like to study the effect of varying the parameter g on the relaxation rate of the open system. This means that we must be able to compare the rates for two system Hamiltonians H_1 and H_2. However, we are not interested in the absolute rate, but rather the rate relative to the time scale of the system. For example, if $H_2 = 2H_1$, then a system with H_2 will relax at a different rate than one with H_1. Both Hamiltonians describe the same dynamics at different time scales. Therefore, we first need to normalize the Hamiltonians with a map $\mathcal{N}$ such that

$$\mathcal{N}(H_S) = \mathcal{N}(\alpha H_S) \tag{2.29}$$

for $\alpha > 0$. A related problem with eq. (2.20) is that we must consider $g \to \infty$ which causes the system energy to diverge. To enable comparison between different values of

g, it would be convenient to consider a parameter in the interval $[0, 1]$. Both of these problems are solved by an appropriate interpolation between the extremal Hamiltonians

$$H_x = -\sum_{i\in\mathbb{Z}_N} \sigma_i^x \sigma_{i+1}^x \quad \text{and} \quad H_z = -\sum_{i\in\mathbb{Z}_N} \sigma_i^z \tag{2.30}$$

of the form

$$H_S = -J(g) \sum_{i\in\mathbb{Z}_N} \left(f(1-g)\sigma_i^x \sigma_{i+1}^x + f(g)\sigma_i^z \right). \tag{2.31}$$

The map $\mathcal{N}$ is implemented by the normalization $J(g)$ and the compactification is implemented by the function $f(g)$. A natural choice is to redefine g and use spherical linear interpolation to rotate between H_x and H_z with

$$H_S = -\sqrt{|H_x|\cdot|H_z|}\left(\frac{\sin((1-g)\theta)}{\sin\theta}\hat{H}_x + \frac{\sin(g\theta)}{\sin\theta}\hat{H}_z \right), \quad 0 \leqslant g \leqslant 1, \tag{2.32}$$

where a normalized operator $\hat{A} = A/|A|$ and the angle θ between H_x and H_z are defined with respect to the inner product

$$\langle A|B\rangle = \text{tr}\left(A^\dagger B\right). \tag{2.33}$$

An overall magnitude $\sqrt{|H_x|\cdot|H_z|}$ is reintroduced so that systems with diffent numbers of spins may be more easily compared below.

Now we may add in the interaction with the bath. The field Hamiltonian is

$$H_B = \sum_{k,\lambda} \omega_k a_{k,\lambda}^\dagger a_{k,\lambda}, \tag{2.34}$$

which is a collection of harmonic oscillators: one for each wavenumber k and polarization λ of photons that make up the electromagnetic field. The vacuum energy $\sum_{k,\lambda}\omega_k/2$ is dropped, since it diverges in the continuum limit.

The interaction Hamiltonian for electron spins in a magnetic field is [5]

$$H_I = -\int \mathrm{d}r\, \boldsymbol{\mu} \cdot \boldsymbol{B} \tag{2.35}$$

$$= -\int \mathrm{d}r \sum_i \mu_e \delta(r_i)\boldsymbol{\sigma}_i$$
$$\cdot \, \mathrm{i}\sum_{k,\lambda} \sqrt{\frac{1}{2V\omega_k}}\left((k\times e_{k,\lambda})e^{\mathrm{i}k\cdot r}a_{k,\lambda} - \left(k\times e_{k,\lambda}^*\right)e^{-\mathrm{i}k\cdot r}a_{k,\lambda}^\dagger \right) \tag{2.36}$$

$$= -\sum_{i,\mu} \sigma_i^\mu B_i^\mu, \tag{2.37}$$

---

[5]An electron has spin $s = 1/2$ and g-factor $g_e \approx 2$, so its magnetic moment $\mu_e = sg\mu_B$ is approximately the Bohr magneton μ_B. The time dependence of the field is absorbed into the operators $a_{k,\lambda}$, and the prefactor is chosen so that these operators are dimensionless, but $\boldsymbol{B}$ is not.

where the components of the **magnetic field operator** evaluated at r_i are [6]

$$B_i^\mu = i\mu_e \sum_{k,\lambda} \sqrt{\frac{1}{2V\omega_k}} \left(\left(k \times e_{k,\lambda} \right)_\mu e^{ik\cdot r_i} a_{k,\lambda} - \left(k \times e_{k,\lambda}^* \right)_\mu e^{-ik\cdot r_i} a_{k,\lambda}^\dagger \right). \tag{2.38}$$

This magnetic field operator includes the electron's magnetic moment so that the final rate γ (eq. (2.69)) carries the dimensions of frequency in the dissipator (eq. (1.85)).

To summarize, the composite Hamiltonian that we will study is

$$H = H_S \otimes 1 + 1 \otimes H_B + H_I \tag{2.39}$$

$$= -J(g) \sum_{i\in\mathbb{Z}_N} \left(f(1-g)\sigma_i^x \sigma_{i+1}^x + f(g)\sigma_i^z \right) \otimes 1 + 1 \otimes \sum_{k,\lambda} \omega_k a_{k,\lambda}^\dagger a_{k,\lambda} - \sum_{i,\mu} \sigma_i^\mu \otimes B_i^\mu,$$

$$\tag{2.40}$$

where

- $J(g) > 0$ for $0 \leqslant g \leqslant 1$,

- $f(g)$ is monotonic for $0 \leqslant g \leqslant 1$, $f(0) = 0$, and $f(1) = 1$, like for $f(g) = g$,

- The bath is a 3D continuum of modes according to eq. (2.55),

- The spin positions in eq. (2.38) are $r_i = ai\hat{z}$ for some spacing a,

- The dipole approximation is valid. This requires that $a \ll c/\omega_k$ for ω_k up to the largest transition energy possible for H_S.

We will later nondimensionalize energy and time with respect to the system energy scale $J(g)$ so that the rates γ and S in the Lindblad equation (eq. (1.83)) are relative to the system timescale $\tau_S = 1/J(g)$.

In the interaction picture:

$$B_i^\mu(t) = e^{iH_Bt} B_i^\mu e^{-iH_Bt} \tag{2.41}$$

$$= i\mu_e \sum_{k,\lambda} \sqrt{\frac{1}{2V\omega_k}} \left(\left(k \times e_{k,\lambda} \right)_\mu e^{i(k\cdot r_i - \omega_k t)} a_{k,\lambda} - \left(k \times e_{k,\lambda}^* \right)_\mu e^{-i(k\cdot r_i - \omega_k t)} a_{k,\lambda}^\dagger \right).$$

$$\tag{2.42}$$

---

[6]This operator arises from quantizing the electromagnetic field. See the discussion of field quantization in [25, p. 506] for more details.

The spectral correlation tensor is then

$$\Gamma_{i\mu,j\nu}(\omega) = \int_0^\infty ds\, e^{i\omega s} \left\langle B_i^\mu(t)^\dagger B_j^\nu(t-s) \right\rangle \tag{2.43}$$

$$= -\frac{\mu_e^2}{2V} \int_0^\infty ds \sum_{k,k',\lambda,\lambda'} \sqrt{\frac{1}{\omega_k \omega_{k'}}} \quad : $$

$$(k \times e_{k,\lambda})_\mu (k' \times e_{k',\lambda'})_\nu e^{i(k\cdot r_i - \omega_k t + k'\cdot r_j - \omega_{k'}(t-s)+\omega s)} \left\langle a_{k,\lambda} a_{k',\lambda'} \right\rangle$$

$$- (k \times e_{k,\lambda})_\mu (k' \times e_{k',\lambda'}^*)_\nu e^{i(k\cdot r_i - \omega_k t - k'\cdot r_j + \omega_{k'}(t-s)+\omega s)} \left\langle a_{k,\lambda} a_{k',\lambda'}^\dagger \right\rangle \tag{2.44}$$

$$- (k \times e_{k,\lambda}^*)_\mu (k' \times e_{k',\lambda'})_\nu e^{-i(k\cdot r_i - \omega_k t - k'\cdot r_j + \omega_{k'}(t-s)-\omega s)} \left\langle a_{k,\lambda}^\dagger a_{k',\lambda'} \right\rangle$$

$$+ (k \times e_{k,\lambda}^*)_\mu (k \times e_{k',\lambda'}^*)_\nu e^{-i(k\cdot r_i - \omega_k t + k'\cdot r_j - \omega_{k'}(t-s)-\omega s)} \left\langle a_{k,\lambda}^\dagger a_{k',\lambda'}^\dagger \right\rangle.$$

In the thermal state

$$\rho_B = \frac{e^{-\beta H_B}}{\operatorname{tr} e^{-\beta H_B}} = \prod_{k,\lambda} \left(1 - e^{-\beta \omega_k}\right) e^{-\beta \omega_k a_{k,\lambda}^\dagger a_{k,\lambda}} \tag{2.45}$$

Since $\left[a_{k,\lambda}, a_{k',\lambda'}^\dagger \right] = \delta_{kk'} \delta_{\lambda\lambda'} \mathbb{1}$,

$$\left\langle a_{k,\lambda}^\dagger a_{k',\lambda'} \right\rangle = \operatorname{tr}\!\left(e^{-\beta H_B}\right)^{-1} \operatorname{tr}\!\left(e^{-\beta H_B} a_{k,\lambda}^\dagger a_{k',\lambda'}\right) \tag{2.46}$$

$$= \operatorname{tr}\!\left(e^{-\beta H_B}\right)^{-1} \operatorname{tr}\!\left(e^{-\beta H_B} a_{k',\lambda'} a_{k,\lambda}^\dagger\right) - \delta_{kk'} \delta_{\lambda\lambda'} \tag{2.47}$$

$$= \operatorname{tr}\!\left(e^{-\beta H_B}\right)^{-1} \operatorname{tr}\!\left(e^{\beta \omega_k} a_{k',\lambda'} e^{-\beta H_B} a_{k,\lambda}^\dagger\right) - \delta_{kk'} \delta_{\lambda\lambda'} \tag{2.48}$$

$$= e^{\beta \omega_k} \left\langle a_{k,\lambda}^\dagger a_{k',\lambda'} \right\rangle - \delta_{kk'} \delta_{\lambda\lambda'} \tag{2.49}$$

$$= \delta_{kk'} \delta_{\lambda\lambda'} n_B(\omega_k), \tag{2.50}$$

where

$$n_B(\omega) = \frac{1}{e^{\beta \omega} - 1}. \tag{2.51}$$

Similarly,

$$\left\langle a_{k,\lambda} a_{k',\lambda'} \right\rangle = \left\langle a_{k,\lambda}^\dagger a_{k',\lambda'}^\dagger \right\rangle = 0 \tag{2.52}$$

$$\left\langle a_{k,\lambda} a_{k',\lambda'}^\dagger \right\rangle = \delta_{kk'} \delta_{\lambda\lambda'} (1 + n_B(\omega_k)). \tag{2.53}$$

Then for a thermal bath, the spectral correlation tensor becomes

$$\Gamma_{i\mu,j\nu}(\omega) = \frac{\mu_e^2}{2V} \int_0^\infty ds \sum_{k,\lambda} \frac{1}{\omega_k} \quad : $$

$$(k \times e_{k,\lambda})_\mu (k \times e_{k,\lambda}^*)_\nu e^{i(k\cdot(r_i - r_j)+s(\omega - \omega_k))}(1 + n_B(\omega_k)) \tag{2.54}$$

$$+ (k \times e_{k,\lambda}^*)_\mu (k \times e_{k,\lambda})_\nu e^{-i(k\cdot(r_i - r_j)-s(\omega+\omega_k))} n_B(\omega_k).$$

To evaluate eq. (2.54), we now consider a chain of N spins along the z-axis, so that $\boldsymbol{r}_i = r_i \hat{\boldsymbol{z}}$.[7]
Then $\boldsymbol{k} \cdot (\boldsymbol{r}_i - \boldsymbol{r}_j) = k_z \Delta r_{ij}$.

