Interacting Spins Decay as Open Quantum Systems

Draft

A Thesis

Presented to

The Division of Mathematics and Natural Sciences

Reed College

In Partial Fulfillment

of the Requirements for the Degree

Bachelor of Arts

Alex Striff

April 13, 2021

Approved for the Division
(Physics)

Darrell Schroeter

Acknowledgements

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	$\lvert v\rangle$
$\lvert v\rangle$ in coordinates	$\boldsymbol{v}$
Tuple	$\boldsymbol{n}$
Operator	A
Vector operator	$\boldsymbol{B}$
A in coordinates	$\boldsymbol{A}$
Superoperator	$\mathcal{A}$
One	1
Identity operator	1
Identity superoperator	$\mathbb{1}$
Zero	0
Zero operator	0
Zero superoperator	$\mathbb{0}$
Sign of x	$\operatorname{sgn} x$
Sinc function	$\operatorname{sinc} x = \dfrac{\sin x}{x}$

Real numbers	$\mathbb{R}$
Complex numbers	$\mathbb{C}$
Integers modulo n	$\mathbb{Z}_n$
Hilbert space	$\mathcal{H}$
Bounded operators	$\mathcal{B}(\mathcal{H})$
Liouville space	$\mathcal{L}(\mathcal{H})$
Hamiltonian operator	H
Density operator	ρ
Pauli operators	σ_i
Spin operators	$S_i = \hbar\sigma_i/2$
Inner product on $\mathcal{L}$	$\langle A\vert B\rangle$
Transpose of $\boldsymbol{A}$	$\boldsymbol{A}^\intercal$
Adjoint of A	$A^\dagger$
Trace of A	$\operatorname{tr} A$
Partial trace over S	tr_S
Expected value of A	$\langle A\rangle = \operatorname{tr}(\rho A)$
Hermitian part of A	$\operatorname{He} A = \dfrac{A + A^\dagger}{2}$

Chapter 1

Open quantum systems

What happens after performing an operation on a physical system? Our actions are uncertain, so the best we can do is to assign probabilities to the possible outcomes. Quantum mechanics is a theory for determining the probabilities of such outcomes. Physical theories model the relevant aspects of phenomena by abstracting away unnecessary information. Newtonian mechanics considers point masses while neglecting the material composition of bodies. This enables a simpler description of motion. Just as Newtonian mechanics models physical systems as "Newtonian systems" of point masses, quantum mechanics models physical systems with **quantum states** which represent only the probabilistic description of operation outcomes. A penny and a quarter are different physical systems that correspond to the same "quantum system," as far as the outcomes of coin tosses are concerned.[1]

1.1 A sketch of quantum mechanics

What follows is a sketch of quantum theory that helps motivate the mathematical formalism we use later.

We are interested in performing operations that have consistent effects, for otherwise we could make little sense of the world. Consider performing an operation with m outcomes on a quantum system. Given a particular outcome, this operation is a **measurement** if repeating the operation gives the same outcome with probability one.[2]

---

[1]That is, in an ideal sense. Actual coins made from many atoms are not two-outcome systems. For example, the coin atoms could melt into a blob, rendering them unflippable.

[2]On this view, the result of a measurement is defined operationally. This avoids confusion with prop-

We may then characterize a quantum system by its **dimension** N, which is the maximum number of outcomes distinguishable by a measurement.[3] This means that a $(N+1)$-outcome operation cannot be a measurement on a N-dimensional system. Repeating such an operation cannot produce the same outcome with certainty.

1.1.1 ENTROPY

Since quantum states encode the probabilities of outcomes, it is relevant to have a measure for how uncertain we are about which outcome will happen.

To do so, we must quantify the uncertainty expressed by a probability distribution of outcomes. The most successful definition of this uncertainty due to Shannon considers the **surprisal** I of an event with probability p [1]. This is a function I that has the following intuitive properties:[4]

1. $I(1) = 0$: Certain events are unsurprising.
2. $I(p) < I(p')$ if $p' < p$: Less probable events are more surprising.
3. $I(p) \geqslant 0$: Surprisal cannot be negative.
4. $I(p, p') = I(p) + I(p')$: The surprisal of independent events is the sum of the surprisals for each event.