In the continuum limit,

$$\frac{1}{V} \sum_{\boldsymbol{k}} \mapsto \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3} = \frac{1}{(2\pi c)^3} \int_0^\infty \mathrm{d}\omega_k\, \omega_k^2 \int \mathrm{d}\Omega, \tag{2.55}$$

where the integral over solid angle is

$$\int \mathrm{d}\Omega = \int \mathrm{d}\phi \int \mathrm{d}\theta \sin\theta. \tag{2.56}$$

To apply this limit to eq. (2.54), we first note that

$$\sum_\lambda \left(\boldsymbol{k} \times \boldsymbol{e}_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k} \times \boldsymbol{e}_{\boldsymbol{k},\lambda}^*\right)_\nu = \sum_{abcd} \varepsilon_{\mu ab} \varepsilon_{\nu cd} k^a k^c \sum_\lambda e_{\boldsymbol{k},\lambda}^b \left(e_{\boldsymbol{k},\lambda}^d\right)^* \tag{2.57}$$

$$= \sum_{abcd} \varepsilon_{\mu ab} \varepsilon_{\nu cd} k^a k^c \left(\delta_{bd} - \frac{k^b k^d}{k^2}\right) \tag{2.58}$$

$$= \sum_{abc} \varepsilon_{\mu ab} \varepsilon_{\nu cb} k^a k^c \tag{2.59}$$

$$= \sum_{ac} \left(\delta_{\mu\nu} \delta_{ac} - \delta_{\mu c} \delta_{a\nu}\right) k^a k^c \tag{2.60}$$

$$= k^2 \delta_{\mu\nu} - k^\mu k^\nu. \tag{2.61}$$

Thus

$$\int \mathrm{d}\Omega\, e^{\pm i k_z \Delta r_{ij}} \sum_\lambda \left(\boldsymbol{k} \times \boldsymbol{e}_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k} \times \boldsymbol{e}_{\boldsymbol{k},\lambda}^*\right)_\nu = \frac{8\pi \omega_k^2}{3c^2} \delta_{\mu\nu} G_\nu\left(\frac{\omega_k \Delta r_{ij}}{c}\right), \tag{2.62}$$

where

$$G_\nu(u) = \left(\delta_{\nu z} - \frac{\delta_{\nu x} + \delta_{\nu y}}{2}\right) \frac{\operatorname{sinc} u - \cos u}{u^2} + \frac{\delta_{\nu x} + \delta_{\nu y}}{2} \operatorname{sinc} u. \tag{2.63}$$

Note that in the dipole approximation

$$\lim_{u \to 0} G_\nu(u) = \left(\delta_{\nu z} - \frac{\delta_{\nu x} + \delta_{\nu y}}{2}\right) \frac{1}{3} + \frac{\delta_{\nu x} + \delta_{\nu y}}{2} = \frac{1}{3}. \tag{2.64}$$

Now eq. (2.62) gives that the continuum limit of the spectral correlation tensor for the spin chain is

$$\Gamma_{i\mu,j\nu}(\omega) = \delta_{\mu\nu} \frac{1}{6\pi^2 \mu_e^2} \int_0^\infty \mathrm{d}\omega_k\, \omega_k^3 G_\nu\left(\frac{\omega_k \Delta r_{ij}}{c}\right) :$$

$$(1 + n_B(\omega_k)) \int_0^\infty \mathrm{d}s\, e^{is(\omega - \omega_k)} + n_B(\omega_k) \int_0^\infty \mathrm{d}s\, e^{is(\omega + \omega_k)}. \tag{2.65}$$

---

[7]We could consider any axis given the spherical symmetry, but the z-axis is the simplest to evaluate.

We now use that

$$n_B(-\omega) = -(1 + n_B(\omega)) \tag{2.66}$$

and

$$\int_0^\infty ds\, e^{-i\omega s} = \pi \delta(\omega) - i\mathcal{P}\frac{1}{\omega}, \tag{2.67}$$

where $\mathcal{P}$ denotes the Cauchy principal value, to find

$$\Gamma_{i\mu,j\nu}(\omega) = \frac{1}{2}\gamma_{i\mu,j\nu}(\omega) + iS_{i\mu,j\nu}(\omega), \tag{2.68}$$

where

$$\gamma_{i\mu,j\nu}(\omega) = \delta_{\mu\nu}\frac{\mu_e^2\omega^3}{3\pi}G_\nu\left(\frac{|\omega|\Delta r_{ij}}{c}\right)(1 + n_B(\omega)) \tag{2.69}$$

$$S_{i\mu,j\nu}(\omega) = \delta_{\mu\nu}\frac{\mu_e^2}{6\pi^2}\mathcal{P}\int_0^\infty d\omega_k\, \omega_k^3 G_\nu\left(\frac{\omega_k\Delta r_{ij}}{c}\right)\left(\frac{1 + n_B(\omega_k)}{\omega - \omega_k} + \frac{n_B(\omega_k)}{\omega + \omega_k}\right). \tag{2.70}$$

The dipole approximation then leaves

$$\gamma(\omega) = \frac{\mu_e^2\omega^3}{9\pi}(1 + n_B(\omega)) \tag{2.71}$$

for all spins and polarizations.

We will now nondimensionalize γ and S. Letting $\tilde{\gamma} = \gamma\tau_S$ and $\tilde{\omega} = \omega\tau_S$ gives

$$\tilde{\gamma}(\tilde{\omega}) = \left(\frac{\tau_0}{\tau_S}\right)^2 \tilde{\omega}^3\left(1 + \frac{1}{e^{\tau_B\tilde{\omega}/\tau_S} - 1}\right) \tag{2.72}$$

in terms of the thermal correlation time $\tau_B = \beta$ and the **vacuum magnetic timescale**

$$\tau_0 = \sqrt{\frac{\mu_e^2}{9\pi}} = 3.67 \times 10^{-23}\,\text{s}. \tag{2.73}$$

In the high-temperature limit where $\tau_B\tilde{\omega}/\tau_S \ll 1$, $\tilde{\gamma}$ becomes

$$\tilde{\gamma}(\tilde{\omega}) \approx \frac{\tau_0^2}{\tau_B\tau_S}\tilde{\omega}^2. \tag{2.74}$$

The other limit where $\tau_B\tilde{\omega}/\tau_S \gg 1$ motivates the definition of the typical zero-temperature decay rate

$$\tilde{\gamma}_0 = \lim_{\tau_B\to\infty}\tilde{\gamma}(1) = \left(\frac{\tau_0}{\tau_S}\right)^2. \tag{2.75}$$

What about $\tilde{S} = S\tau_S$? Applying the dipole approximation and letting $\tilde{\omega} = \omega\tau_S$ gives

$$\tilde{S}(\tilde{\omega}) = \frac{1}{2\pi}\left(\frac{\tau_0}{\tau_S}\right)^2 \mathcal{P} \int_0^\infty \mathrm{d}\tilde{\omega}_k\, \tilde{\omega}_k^3\left(\frac{1 + \tilde{n}_B(\tilde{\omega}_k)}{\tilde{\omega} - \tilde{\omega}_k} + \frac{\tilde{n}_B(\tilde{\omega}_k)}{\tilde{\omega} + \tilde{\omega}_k}\right), \tag{2.76}$$

where

$$\tilde{n}_B(\tilde{\omega}) = \frac{1}{e^{\tau_B\tilde{\omega}/\tau_S} - 1}. \tag{2.77}$$

To avoid the divergence of eq. (2.76), we introduce an upper frequency cutoff $\tilde{\Omega}$. Physically, one expects the coupling to high-frequency modes of the bath to weaken.[8] For simplicity, we just set the upper limit of the integral to $\tilde{\Omega}$, though other cutoffs like $e^{-\tilde{\omega}_k/\tilde{\Omega}}$ are common. As we will see, the exact functional form does not matter. If we set the frequency cutoff $\tilde{\Omega} \gg \tilde{\omega}$ to be far above any system frequency, we have the following limits.

- In the high-temperature limit where $\tau_B\tilde{\Omega}/\tau_S \ll 1$, $\tilde{S}$ simplifies to

$$\tilde{S}(\tilde{\omega}) \approx \frac{1}{2\pi}\frac{\tau_0^2}{\tau_B\tau_S}\mathcal{P}\int_0^{\tilde{\Omega}} \mathrm{d}\tilde{\omega}_k\, \tilde{\omega}_k^2\left(\frac{1}{\tilde{\omega} - \tilde{\omega}_k} + \frac{1}{\tilde{\omega} + \tilde{\omega}_k}\right) \tag{2.78}$$

$$= \frac{\tau_0^2}{\tau_B\tau_S}\frac{\tilde{\omega}}{\pi}\left(\tilde{\omega}\,\mathrm{atanh}\left(\frac{\tilde{\omega}}{\tilde{\Omega}}\right) - \tilde{\Omega}\right) \tag{2.79}$$

$$\approx -\frac{\tau_0^2}{\tau_B\tau_S}\frac{\tilde{\Omega}}{\pi}\tilde{\omega}. \tag{2.80}$$

- In the low-temperature limit where $\tau_B\tilde{\Omega}/\tau_S \gg 1$, $\tilde{S}$ simplifies to

$$\tilde{S}(\tilde{\omega}) \approx \frac{1}{2\pi}\left(\frac{\tau_0}{\tau_S}\right)^2 \mathcal{P}\int_0^{\tilde{\Omega}} \mathrm{d}\tilde{\omega}_k\, \frac{\tilde{\omega}_k^2}{\tilde{\omega} - \tilde{\omega}_k} \tag{2.81}$$

$$= -\frac{1}{2\pi}\left(\frac{\tau_0}{\tau_S}\right)^2\left(\frac{\tilde{\Omega}^2}{2} + \tilde{\Omega}\tilde{\omega} - \tilde{\omega}^2 \log\left(\frac{\tilde{\omega}}{\tilde{\Omega} - \tilde{\omega}}\right)\right) \tag{2.82}$$

$$\approx -\frac{1}{2\pi}\left(\frac{\tau_0}{\tau_S}\right)^2\left(\frac{\tilde{\Omega}^2}{2} + \tilde{\Omega}\tilde{\omega}\right). \tag{2.83}$$

In either case, the Lamb-shift Hamiltonian may be neglected since $\tilde{\Omega}\tau_0 \ll \tau_S$.

We may verify that the reservoir correlation functions do decay over a time scale that is much less than the relaxation time τ_R.[9] Recall that the rate $\gamma(\omega)$ is given by the Fourier transform of the reservoir correlation functions $\left\langle B_i^\mu(t)^\dagger B_j^\nu(t - s)\right\rangle$, which are constant in t

---

[8]This is not the case for the electromagnetic field, but in other contexts, one may view the bath as merely an effective model, and this cutoff is used to describe the effective interaction.

[9]Analogous results for the electric field are given in [16, p. 574].

and the same for all sites and polarizations. The correlation functions are then the inverse Fourier transform of γ:

$$\left\langle B_i^\mu(t)^\dagger B_j^\nu(t-s) \right\rangle = \frac{1}{2\pi} \int_{-\infty}^\infty d\omega \, e^{-i\omega s} \gamma(\omega). \tag{2.84}$$

Using the dimensionless time $\tilde{s} = s/\tau_S$ and introducing the parameter $\eta = \tau_B/\tau_S$, we find that

$$\frac{1}{\tau_S^2} \left\langle B_i^\mu(\tilde{s})^\dagger B_j^\nu(0) \right\rangle = \frac{1}{2\pi} \int_{-\infty}^\infty d\tilde{\omega} \, e^{-i\tilde{\omega}\tilde{s}} \tilde{\gamma}(\tilde{\omega}) \tag{2.85}$$

$$= \left(\frac{\tau_0}{\tau_S} \right)^2 \frac{\pi^3}{\eta^4} \sinh\left(\frac{\pi\tilde{s}}{\eta} \right)^{-4} \left(1 + 2\cosh\left(\frac{\pi\tilde{s}}{\eta} \right)^2 \right). \tag{2.86}$$

At low temperatures $\tilde{s} \ll \eta$ and

$$\frac{1}{\tau_S^2} \left\langle B_i^\mu(\tilde{s})^\dagger B_j^\nu(0) \right\rangle = \left(\frac{\tau_0}{\tau_S} \right)^2 \frac{3}{\pi\tilde{s}^4}, \tag{2.87}$$

while at high temperatures $\tilde{s} \gg \eta$ and

$$\frac{1}{\tau_S^2} \left\langle B_i^\mu(\tilde{s})^\dagger B_j^\nu(0) \right\rangle = \left(\frac{\tau_0}{\tau_S} \right)^2 \frac{8\pi^3}{\eta^4} e^{-2\pi\tilde{s}/\eta} \tag{2.88}$$

$$= \left(\frac{\tau_0^2}{\tau_B \tau_S} \right) \frac{8\pi^3}{\eta^3} e^{-2\pi\tilde{s}/\eta}. \tag{2.89}$$

Thus if $\tau_B \ll \tau_S$, the reservoir correlation time is $\tau_C = \tau_B/2\pi$, which is comparable to the thermal correlation time. In either case, the correlation functions decay quickly for $\tilde{s} > 1$. Since $\tau_S \ll \tau_R$, this establishes the validity of the Markov approximation.

CHAPTER 3

COMPUTING JUMP OPERATORS

Here we go.[1]

```
n = 5;
```

3.1 INTERPOLATING HAMILTONIANS

```
trnorm(A) = sum(svdvals(A)) # tr(√(A' * A))
trnormalize(A) = A / trnorm(A)
∠(A, B) = acos(tr(A' * B)) # For normalized A, B
function normslerp(A, B, g)
    a, b = trnorm(A), trnorm(B)
    A /= a
    B /= b
    θ = ∠(A, B)
    √(a * b) * trnormalize((sin((1-g)*θ)*A + sin(g*θ)*B) / sin(θ))
end
Hinterp(A, B) = g → normslerp(A, B, g);
```

---

[1]A spaghetti diagram [26].

Spaghetti Diagrams

The Ising interaction and transverse-field Hamiltonians are

```
Hx(n) = -sum(siteop(σx, i, n) * siteop(σx, i+1, n) for i in 1:n)
Hz(n) = -sum(siteop(σz, i, n) for i in 1:n)
Hint = Hinterp(Hx(n), Hz(n));

grange(points) = range(1e-3, 1-1e-3, length=points)
lgs = grange(64)
energies = [eigvals(Hint(g)) for g in lgs];
plot(lgs, hcat(energies...)', color=:black, alpha=0.25, key=false, xlabel=L"Hamiltonian
  ↪  parameter $g$", ylabel=L"Dimensionless energy $\tilde{E}$")
```
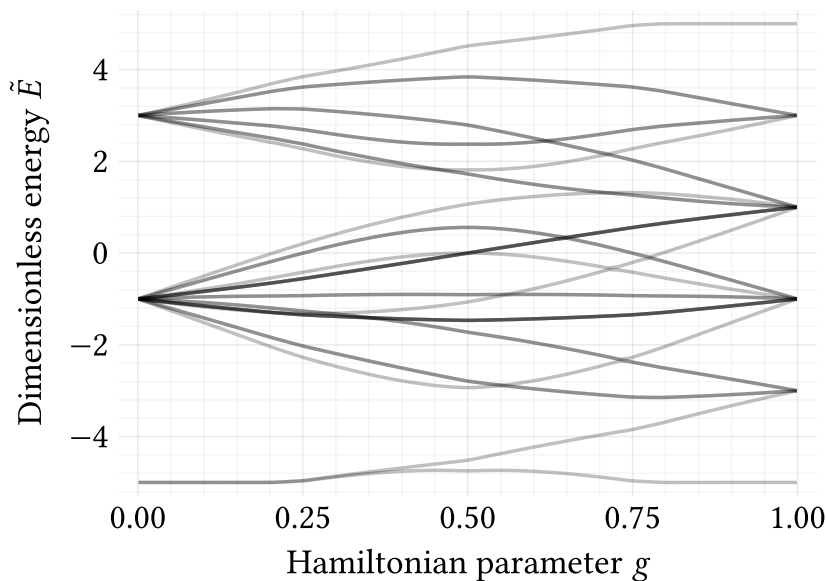

Figure 3.1

3.2   COMPUTATION OF JUMP OPERATORS

```
function addentry!(dict, key, value; isequal=isequal)
    for k in keys(dict)
        if isequal(k, key)
            push!(dict[k], value)
            return dict
        end
    end
    dict[key] = [value]
    dict
end;

function incentry!(dict, key; isequal=isequal)
    for k in keys(dict)
```

```julia
            if isequal(k, key)
                dict[k] += 1
                return dict
            end
        end
        dict[key] = 1
        dict
end;

firstvalue(i, (x, y)) = x
lastvalue(i, (x, y)) = y
dictmap(f, dict) = Dict(key ⇒ f(value) for (key, value) in dict)
function dictby(A; isequal=isequal, keyof=firstvalue, valof=lastvalue)
    i0, x0 = 1, first(A)
    k0, v0 = keyof(i0, x0), valof(i0, x0)
    dict = Dict(k0 ⇒ typeof(v0)[])
    dict = Dict()
    for (i, x) in enumerate(A)
        k, v = keyof(i, x), valof(i, x)
        addentry!(dict, k, v, isequal=isequal)
    end
    dict
end;

sumprojector(A) = sum(a * a' for a in A)
projectors(eigdict) = dictmap(sumprojector, eigdict);

function combinejumps(Js)
    d = Dict()
    for J in Js
        incentry!(d, J)
    end
    [√(one(eltype(J)) * N)*J for (J, N) in d]
end;

isequalto(atol=1e-9) = (x, y) → isapprox(x, y, atol=atol)
function jumps(vals, vecs, As; combine=true, isequal=isequalto())
    eigendict = dictby(zip(vals, vecs))
    ωs = dictby(((E2 - E1, (E1, E2)) for E1 in keys(eigendict), E2 in keys(eigendict)),
        isequal=isequal)
    Πs = projectors(eigendict)
    Jωs = dictmap(ωs) do ΔEs
        filter(x → !isequal(x, zero(x)),
            [sum(Πs[E1]*A*Πs[E2] for (E1, E2) in ΔEs) for A in As])
    end
    combine ? dictmap(combinejumps, Jωs) : Jωs
end

op_to_spindim(H) = Int(log2(size(H)[1]))
dipole_interactions(n) = vcat(map(A → [siteop(A, i, n) for i in 1:n], [σx, σy, σz])...)
function dipolejumps(H; kwargs...)
    vals, vecs = eigen(H)
    jumps(vals, eachcol(vecs), dipole_interactions(op_to_spindim(H)); kwargs...)
end;
```

3.3 Numerical solution of the Lindblad equation

```julia
g = 0.5
Hsys = Hint(g)
b = SpinBasis(1//2)
sys = ⊗(repeat([b], n)...)
Jωs = dipolejumps(Hsys)
η = 1e1
α = 1e-2 # Large α means that Lamb shift dominates. For relaxation illustration only.
up = spinup(b)
ψ0 = ⊗(repeat([up], n)...)
ρ0 = projector(ψ0)
op = dense(embed(sys, 1, sigmaz(b)));


jumpops, rates = [], Float64[]
γ(ω, η) = (1e-1 < η*ω ? ω^3 * (1 + 1 / (exp(η*ω) - 1)) : ω^2 / η)
for (ω, Js) in Jωs
    for J in Js
        push!(rates, α * γ(ω, η))
        push!(jumpops, DenseOperator(sys, J))
    end
end


function fout(t, ρ)
    ρ = normalize(ρ)
    real(expect(op, ρ))
end
Hspin = DenseOperator(sys, Hsys)
opth = fout(0.0, thermalstate(Hspin, 1e0))
tf = 2e-1 / (α * γ(1.0, η))
ts = range(0.0, tf, length=501);


_, closed_σzs = timeevolution.schroedinger(ts, ψ0, Hspin; fout=fout)
_, open_σzs   = timeevolution.master(ts, ρ0, Hspin, jumpops; rates=rates, fout=fout)
_, diss_σzs   = timeevolution.master(ts, ρ0, 0*Hspin, jumpops; rates=rates, fout=fout);


plot(
    title=L"Solution for $N = %$n$, $g = %$g$, $\tau_B / \tau_S = %$η$, ${(\tau_0 /
    ↪  \tau_S)}^2 = %$α$",
    xlabel=L"Time ($t / \tau_S$)",
    ylabel=L"\ev{\pauli_1^z}",
)
plot!(ts, [closed_σzs open_σzs diss_σzs], label=["Closed" "Open" "Dissipator"])
```
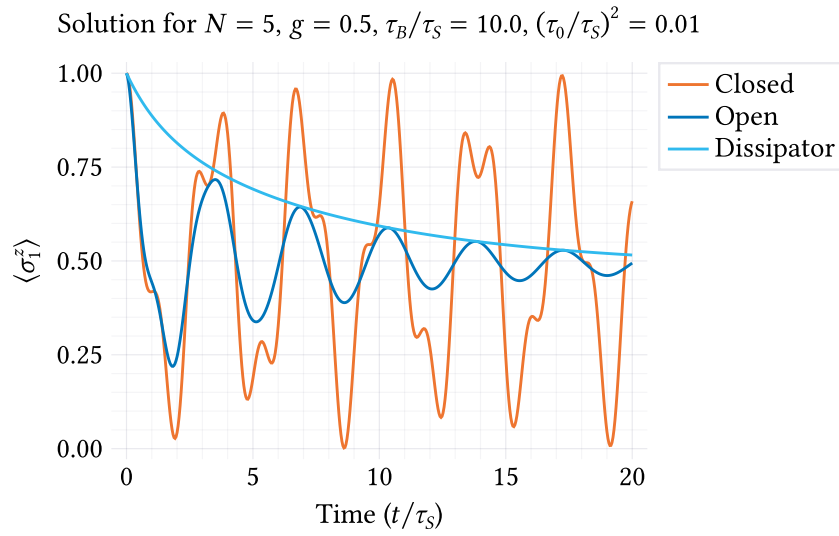
Figure 3.2

```
@. decay_exponential(x, p) = diss_σzs[end] + p[1]*exp(x*p[2])
p0 = [1.0, α * γ(1, η)]
fit = curve_fit(decay_exponential, ts, diss_σzs, p0);

plot(ts, diss_σzs, label=L"\dot{\dop} = \sopr{D}\dop",
    legend=:topright,
    title="Exponential fit over short and medium times",
    xlabel=L"Time ($t / \tau_S$)",
    ylabel=L"\ev{\pauli_1^z}")
plot!(ts, decay_exponential(ts, coef(fit)), label=L"Fit: $Ae^{-s t} +
↪   \ev{\pauli_1^z}_\text{eq}$")
```
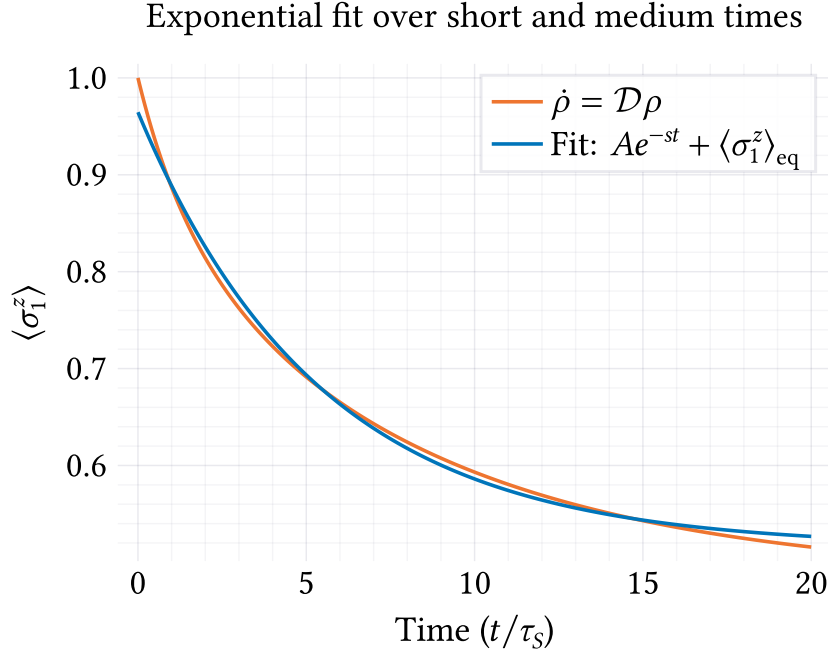
Exponential fit over short and medium times