The only functions with these properties are of the form $I(p) = b \log p$ for $b < 0$. Choosing b amounts to choosing the base of the logarithm and the unit of information. It is standard to use base two for which the unit of the surprisal

$$I(p) = -\log p \tag{1.1}$$

is the **bit**. The uncertainty expressed by a probability distribution of outcomes is called the **Shannon entropy**, and is defined as the expected surprisal of an outcome:

$$\begin{aligned} H &= \langle I \rangle \qquad (1.2) \\ &= -\sum_i p_i \log p_i, \qquad (1.3) \end{aligned}$$

erties of *physical* systems: an outcome with probability one is a different kind of thing than a physical property.

[3] This supposes that such systems exist, which requires experimental verification. For example, Stern-Gerlach type experiments demonstrate the existence of a two-dimensional quantum system. As far as we are concerned, we have examples of quantum systems for all dimensions.

[4] Technically, I is defined for a random variable X with support $\mathcal{X}$, so that $I : \mathcal{X} \to \mathbb{R}$ is a function of the probability of an event: $I(x) = f(P(x))$.

where $0 \log 0 := \lim_{p \to 0} p \log p = 0$. Thus an operation with a certain outcome has $H = 0$. The most uncertain one can be in a m-outcome operation is to have $p_i = 1/m$. In that case, $H = \log m$.

We now define the **von Neumann entropy** S of a quantum state ρ to be the minimum entropy of any measurement of the state. If $S(\rho) = 0$, there is a measurement with a definite outcome for ρ. Since the other outcomes are excluded, ρ is called a **pure state**, rather than a **mixed state** which has probability spread out over more than one outcome.

1.1.2 Hardy's postulates

TODO: Rewrite as quantum logic.

Now that we have the notion of a pure state, we may indicate postulates of quantum theory.

We expect that K real numbers are needed to describe a quantum state ρ and to predict the probabilities of outcomes. In quantum theory, we posulate the following statements about N and K:

1. K is a function of N, which we may select to be the smallest value consistent with the remaining postulates.

2. A N-dimensional system constrained to only M states distinguishable by measurement behaves like a system of dimension M.

3. A composite system consisting of subsystems A and B satisfies $N = N_A N_B$ and $K = K_A K_B$.

These statements apply equally well to classical probability theory. Quantum theory is distinguished by the final postulate:

4. There is a continuous and reversible transformation between any two pure states of a system.

These postulates are enough to reproduce quantum mechanics as we know it. While this has been just a sketch, Hardy gives a more precise description and demonstrates agreement with the formalism to follow [2]. In particular, Hardy shows that $K = N^2$, which corresponds to considering a complex Hilbert space.

1.2 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. Motivated by section 1.1.2, we now make the following postulates:

Postulate 1. A quantum system is described by a separable complex Hilbert space $\mathcal{H}$.[5]

Postulate 2. An outcome corresponds to an **effect** E, which is a self-adjoint operator on $\mathcal{H}$ such that $0 \leqslant E \leqslant 1$.[6]

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

$$\left(\sum_i p_i P_i\right)(E) = \sum_i p_i P_i(E). \tag{1.4}$$

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

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

$$P(E) = \operatorname{tr}(\rho E), \tag{1.5}$$

where $\rho \geqslant 0$ is a self-adjoint operator known as a **density operator** [3, 4].[7] Equation (1.5) implies that $\operatorname{tr}\rho = 1$ 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.

[5]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.

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

[7]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 [5].

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 valued measure** (PVM). 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

$$\rho'_m = P(m)^{-1}\mathcal{O}_m\rho. \tag{1.6}$$

Inherent in postulate 5 is the normalization condition $\operatorname{tr}\rho' = 1$, which implies that $\operatorname{tr}\mathcal{O}_m\rho = \operatorname{tr}(\rho E_m)$, as well as the requirement that $\mathcal{O}_m\rho \geqslant 0$. If an operation is performed but the outcome is unknown, we may assign the state

$$\rho' = \sum_m P(m)\rho'_m = \sum_m \mathcal{O}_m\rho, \tag{1.7}$$

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

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

$$\frac{\mathcal{O}_m\rho}{\operatorname{tr}\mathcal{O}_m\rho} = \sum_i P(i\,|\,m)\frac{\mathcal{O}_m\rho_i}{\operatorname{tr}\mathcal{O}_m\rho_i} \tag{1.8}$$

By Bayes' theorem,

$$P(i\,|\,m) = \frac{P(i)P(m\,|\,i)}{P(m)} = \frac{p_i \operatorname{tr}\mathcal{O}_m\rho_i}{\operatorname{tr}\mathcal{O}_m\rho}. \tag{1.9}$$

Now eq. (1.8) becomes

$$\mathcal{O}_m\left(\sum_i p_i\rho_i\right) = \sum_i p_i\mathcal{O}_m\rho_i. \tag{1.10}$$

Thus operations are convex linear.