Figure 3.3

3.4   OBTAINING RELAXATION FROM SPAGHETTI (DIAGRAMS)

$$\rho_S(t) = \sum_i c_i(0)e^{-s_i t}V_i \tag{3.1}$$

```julia
@. decay_exponential(x, p) = p[1]*exp(x*p[2])
function effective_rate(ℒrates, ℒops, ρ0, op, η)
    cs = hcat([vec(V.data) for V in ℒops]...) \ vec(ρ0.data)
    V0s = [tr(op * V) for V in ℒops]
    t0, tf = (0.0, 1e-2) ./ γ(1.0, η)
    ts = range(t0, tf, length=501)
    ys = real(sum(@. c * V0 * exp(real(s)*ts) for (s, c, V0) in zip(ℒrates, cs, V0s)))
    p0 = [1.0, -1.0 / η]
    yf = real(cs[1] * V0s[1])
    fit = curve_fit(decay_exponential, ts, ys .- yf, p0)
    fit.converged || error("Could not fit an effective exponential.")
    coef(fit)[2], stderror(fit)[2]
end

function 𝒟_rates(H, n = op_to_spindim(H); η, ρ0, op)
    Jωs = dipolejumps(H)
```

```julia
    sys = ρ0.basis_r
    jumpops, rates = [], Float64[]
    for (ω, Js) in Jωs
        for J in Js
            push!(rates, γ(ω, η))
            push!(jumpops, DenseOperator(sys, J))
        end
    end
    𝓛 = steadystate.liouvillian(0*DenseOperator(sys), jumpops; rates=rates)
    𝓛rates, 𝓛ops = steadystate.liouvillianspectrum(𝓛; nev=4^n)
    effrate = effective_rate(𝓛rates, 𝓛ops, ρ0, op, η)
    sort(real(𝓛rates)), effrate...
end;


function plot_𝒟_rates(Hint;
        points=16, η=1.0, ρ0, op, onplot=false,
        spectrum=true, extremes=true, effective=true,
        kwargs...)
    g0s = grange(points)
    outs = map(g → 𝒟_rates(Hint(g); η, ρ0, op), g0s)
    rates = [o[1] for o in outs]
    r0 = [o[2] for o in outs]
    σr0 = [o[3] for o in outs]

    p = onplot
    if onplot == false
        p = plot(
            xlabel=L"Hamiltonian parameter $g$",
            ylabel=L"Dissipaton rates ($\tilde{\gamma} / \tilde{\gamma}_0$)",
            legendtitle=L"\log\eta",
            legend=:topright;
            kwargs...)
    end
    if spectrum
        plot!(p, g0s, -hcat(rates...)', color=:black, alpha=0.25, label=false)

        if extremes
            rates0 = 𝒟_rates(Hint(0); η, ρ0, op)[1]
            rates1 = 𝒟_rates(Hint(1); η, ρ0, op)[1]
            scatter!(p, repeat([g0s[1] - 2e-2], length(rates0)), -rates0,
                marker=(:rtriangle, 2, rubric), markerstrokecolor=rubric, label=false)
            scatter!(p, repeat([g0s[end] + 2e-2], length(rates1)), -rates1,
                marker=(:ltriangle, 2, rubric), markerstrokecolor=rubric, label=false)
        end
    end
    if effective
        plot!(p, g0s, -r0, ribbon=σr0, label=L"%$(round(log10(η), digits=1))",
            color = (onplot == false) ? rubric : :auto)
    end
    p
end;


plot_𝒟_rates(Hint; η, ρ0, op)
```
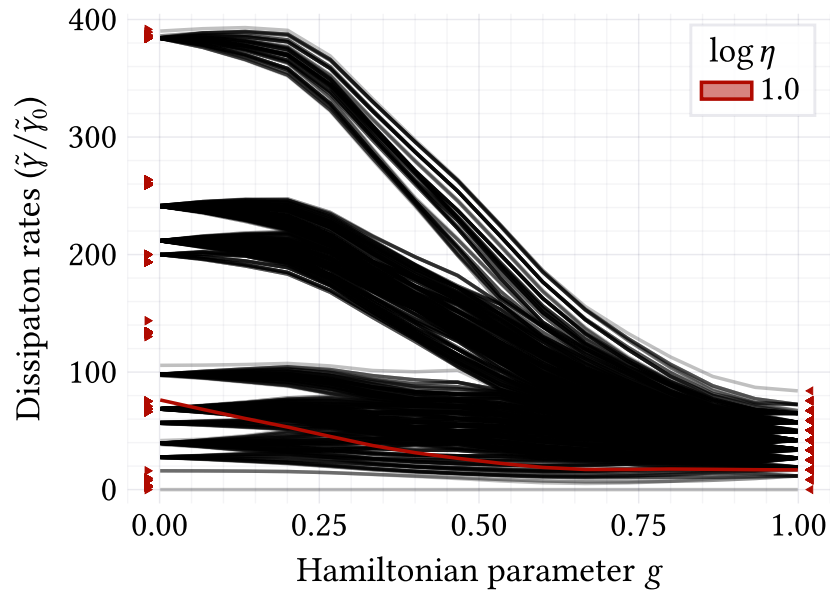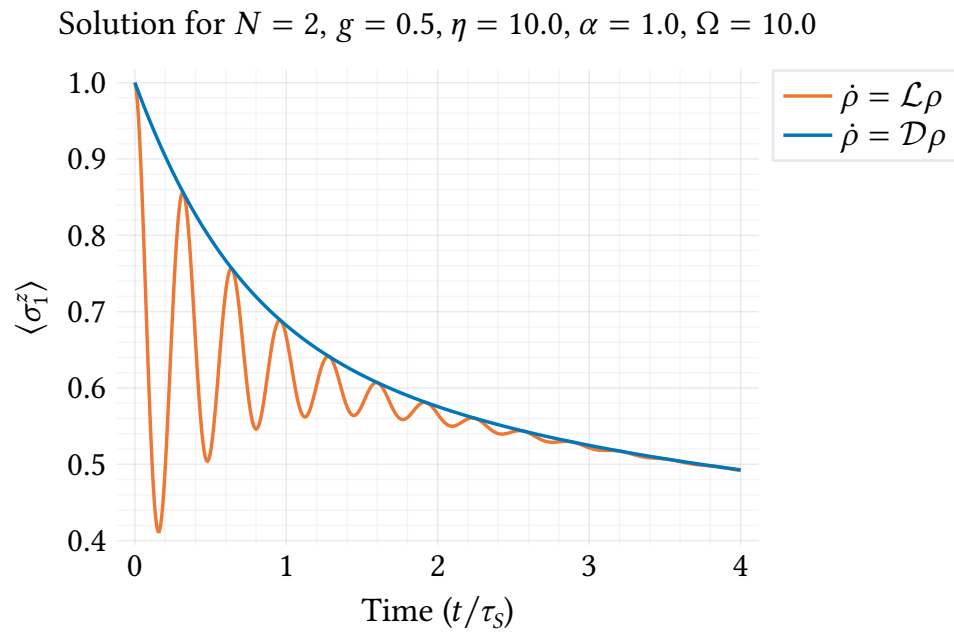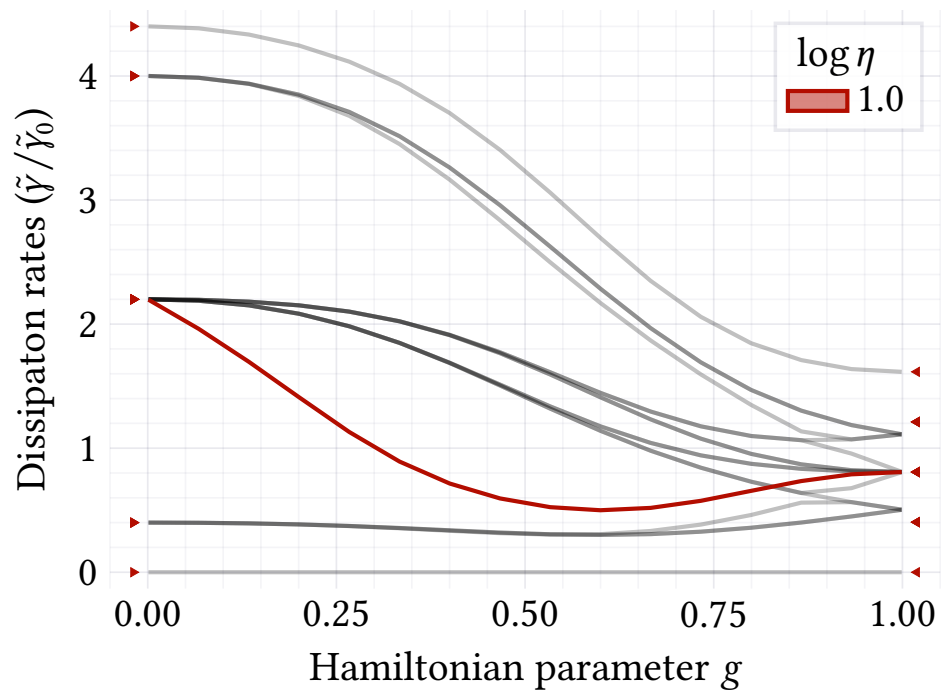
Figure 3.4

```
plot([reduce((p, η) →
        plot_𝒟_rates(Hint; η, ρ0, op, spectrum=false, onplot=p),
        10 .^ range(lη, lη + 1, length=4);
        init = plot(size=2 .* (400, 300 * 3//2),
            xlabel=L"Hamiltonian parameter $g$",
            ylabel=L"Decay rates for $\pauli_1^z$ ($\tilde{\gamma} /
            ↪  \tilde{\gamma}_0$)",
            legend=:topright,
            legendtitle=L"\log\eta"))
    for lη in -2:3]...,
  layout=(3,2))
```

Figure 3.5: Example time evolution for $N = 2$ spins.

Figure 3.6: Dissipation rate spaghetti diagram for $N = 2$ spins.