1.2.1 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.[8]

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

$$\operatorname{tr}(\rho f_i(E_i)) = \operatorname{tr}(g_i(\rho)E_i) \tag{1.11}$$

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

$$\left(\sum_i \alpha_i \rho_i^A, \sum_j \beta_j \rho_j^B \right) \sim \sum_{ij} \alpha_i \beta_j \big(\rho_i^A, \rho_j^B \big) \tag{1.12}$$

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 $\mathcal{B}(\mathcal{H}_A) \otimes \mathcal{B}(\mathcal{H}_B) \cong \mathcal{B}(\mathcal{H})$.[9] 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 $(\rho_A \otimes \rho_B)(E_A \otimes E_B) = \rho_A E_A \otimes \rho_B E_B$.

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

$$\operatorname{tr}(A \otimes B) = \operatorname{tr} A \operatorname{tr} B. \tag{1.13}$$

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

---

[8]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.

[9]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 [6, pp. 84–87].

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. (1.11),

$$\operatorname{tr}\left(\rho \sum_a f(E_a)\right) = \sum_a \operatorname{tr}(\rho f(E_a)) \tag{1.14}$$

$$= \sum_a \operatorname{tr}(g(\rho)E_a) \tag{1.15}$$

$$= \operatorname{tr}\left(g(\rho) \sum_a E_a\right) \tag{1.16}$$

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

for all ρ. Thus f is countably additive. If $E_1 \leqslant E_2$, then $0 \leqslant \operatorname{tr}(g(\rho)(E_2 - E_1)) = \operatorname{tr}(\rho f(E_2 - E_1))$ so $f(E_1) \leqslant f(E_2)$. It then follows that the f_i are convex.[10] 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

$$g_A(\rho) = \operatorname{tr}_B(\rho_A \otimes \rho_B) \equiv \rho_A \operatorname{tr} \rho_B = \rho_A, \tag{1.18}$$

and is extended linearly to combinations of product states.

1.2.2 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.

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. (1.10). Since the information in the state ρ cannot change, $\mathcal{O}$ must be invertible. Kadison's theorem[11] states that all such operations have the form

$$\mathcal{O}\rho = U\rho U^\dagger, \tag{1.19}$$

where the operator U is either **unitary** ($U^\dagger U = 1$) or **antiunitary** ($U^\dagger U = -1$) [7, 10].

[10] The argument is the same as that for the real linearity of a probability measure on effects given in [3].

[11] Wigner's theorem on symmetries of pure states is a special case [7, p. 77]. Many similar results hold, such as that only unitary transformations preserve the entropy (relative or not) [8, 9].

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

$$\rho(t) = U(t)\rho(0)U^\dagger(t) \tag{1.20}$$

as a function of time. We expect that $U(t)$ changes continuously[12] and satisfies

$$U(t + t') = U(t)U(t') \tag{1.21}$$

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 [12], which states that there is a self-adjoint operator H such that

$$U(t) = e^{-\mathrm{i}Ht}. \tag{1.22}$$

This allows us to differentiate eq. (1.20) to find

$$\begin{align}
\dot{\rho} &= \dot{U}(t)\rho(0)U^\dagger(t) + U(t)\rho(0)\dot{U}^\dagger(t) \tag{1.23}\\
&= -\mathrm{i}H\big(U(t)\rho(0)U^\dagger(t)\big) + \big(U(t)\rho(0)U^\dagger(t)\big)\mathrm{i}H \tag{1.24}\\
&= -\mathrm{i}[H, \rho], \tag{1.25}
\end{align}$$

which is known as the **Liouville** or **von Neumann equation**.[13]

TODO: Explain the link to classical phase space and canonical commutation. Why is H the Hamiltonian?

TODO: Dynamical pictures

1.2.3 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 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.

[12]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 [11].

[13]Equation (1.25) is given in **Planck units** where $\hbar = c = G = k_B = 1$. Otherwise $\dot{\rho} = -\mathrm{i}[H, \rho]/\hbar$.

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: [13]

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

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

   (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 $\rho_S(t) = \operatorname{tr}_B \rho(t)$.