Solution for $N = 3$, $g = 0.5$, $\eta = 10.0$, $\alpha = 1.0$, $\Omega = 10.0$
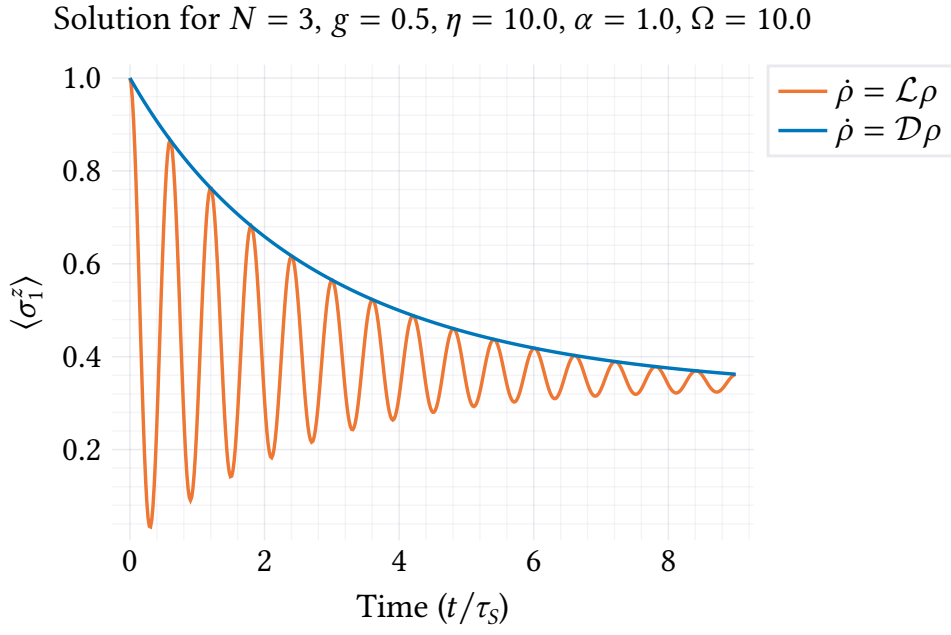
Figure 3.7: Example time evolution for $N = 3$ spins.
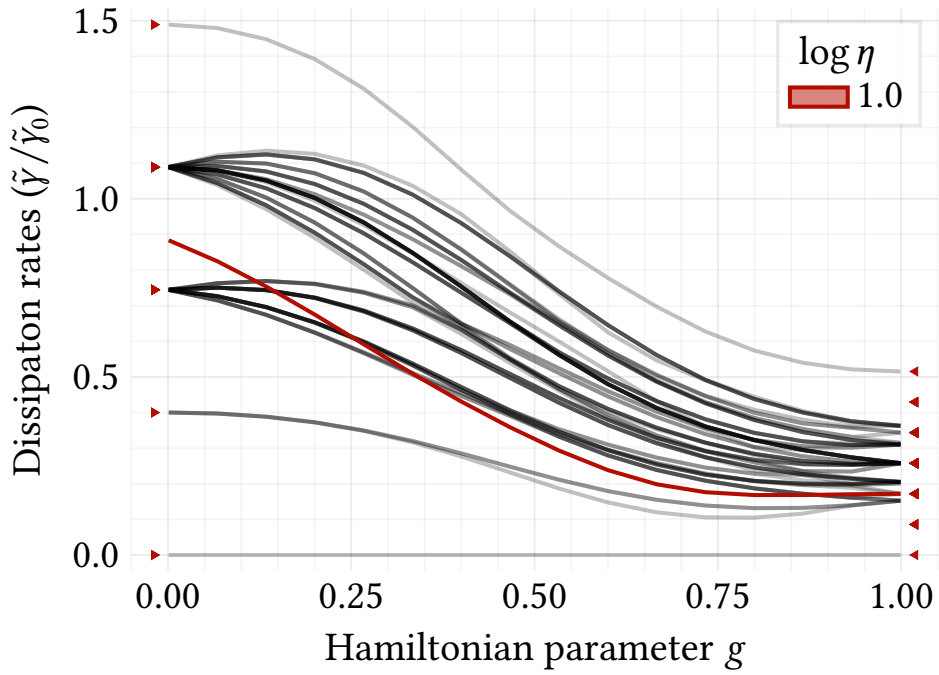
Figure 3.8: Dissipation rate spaghetti diagram for $N = 3$ spins.
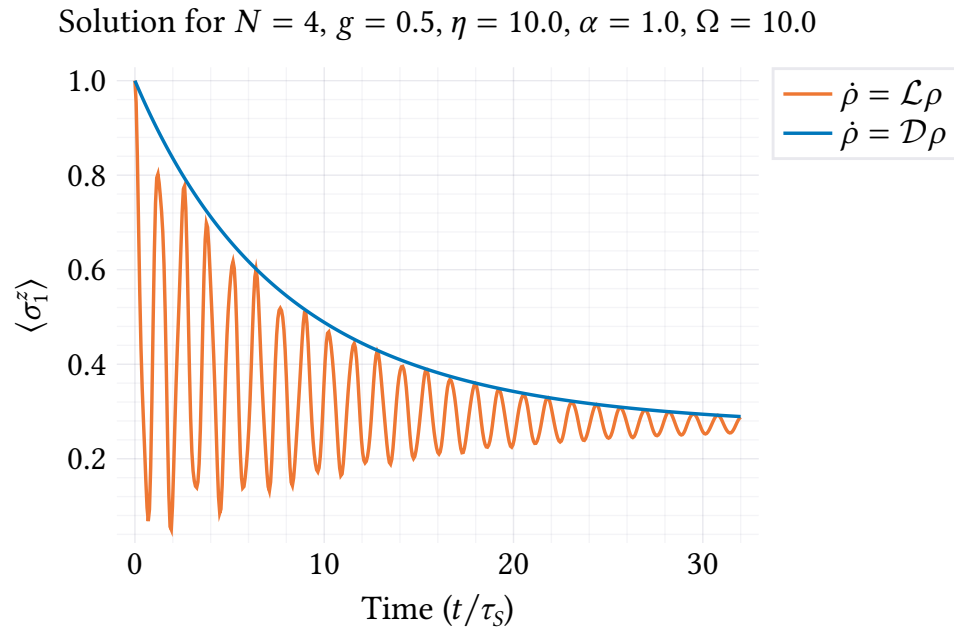
Figure 3.9: Example time evolution for $N = 4$ spins.
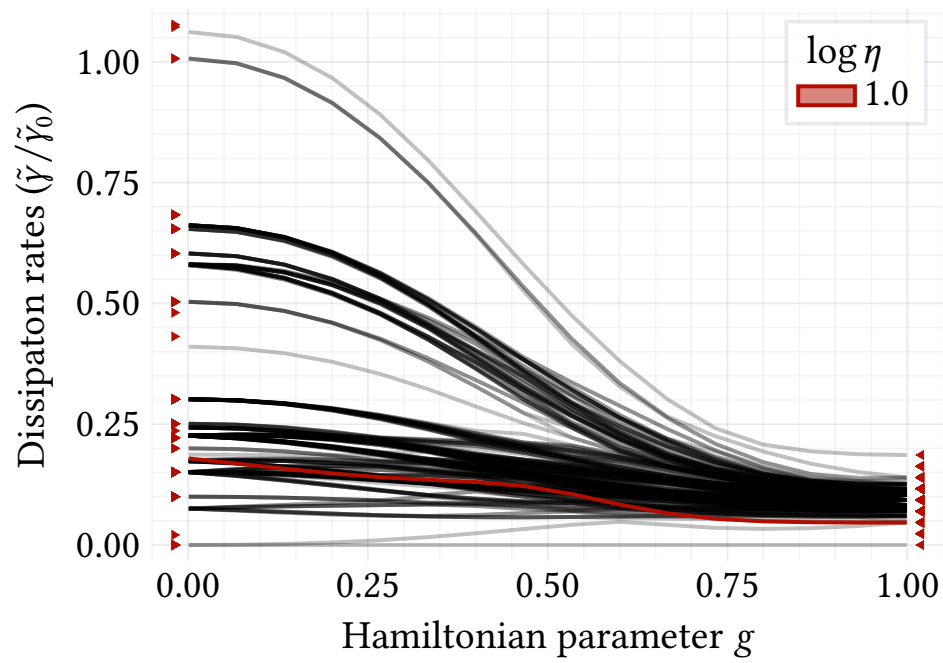
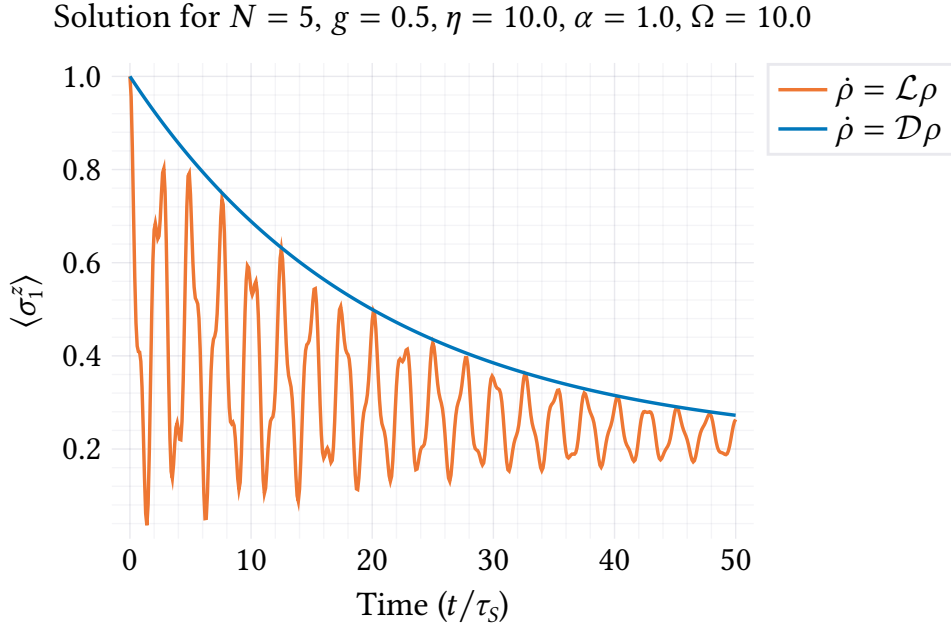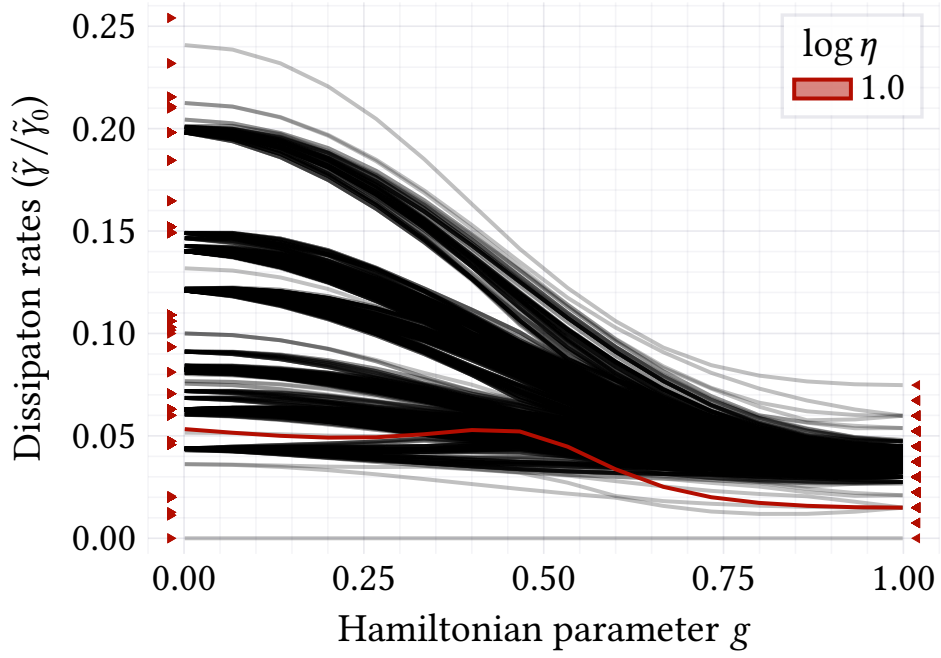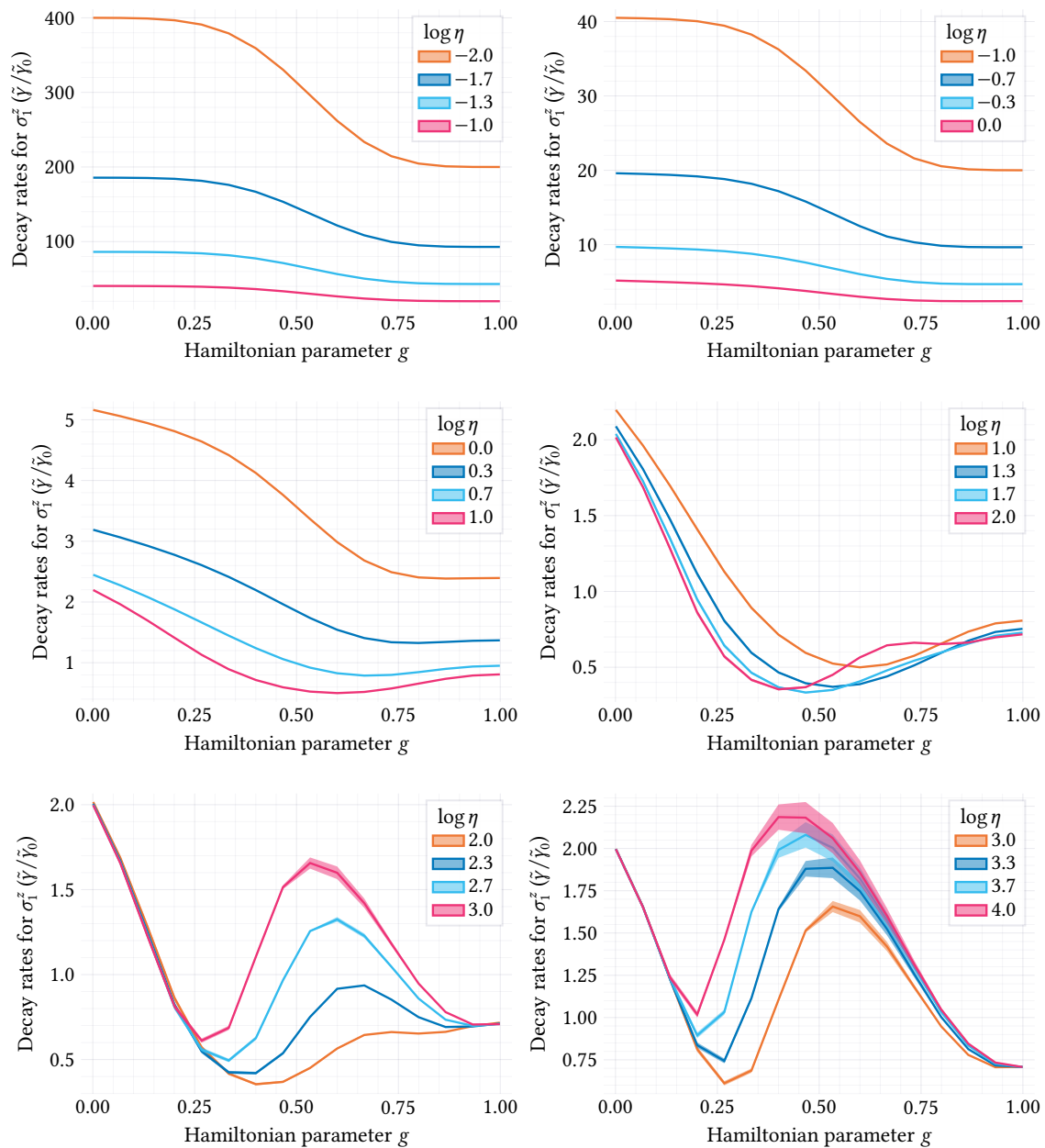**Figure 3.10:** Dissipation rate spaghetti diagram for $N = 4$ spins.

Solution for $N = 5$, $g = 0.5$, $\eta = 10.0$, $\alpha = 1.0$, $\Omega = 10.0$

Figure 3.11: Example time evolution for $N = 5$ spins.

Figure 3.12: Dissipation rate spaghetti diagram for $N = 5$ spins.

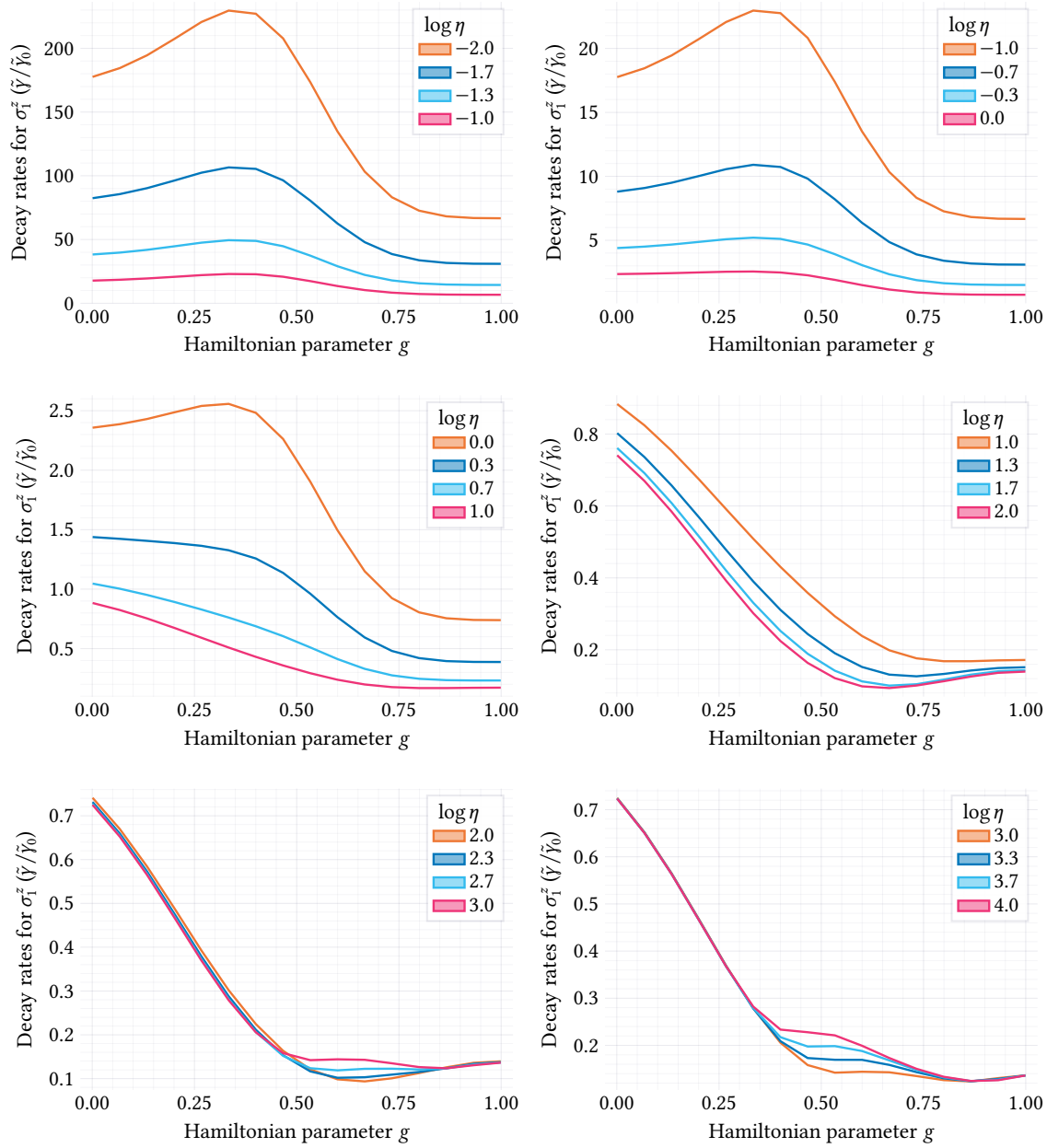**Figure 3.13:** Single-spin relaxation rates in different temperature regimes for $N = 2$ spins.