In summary, the state at time t is

$$\rho_S(t) = \operatorname{tr}_B(U(t)\mathcal{A}(\rho_0)U^\dagger(t)). \tag{1.26}$$

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 $\mathcal{H}_B$ [14]. 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 $\mathcal{A}$? Since ρ_B does not change in time, this would require 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_S where the system changes appreciably. If the timescale of the excitations in the bath is τ_B, then from the perspective of a system with $\tau_B \ll \tau_S$, 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. (1.26) for the coarse-graining to be possible. Since the system must be weakly coupled to the bath for the bath to remain stationary, these simplifications are collectively called the **weak-coupling limit**.

Assume completely positive [14, 15, 16].

We will find that the most general form of $\mathcal{L}$ is given by the **Lindblad equation** eq. (1.41). To obtain this result, first consider diagonalizing ρ_B as $\rho_B = \sum_j \lambda_j |\phi_j\rangle\langle\phi_j|$ with orthonormal vectors $\phi_j \in \mathcal{H}_B$, where $\sum_j \lambda_j = 1$. Then eq. (1.26) becomes (writing ρ_S as ρ)

$$\rho(t) = \sum_{ij} \langle\phi_i|U(t)\big(\rho(0) \otimes \lambda_j |\phi_j\rangle\langle\phi_j|\big)U^\dagger(t)|\phi_i\rangle \tag{1.27}$$

$$= \sum_{ij} \lambda_j \langle\phi_i|U(t)|\phi_j\rangle\, \rho(0)\, \langle\phi_j|U^\dagger(t)|\phi_i\rangle \tag{1.28}$$

$$= \sum_{ij} M_{ij}(t)\rho(0)M_{ij}^\dagger(t), \tag{1.29}$$

where $M_{ij}(t) \equiv \sqrt{\lambda_j}\,\langle\phi_i|U(t)|\phi_j\rangle$. This decomposition in terms of the M_{ij} is an instance of the Choi-Kraus representation theorem (theorem 2.1.4). We can express the M_{ij} in terms of an orthonormal complete basis $\{F_n\}$ for $\mathcal{L}(\mathcal{H}_S)$ as $M_{ij} = \sum_k F_k \langle F_k|M_{ij}\rangle$. Then eq. (1.29) becomes

$$\rho(t) = \sum_{mn} c_{mn}(t)F_m\rho(0)F_n^\dagger, \tag{1.30}$$

where

$$c_{mn}(t) \equiv \sum_{ij} \big\langle F_m\big|M_{ij}(t)\big\rangle \big\langle M_{ij}(t)\big|F_n\big\rangle\,. \tag{1.31}$$

For convenience, we may choose $F_{d^2} = 1/\sqrt{d}$, where $d = \dim(\mathcal{H}_S)$. With an eye towards simplifying eq. (1.36), we eliminate the explicit time dependence of eq. (1.31) by defining

$$a_{mn} \equiv \lim_{t\to 0^+} \frac{c_{mn}(t) - d\delta_{d^2d^2}}{t} \tag{1.32}$$

and introduce the sum of Kraus operators

$$F = \frac{1}{\sqrt{d}} \sum_{n=1}^{d^2-1} a_{nd^2}F_n \tag{1.33}$$

$$= \frac{F + F^\dagger}{2} + \mathrm{i}\frac{F - F^\dagger}{2\mathrm{i}} \equiv G + H/\mathrm{i}\hbar, \tag{1.34}$$

where we have decomposed the sum F into Hermitian and anti-Hermitian parts and included $\hbar$ so that H will have dimensions of energy. Now we may write the master equation

$\mathcal{L}\rho = \dot{\rho}$ as

$$\dot{\rho} = \lim_{\Delta t \to 0^+} \frac{\mathcal{V}(\Delta t)\rho - \rho}{\Delta t} \tag{1.35}$$

$$= \lim_{\Delta t \to 0^+} \left(\frac{c_{d^2 d^2} - d}{d\Delta t}\rho + \sum_{m,n=1}^{d^2-1} \frac{c_{mn}(\Delta t)}{\Delta t} F_m \rho F_n^\dagger + \frac{1}{\sqrt{d}} \sum_{n=1}^{d^2-1} \left(\frac{c_{nd^2}(\Delta t)}{\Delta t} F_n \rho + \frac{c_{d^2 n}(\Delta t)}{\Delta t} \rho F_n^\dagger \right) \right) \tag{1.36}$$