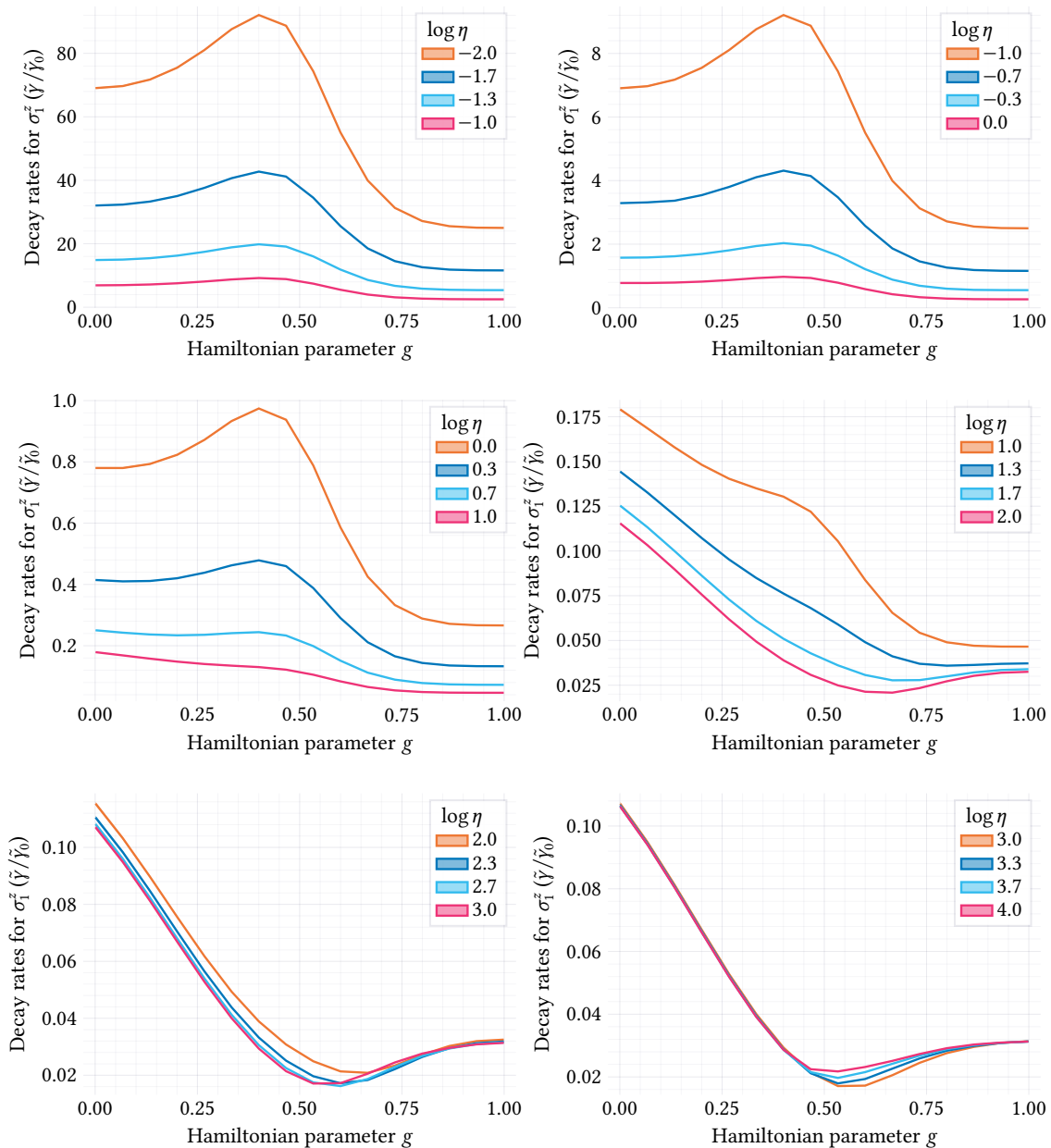**Figure 3.14:** Single-spin relaxation rates in different temperature regimes for $N = 3$ spins.

Figure 3.15: Single-spin relaxation rates in different temperature regimes for $N = 4$ spins.
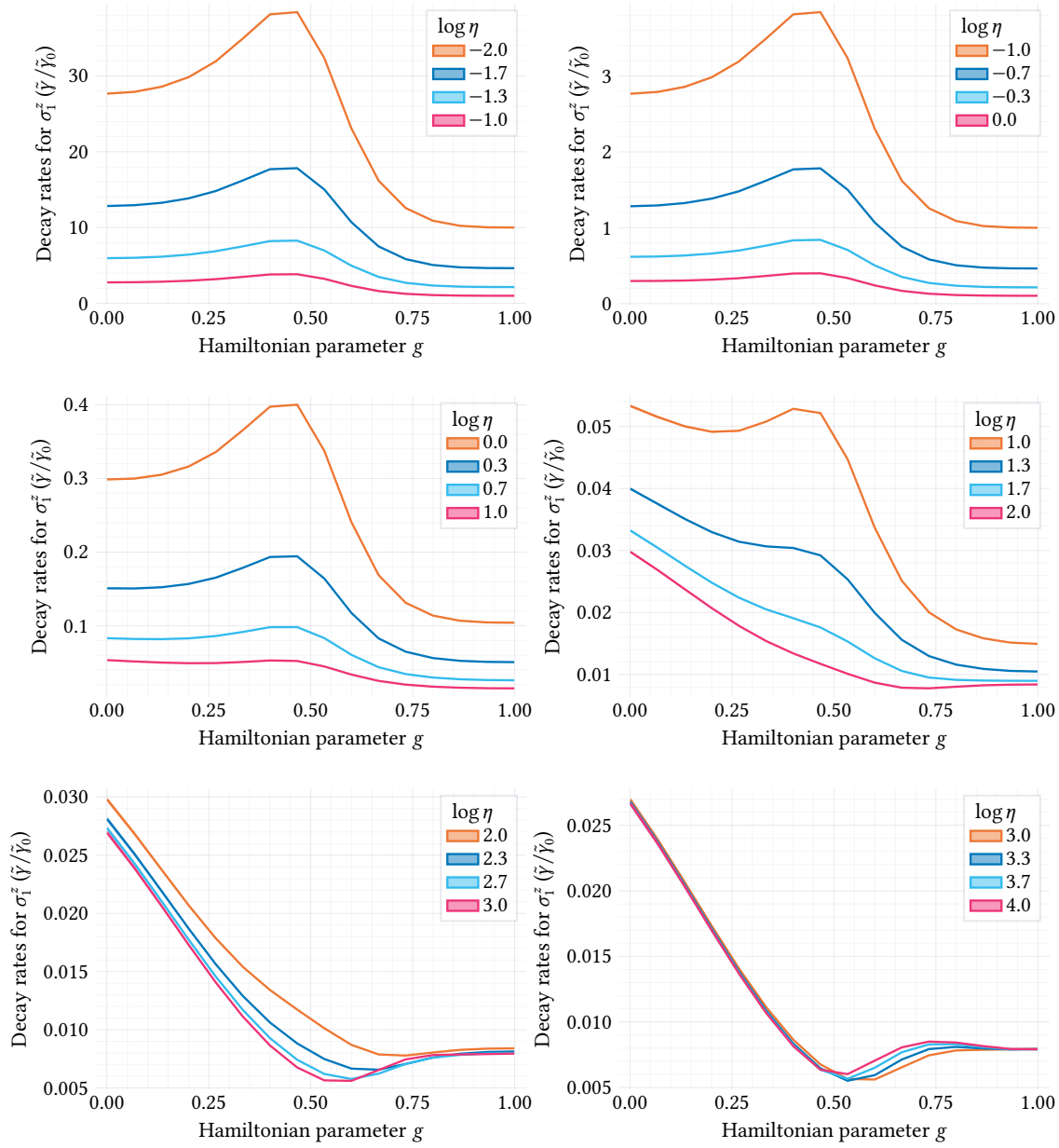
Figure 3.16: Single-spin relaxation rates in different temperature regimes for $N = 5$ spins.

Conclusion

Here's a conclusion, demonstrating the use of all that manual incrementing and table of contents adding that has to happen if you use the starred form of the chapter command. The deal is, the chapter command in LaTeX does a lot of things: it increments the chapter counter, it resets the section counter to zero, it puts the name of the chapter into the table of contents and the running headers, and probably some other stuff.

Appendix A

The generator of a quantum dynamical semigroup

The contents of this appendix follow [16].

Let $\mathcal{V}(t)$ for $t \geqslant 0$ be a family of completely positive and trace-preserving CPTP maps on $\mathcal{L}(\mathcal{H})$ with the **semigroup property** that

$$\mathcal{V}(t)\mathcal{V}(s) = \mathcal{V}(t + s). \tag{A.1}$$

In the physical context, $\mathcal{V}(t)$ is a dynamical map for the reduced dynamics of a system, and the semigroup property is that the dynamics are Markovian or memoryless, just like when one coarse-grains to the system time in the weak-coupling limit.

By analogy to Stone's theorem, we expect that there is a generator $\mathcal{L}$ of the semigroup such that

$$\mathcal{V}(t) = e^{\mathcal{L}t}. \tag{A.2}$$

We are interested in obtaining a **master equation** of the form

$$\dot{\rho} = \mathcal{L}\rho. \tag{A.3}$$

We may find $\mathcal{L}$ as follows. Since $\mathcal{V}(t)$ is CPTP, it may be decomposed with the help of the Kraus representation theorem as

$$\mathcal{V}(t)\rho = \sum_i M_i(t)\rho M_i^\dagger(t), \tag{A.4}$$

where $\sum_i M_i^\dagger(t)M_i = 1$. We can express the M_i in terms of an orthonormal complete basis $\{F_n\}$ for $\mathcal{L}(\mathcal{H})$ as $M_i = \sum_n F_n \langle F_n|M_i\rangle$. Then eq. (A.4) becomes

$$\mathcal{V}(t)\rho = \sum_{mn} c_{mn}(t)F_m\rho F_n^\dagger, \tag{A.5}$$

where

$$c_{mn}(t) \equiv \sum_i \langle F_m|M_i(t)\rangle \langle M_i(t)|F_n\rangle. \tag{A.6}$$

For convenience, we may choose $F_{d^2} = 1/\sqrt{d}$, where $d = \dim(\mathcal{H})$. With an eye towards simplifying eq. (A.11), we eliminate the explicit time dependence of eq. (A.6) by defining

$$a_{mn} \equiv \lim_{t\to0^+} \frac{c_{mn}(t) - d\delta_{d^2d^2}}{t} \tag{A.7}$$

and introduce the sum of Kraus operators

$$F = \frac{1}{\sqrt{d}}\sum_{n=1}^{d^2-1} a_{nd^2}F_n \tag{A.8}$$

$$= \frac{F+F^\dagger}{2} + i\frac{F-F^\dagger}{2i} \equiv G - iH, \tag{A.9}$$

where we have decomposed the sum F into Hermitian and anti-Hermitian parts. Now we may write the master equation $\dot\rho = \mathcal{L}\rho$ as

$$\dot\rho = \lim_{\Delta t\to0^+} \frac{\mathcal{V}(\Delta t)\rho - \rho}{\Delta t} \tag{A.10}$$

$$= \lim_{\Delta t\to0^+} \left(\frac{c_{d^2d^2} - d}{d\Delta t}\rho + \sum_{m,n=1}^{d^2-1} \frac{c_{mn}(\Delta t)}{\Delta t}F_m\rho F_n^\dagger \right.$$

$$\left. + \frac{1}{\sqrt{d}}\sum_{n=1}^{d^2-1} \left(\frac{c_{nd^2}(\Delta t)}{\Delta t}F_n\rho + \frac{c_{d^2n}(\Delta t)}{\Delta t}\rho F_n^\dagger \right) \right) \tag{A.11}$$

$$= \frac{a_{d^2d^2}}{d}\rho + F\rho + \rho F^\dagger + \sum_{m,n=1}^{d^2-1} a_{mn}F_m\rho F_n^\dagger \tag{A.12}$$

$$= \frac{a_{d^2d^2}}{d}\rho + \{G,\rho\} - i[H,\rho] + \sum_{m,n=1}^{d^2-1} a_{mn}F_m\rho F_n^\dagger \tag{A.13}$$

$$= \{G',\rho\} - i[H,\rho] + \sum_{m,n=1}^{d^2-1} a_{mn}F_m\rho F_n^\dagger, \tag{A.14}$$

where $G' = G + a_{d^2 d^2} 1/d$. Since $\mathcal{V}(t)$ is trace-preserving, $\text{tr}\,\dot{\rho} = 0$. Applying this condition to eq. (A.14) and cycling the trace gives

$$0 = \text{tr}\left(2G'\rho + \sum_{m,n=1}^{d^2-1} a_{mn} F_n^\dagger F_m \rho\right), \tag{A.15}$$

so $G' = -\sum_{m,n=1}^{d^2-1} a_{mn} F_n^\dagger F_m / 2$. This allows us to write eq. (A.14) as

$$\dot{\rho} = -\text{i}[H, \rho] + \sum_{m,n=1}^{d^2-1} a_{mn}\left(F_m \rho F_n^\dagger - \frac{1}{2}\left\{F_n^\dagger F_m, \rho\right\}\right), \tag{A.16}$$

which is the first form of the **Lindblad equation**. This may be simplified further if we diagonalize the coefficient matrix a by applying a unitary transformation u to give $a = u\gamma u^\dagger$, where the $\{\gamma_k\}_{k=1}^{d^2-1}$ are the non-negative eigenvalues of a. This is possible since the coefficient matrix c is seen from eq. (A.6) to be Hermitian, and eq. (A.7) then gives that a is Hermitian. We may then express $F_{n \neq d^2} = \sum_{k=1}^{d^2-1} L_n u_{nk}$ in terms of the **Lindblad** or **jump operators** L_n to find

$$\dot{\rho} = -\text{i}[H, \rho] + \sum_{k=1}^{d^2-1} \gamma_k\left(L_k \rho L_k^\dagger - \frac{1}{2}\left\{L_k^\dagger L_k, \rho\right\}\right), \tag{A.17}$$

which is the diagonal form of the Lindblad equation.

It has been proven that that this is the most general generator for a quantum dynamical semigroup when the system is finite-dimensional [27] and when the system is infinite-dimensional but $\mathcal{L}$ is bounded [28]. This is not much help, since the Hamiltonians for even simple infinite-dimensional systems like the harmonic oscillator are unbounded. Regardless, most examples where $\mathcal{L}$ is unbounded may still be cast into Lindblad form with little or no modification.

Appendix B

The transverse-field Ising model

We would like to solve the Hamiltonian eq. (2.20), which we nondimensionalize as

$$\frac{4}{J}H = -\sum_{i\in\mathbb{Z}_N}\left(\sigma_i^x\sigma_{i+1}^x + g\sigma_i^z\right) \tag{B.1}$$

for the periodic transverse-field Ising chain with N spins. We will drop the $4/J$ in what follows. We notice that the operators

$$\sigma_i^\pm = \frac{\sigma_i^x \pm \mathrm{i}\sigma_i^y}{2} \tag{B.2}$$

satisfy

$$\sigma_i^z = 2\sigma_i^+\sigma_i^- - 1 \tag{B.3}$$

and have commutators

$$\left[\sigma_i^+, \sigma_j^-\right] = \frac{1}{4}\left[\sigma_i^x + \mathrm{i}\sigma_i^y, \sigma_j^x - \mathrm{i}\sigma_j^y\right] \tag{B.4}$$

$$= \frac{1}{4}\left(\left[\sigma_i^x, \sigma_j^x\right] + \left[\sigma_i^y, \sigma_j^y\right] + \mathrm{i}\left[\sigma_i^y, \sigma_j^x\right] - \mathrm{i}\left[\sigma_i^x, \sigma_j^y\right]\right) \tag{B.5}$$

$$= \delta_{ij}\sigma_i^z. \tag{B.6}$$

Thus their anticommutators are

$$\left\{\sigma_i^+, \sigma_j^-\right\} = 2\sigma_i^+\sigma_j^- - \left[\sigma_i^+, \sigma_j^-\right] \tag{B.7}$$

$$= 2\sigma_i^+\sigma_j^- - \delta_{ij}\sigma_i^z \tag{B.8}$$

$$= \delta_{ij}1 + 2\sigma_i^+\sigma_j^-(1 - \delta_{ij}). \tag{B.9}$$

It could be helpful to think of the $\sigma_i^{\pm}$ as fermion creation and annihilation operators, but they do not anticommute at different sites.

How might we construct operators that satisfy the fermionic canonical anticommutation relations (CARs) from the Pauli operators? Suppose we have such operators c_i. Given a tuple $\boldsymbol{n} = (n_i)_{i \in \mathbb{Z}_N}$, we have the corresponding states

$$|\boldsymbol{n}\rangle = \prod_{i \in \mathbb{Z}_N} \left(c_i^{\dagger}\right)^{n_i} |0\rangle, \tag{B.10}$$

where $|0\rangle$ denotes the vacuum state. It then follows that

$$c_i |\boldsymbol{n}\rangle = -n_i (-1)^{n_{<i}} |\boldsymbol{n}_{i \leftarrow 0}\rangle \tag{B.11}$$

$$c_i^{\dagger} |\boldsymbol{n}\rangle = -(1 - n_i)(-1)^{n_{<i}} |\boldsymbol{n}_{i \leftarrow 1}\rangle, \tag{B.12}$$

where $\boldsymbol{n}_{i \leftarrow m} = \boldsymbol{n}$ with $n_i = m$ and $n_{<i} = \sum_{j<i} n_j$.

Thus the number operator is

$$c_i^{\dagger} c_i |\boldsymbol{n}\rangle = (1 - 0)(-1)^{n_{<i}} n_i (-1)^{n_{<i}} |\boldsymbol{n}_{i \leftarrow 1}\rangle \tag{B.13}$$

$$= n_i |\boldsymbol{n}\rangle. \tag{B.14}$$

This leads us to consider

$$c_i = -\left(\prod_{j<i} -\sigma_j^z\right)\sigma_i^- \tag{B.15}$$

acting on the states

$$|\boldsymbol{n}\rangle = \prod_{i \in \mathbb{Z}_N} \left(\sigma_i^+\right)^{n_i} |0\rangle, \tag{B.16}$$

where $|0\rangle = |\uparrow\rangle^{\otimes N}$ is the state with all z-spins up, or all zero qubits. This gives the same result as eq. (B.11), so the c_i satisfy the CARs. This process of mapping spin-1/2 sites to non-local fermions is known as the **Jordan-Wigner transformation**. We may then compute that the inverse transformations are

$$\sigma_i^+ \sigma_i^- = c_i^{\dagger} c_i \tag{B.17}$$

$$\sigma_i^z = 2c_i^{\dagger} c_i - 1 \tag{B.18}$$

$$\sigma_i^x = -\left(\prod_{j<i}\left(1 - 2c_j^{\dagger} c_j\right)\right)\left(c_i^{\dagger} + c_i\right) \tag{B.19}$$

$$\sigma_i^y = i\left(\prod_{j<i}\left(1 - 2c_j^{\dagger} c_j\right)\right)\left(c_i^{\dagger} - c_i\right). \tag{B.20}$$

While σ_i^x remains complicated, the product $\sigma_i^x \sigma_{i+1}^x$ does not. For $i < N - 1$,

$$\sigma_i^x \sigma_{i+1}^x = \left(\prod_{j<i} \left(2c_j^\dagger c_j - 1 \right) \right) \left(c_i^\dagger + c_i \right) \left(\prod_{j<i+1} \left(2c_j^\dagger c_j - 1 \right) \right) \left(c_{i+1}^\dagger + c_{i+1} \right) \tag{B.21}$$

$$= \left(c_i^\dagger + c_i \right) \left(1 - 2c_i^\dagger c_i \right) \left(c_{i+1}^\dagger + c_{i+1} \right) \tag{B.22}$$

$$= \left(c_i^\dagger - c_i \right) \left(c_{i+1}^\dagger + c_{i+1} \right), \tag{B.23}$$

and for $i = N - 1$,

$$\sigma_{N-1}^x \sigma_0^x = \left(\prod_{j<N-1} \left(2c_j^\dagger c_j - 1 \right) \right) \left(c_{N-1}^\dagger + c_{N-1} \right) \left(c_0^\dagger + c_0 \right). \tag{B.24}$$

We may now perform the Jordan-Wigner transformation of eq. (B.1) to obtain

$$H = \sum_i \left(c_i - c_i^\dagger \right) \left(c_{i+1}^\dagger + c_{i+1} \right) - g \sum_i 2c_i^\dagger c_i + gN1$$

$$- \left(1 - \prod_{j<N-1} \left(2c_j^\dagger c_j - 1 \right) \right) \left(c_{N-1} - c_{N-1}^\dagger \right) \left(c_0^\dagger + c_0 \right). \tag{B.25}$$

We now Fourier transform with

$$c_i = \frac{1}{\sqrt{N}} \sum_k e^{iki} C_k \tag{B.26a}$$

$$C_k = \frac{1}{\sqrt{N}} \sum_i e^{-iki} c_i \tag{B.26b}$$

and

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-iki} C_k^\dagger \tag{B.26c}$$

$$C_k^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{iki} c_i^\dagger. \tag{B.26d}$$

We now propagate the periodic boundary conditions to the Fourier-transformed operators.

$$c_0 = \frac{1}{\sqrt{N}} \sum_k C_k \tag{B.27}$$

$$c_N = \frac{1}{\sqrt{N}} \sum_k e^{ikN} C_k. \tag{B.28}$$

We then must require that

$$kN \equiv 0 \pmod{2\pi} \tag{B.29}$$

$$k = \frac{2\pi n}{N} - \frac{N - [N \text{ odd}]}{N}\pi, \quad n \in \mathbb{Z}_N. \tag{B.30}$$

For N odd, what is C_π?

$$C_\pi = \frac{1}{\sqrt{N}} \sum_i e^{-i\pi i} c_i. \tag{B.31}$$

Since $e^{-i\pi i} = e^{i\pi i}$, $C_\pi = C_{-\pi}$.

We now verify that this operator Fourier transformation is a unitary operation. That is, it preserves the fermionic CARs.

Proof. Consider N fermionic operators c_i and a $N \times N$ unitary matrix U. We may change bases with

$$C_k^\dagger = \sum_i U_{ik} c_i^\dagger. \tag{B.32}$$

Then

$$\left\{ C_k, C_{k'}^\dagger \right\} = \sum_{ij} U_{ik}^* U_{jk'} \left\{ c_i, c_j^\dagger \right\} \tag{B.33}$$

$$= \sum_i U_{ik}^* U_{ik'} \tag{B.34}$$

$$= \left(U^\dagger U \right)_{kk'} \tag{B.35}$$

$$= \delta_{kk'}, \tag{B.36}$$

and similar for the other fermionic (anti-)commutation relations.

For the Fourier transform,

$$F_{ik} = \frac{1}{\sqrt{N}} e^{iki}. \tag{B.37}$$

We may then confirm that

$$\left(F^\dagger F \right)_{kk'} = \sum_i \frac{1}{N} e^{i(k'-k)i} \tag{B.38}$$

$$= \delta_{kk'}. \tag{B.39}$$

Thus the Fourier transform is unitary.   □

We are now equipped to Fourier transform eq. (B.25) as follows. Since

$$\frac{1}{N}\sum_{i\in\mathbb{Z}_N} e^{i(k'-k)i} = \delta_{kk'}, \tag{B.40}$$

and also

$$C_{-k} = C_k^* \tag{B.41}$$

$$= \frac{1}{\sqrt{N}}\sum_i e^{-i(-k)i}c_i \tag{B.42}$$

$$= \frac{1}{N}\sum_{ik'} e^{i(k'+k)i}C_{k'}, \tag{B.43}$$

we have that

$$\sum_i c_i^\dagger c_i = \frac{1}{N}\sum_{ikk'} e^{i(k'-k)i}C_k^\dagger C_{k'} \tag{B.44}$$

$$= \sum_k C_k^\dagger C_k, \tag{B.45}$$

$$\sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right) = \frac{1}{N}\sum_{ikk'} e^{i(k'-k)i}\left(e^{ik'} + e^{-ik}\right)C_k^\dagger C_{k'} \tag{B.46}$$

$$= \sum_k 2\cos k\, C_k^\dagger C_k, \tag{B.47}$$

$$\sum_i \left(c_{i+1}c_i + c_i^\dagger c_{i+1}^\dagger\right) = \frac{1}{N}\sum_{ikk'} \left(e^{i(k'+k)i}e^{ik}C_kC_{k'} + e^{-i(k'+k)i}e^{-ik'}C_k^\dagger C_{k'}^\dagger\right) \tag{B.48}$$

$$= \sum_k \left(e^{-ik}C_{-k}C_k + e^{ik}C_k^\dagger C_{-k}^\dagger\right). \tag{B.49}$$

Thus eq. (B.25) is now

$$H = -\sum_k 2\cos k\, C_k^\dagger C_k + \sum_k \left(e^{-ik}C_{-k}C_k + e^{ik}C_k^\dagger C_{-k}^\dagger\right) - \sum_k 2gC_k^\dagger C_k + gN\mathbb{1} \tag{B.50}$$

$$= -\sum_k (g + \cos k)\left(C_k^\dagger C_k + C_{-k}^\dagger C_{-k}\right) + \sum_k i\sin k\left(C_{-k}C_k - C_k^\dagger C_{-k}^\dagger\right) + gN\mathbb{1} \tag{B.51}$$

$$= -\sum_k (g + \cos k)\left(C_k^\dagger C_k - C_{-k}C_{-k}^\dagger\right) + \sum_k i\sin k\left(C_{-k}C_k - C_k^\dagger C_{-k}^\dagger\right) \tag{B.52}$$

$$= \sum_k v_k^\dagger H_k v_k, \tag{B.53}$$

where

$$H_k = \begin{bmatrix} -(g + \cos k) & -i\sin k \\ i\sin k & g + \cos k \end{bmatrix}, \tag{B.54}$$

$$v_k = \begin{bmatrix} C_k \\ C_{-k}^\dagger \end{bmatrix}, \tag{B.55}$$

and we have used that

$$\sum_k \cos k = 0. \tag{B.56}$$

Since the H_k are Hermitian, they may be diagonalized by a unitary transformation of the v_k.[1] The H_k are traceless, so they have the eigenvalues

$$E_k^\pm = \pm\sqrt{-\det H_k} \tag{B.62}$$

$$= \pm\sqrt{g^2 + 2g\cos k + \cos^2 k + \sin^2 k} \tag{B.63}$$

$$= \pm\sqrt{g^2 + 2g\cos k + 1}. \tag{B.64}$$

The eigenvectors are then

$$q_k^\pm = \begin{bmatrix} -i\sin k \\ E_k^\pm + g + \cos k \end{bmatrix}, \tag{B.65}$$

except if $k = 0$ or $-\pi$, in which case

$$q_k^- = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad q_k^+ = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{B.66}$$

---

[1] The unitary transformation of the $C_{\pm k}$ to obtain $\eta_k^\pm$ is an instance of a fermionic **Bogoliubov transformation**:

$$C_k = u f_k + v g_k^\dagger \tag{B.57a}$$

and

$$C_{-k} = -v f_k^\dagger + u g_k. \tag{B.57b}$$

For these transformations to preserve the CARs,

$$\{C_k^\dagger, C_k\} = |u|^2 \{f_k^\dagger, f_k\} + |v|^2 \{g_k, g_k^\dagger\} + u^* v \{f_k^\dagger, g_k^\dagger\} + v^* u \{g_k, f_k\} \tag{B.58}$$

$$= \left(|u|^2 + |v|^2\right) 1, \tag{B.59}$$

so we must have

$$|u|^2 + |v|^2 = 1. \tag{B.60}$$

We may choose

$$u = e^{i\phi_1} \cos\theta \tag{B.61a}$$

$$v = e^{i\phi_2} \sin\theta \tag{B.61b}$$

for real angles ϕ_1, ϕ_2, and θ.

The $k = -\pi$ case does not appear if N is odd. If also $g = 1$, then $H_{-\pi} = 0$. To construct the unitary transformation, we must normalize the $q_k^{\pm}$. We find that

$$\left\| q_k^{\pm} \right\|^2 = \left(E_k^{\pm} + g + \cos k \right)^2 + \sin^2 k \tag{B.67}$$

$$= \left(E_k^{\pm} \right)^2 + g^2 + \cos^2 k + 2g \cos k + 2E_k^{\pm}(g + \cos k) + 1 - \cos^2 k \tag{B.68}$$

$$= 2E_k^{\pm} \left(E_k^{\pm} + g + \cos k \right). \tag{B.69}$$

Now

$$\frac{\left(q_k^{\pm} \right)_1}{\left\| q_k^{\pm} \right\|} = \frac{-i \sin k}{\sqrt{2E_k^{\pm}\left(E_k^{\pm} + g + \cos k \right)}} \tag{B.70}$$

$$= \frac{-i \sin k}{\sqrt{2\left| E_k^{\pm} \right|\left(\left| E_k^{\pm} \right| \pm (g + \cos k) \right)}} \tag{B.71}$$

and

$$\frac{\left(q_k^{\pm} \right)_2}{\left\| q_k^{\pm} \right\|} = \pm \sqrt{\frac{E_k^{\pm} + (g + \cos k)}{2E_k^{\pm}}} \tag{B.72}$$

$$= \pm \sqrt{\frac{\left| E_k^{\pm} \right| \pm (g + \cos k)}{2\left| E_k^{\pm} \right|}} \tag{B.73}$$

$$U_k^{\dagger} = \begin{bmatrix} \left(\hat{q}_k^{-} \right)^{\dagger} \\ \left(\hat{q}_k^{+} \right)^{\dagger} \end{bmatrix}. \tag{B.74}$$

Then with $E_k = \left| E_k^{\pm} \right|$,

$$\eta_k^{\pm} = \frac{i \sin k}{\sqrt{2E_k(E_k \pm (g + \cos k))}} C_k \pm \sqrt{\frac{E_k \pm (g + \cos k)}{2E_k}} C_{-k}^{\dagger} \tag{B.75}$$

so that

$$\left\{ \left(\eta_k^{\pm} \right)^{\dagger}, \eta_k^{\pm} \right\} = \frac{\sin^2 k}{2E_k(E_k \pm (g + \cos k))} 1 + \frac{E_k \pm (g + \cos k)}{2E_k} 1 \tag{B.76}$$

$$= 1 \tag{B.77}$$

$$\left\{ \left(\eta_k^{\pm} \right)^{\dagger}, \eta_k^{\mp} \right\} = \frac{\sin^2 k}{2E_k\sqrt{E_k \pm (g + \cos k)}\sqrt{E_k \mp (g + \cos k)}} 1$$
$$- \frac{\sqrt{E_k \pm (g + \cos k)}\sqrt{E_k \mp (g + \cos k)}}{2E_k} 1 \tag{B.78}$$

$$= 0. \tag{B.79}$$

Note that eq. (B.75) is consistent with the edge cases in the limits $k \to -\pi$ and $k \to 0$. If also $g = 1$, then we impose that $\eta_{-\pi} = C_\pi^\dagger$, which is the same as if $g \neq 1$.

Equation (B.53) becomes

$$H = \sum_k E_k^+ \left(\eta_k^+\right)^\dagger \eta_k^+ + \sum_k E_k^- \left(\eta_k^-\right)^\dagger \eta_k^-. \tag{B.80}$$

Since

$$\left(\eta_{-k}^-\right)^\dagger = \eta_k^+ =: \eta_k \tag{B.81}$$

and $E_{-k}^\pm = E_k^\pm$, we may reduce eq. (B.80) to

$$H = \sum_k E_k \eta_k^\dagger \eta_k - \sum_k E_k \left(1 - \eta_k^\dagger \eta_k\right) \tag{B.82}$$

$$= \sum_k 2 E_k \eta_k^\dagger \eta_k - 1 \sum_k E_k. \tag{B.83}$$

Appendix C

Computer details

C.1 Julia version information

```
versioninfo()
```

```
Julia Version 1.6.0
Commit f9720dc2eb (2021-03-24 12:55 UTC)
Platform Info:
  OS: Linux (x86_64-pc-linux-gnu)
  CPU: Intel(R) Core(TM) i7-4710MQ CPU @ 2.50GHz
  WORD_SIZE: 64
  LIBM: libopenlibm
  LLVM: libLLVM-11.0.1 (ORCJIT, haswell)
Environment:
  JULIA_PROJECT = .
  JULIA_NUM_THREADS = 8
```

```julia
using Pkg
Pkg.activate(".")
```

```
  Activating environment at `~/drive/thesis/notebooks/Project.toml`
```

```julia
Pkg.status()
```

Status `~/drive/thesis/notebooks/Project.toml`

```
[537997a7] AbstractPlotting v0.15.27
[7d9fca2a] Arpack v0.4.0
[6e4b80f9] BenchmarkTools v0.7.0
[ad839575] Blink v0.12.5
[13f3f980] CairoMakie v0.3.19
[5ae59095] Colors v0.12.7
[150eb455] CoordinateTransformations v0.6.1
[e9467ef8] GLMakie v0.1.30
[7073ff75] IJulia v1.23.2
[d1acc4aa] IntervalArithmetic v0.17.8
[c8e1da08] IterTools v1.3.0
[5ab0869b] KernelDensity v0.6.2
[b964fa9f] LaTeXStrings v1.2.1
[2fda8390] LsqFit v0.12.0
[ee78f7c6] Makie v0.12.0
[eff96d63] Measurements v2.5.0
[3b7a836e] PGFPlots v3.3.6
[ccf2f8ad] PlotThemes v2.0.1
[58dd65bb] Plotly v0.3.0
[91a5bcdd] Plots v1.11.2
[92933f4c] ProgressMeter v1.5.0
[438e738f] PyCall v1.92.3
[6e0679c1] QuantumOptics v0.8.2
[4f57444f] QuantumOpticsBase v0.2.7
[189a3867] Reexport v0.2.0
[f3b207a7] StatsPlots v0.14.19
[24249f21] SymPy v1.0.42
[ac1d9e8a] ThreadsX v0.1.7
[1986cc42] Unitful v1.7.0
[276b4fcb] WGLMakie v0.3.4
[0f1e0344] WebIO v0.8.15
[37e2e46d] LinearAlgebra
```

```julia
using LinearAlgebra
BLAS.vendor()
```

```
:openblas64
```

C.2   NOTEBOOK PREAMBLE

```julia
using Plots, LaTeXStrings
using Unitful, Measurements
using LinearAlgebra, Arpack, QuantumOptics
using LsqFit, Roots
using ThreadsX

import PGFPlotsX
# If reevaluating, so no duplicates
!isempty(PGFPlotsX.CUSTOM_PREAMBLE) && pop!(PGFPlotsX.CUSTOM_PREAMBLE)
push!(PGFPlotsX.CUSTOM_PREAMBLE, "
    \\usepackage{amsmath}
    \\usepackage{physics}
    \\usepackage{siunitx}
    \\usepackage[full]{textcomp} % to get the right copyright, etc.
    \\usepackage[semibold]{libertinus-otf}
    \\usepackage[T1]{fontenc} % LY1 also works
    \\setmainfont[Numbers={OldStyle,Proportional}]{Libertinus Serif}
    \\usepackage[supstfm=libertinesups,supscaled=1.2,raised=-.13em]{superiors}
    \\setmonofont[Scale=MatchLowercase]{JuliaMono} % We need lots of unicode, like ⊗
    \\usepackage[cal=cm,bb=boondox,frak=boondox]{mathalfa}
    \\input{$(pwd())/latexdefs.tex}
    ");
pgfplotsx()

using PlotThemes
_fs = 12
theme(:vibrant,
    size=(400, 300),
    dpi=300,
    titlefontsize = _fs,
    tickfontsize = _fs,
    legendfontsize = _fs,
    guidefontsize = _fs,
    legendtitlefontsize = _fs
)

rubric = RGB(0.7, 0.05, 0.0); # The red color used in the thesis document.

# Pauli matrices
const σ0 = [1 0; 0 1]
const σx = [0 1; 1 0]
const σy = [0 -im; im 0]
const σz = [1 0; 0 -1]
const σp = [0 1; 0 0]
const σm = [0 0; 1 0]

⊗ₖ(a, b) = kron(b, a);
```

```julia
function siteop(A, i, n)
    i = i > 0 ? 1 + ((i - 1) % n) : throw(ArgumentError("Site index must be positive."))
    ops = repeat([one(A)], n)
    ops[i] = A
    reduce(⊗ₖ, ops)
end
```

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Index