$$= \frac{a_{d^2 d^2}}{d}\rho + F\rho + \rho F^\dagger + \sum_{m,n=1}^{d^2-1} a_{mn} F_m \rho F_n^\dagger \tag{1.37}$$

$$= \frac{a_{d^2 d^2}}{d}\rho + \{G, \rho\} + \frac{[H,\rho]}{\mathrm{i}\hbar} + \sum_{m,n=1}^{d^2-1} a_{mn} F_m \rho F_n^\dagger \tag{1.38}$$

$$= \{G', \rho\} + \frac{[H,\rho]}{\mathrm{i}\hbar} + \sum_{m,n=1}^{d^2-1} a_{mn} F_m \rho F_n^\dagger, \tag{1.39}$$

where $G' = G + a_{d^2 d^2} 1 \big/ d$. Since $\mathcal{V}(t)$ is trace-preserving, $\operatorname{tr}\dot{\rho} = 0$. Applying this condition to eq. (1.39) and cycling the trace gives

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

so $G' = -\sum_{m,n=1}^{d^2-1} a_{mn} F_n^\dagger F_m / 2$. This allows us to write eq. (1.39) as

$$\dot{\rho} = \frac{[H,\rho]}{\mathrm{i}\hbar} + \sum_{m,n=1}^{d^2-1} a_{mn} \left(F_m \rho F_n^\dagger - \frac{1}{2}\left\{ F_n^\dagger F_m, \rho \right\} \right), \tag{1.40}$$

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. (1.31) to be Hermitian, and eq. (1.32) 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

$$\dot{\rho} = \frac{[H,\rho]}{\mathrm{i}\hbar} + \sum_{k=1}^{d^2-1} \gamma_k \left(L_k \rho L_k^\dagger - \frac{1}{2}\left\{ L_k^\dagger L_k, \rho \right\} \right) \equiv \mathcal{L}\rho, \tag{1.41}$$

which is the *diagonal form* of the Lindblad equation. The eigenvalues γ_k have dimensions of inverse time and the Lindblad operators may be taken to be traceless. The second term is often called the **dissipator** $\mathcal{D}$ (see section 1.3), so the Lindbladian may be separated into unitary and non-unitary parts.

1.3 THE WEAK-COUPLING LIMIT

Now that we have found the general form for a stochastic CPTP generator, we must now determine the conditions for interaction Hamiltonian in eq. (2.7) to give rise to Markovian dynamics. While there are several different regimes where this is true, we will consider the **weak-coupling** limit which we justify by supposing that the environment is similar to a **harmonic bath** of many harmonic oscillators.

We start by expressing the interaction Hamiltonian in terms of Hermitian operators as

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

We suppose that the system in isolation would have *discrete* energy levels, so the eigenoperators of the superoperator $\mathcal{S} = [H_S, -]$ form a complete basis for $\mathcal{L}(\mathcal{H}_S)$. We then may write $A_\alpha = \sum_\omega A_{\alpha\omega}$, where

$$[H_S, A_{\alpha\omega}] = -\omega A_{\alpha\omega} \tag{1.42}$$

and

$$A_{\alpha\omega} = \sum_{E'-E=\omega} \Pi(E) A_\alpha \Pi(E'). \tag{1.43}$$

Using eq. (1.42) to commute past the exponential in **??** gives $A'_{\alpha\omega} = e^{-\mathrm{i}\omega t} A_{\alpha\omega}$ in the interaction picture. Thus the interaction Hamiltonian in the interaction picture is

$$H'_I = \sum_{\alpha\omega} e^{-\mathrm{i}\omega t} A_{\alpha\omega} \otimes B'_\alpha, \tag{1.44}$$

where $B'_\alpha(t) = e^{-H_B t/\mathrm{i}\hbar} B_\alpha e^{H_B t/\mathrm{i}\hbar}$ per **??**.

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

$$\langle B^\dagger_\alpha(t) B_\beta(t-s)\rangle_{\rho_B} \tag{1.45}$$

and their one-sided Fourier transform

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty \mathrm{d}s\, e^{\mathrm{i}\omega s} \left\langle B^\dagger_\alpha(t) B_\beta(t-s)\right\rangle_{\rho_B} \tag{1.46}$$

$$\equiv \mathrm{i} S_{\alpha\beta}(\omega) + \gamma_{\alpha\beta}(\omega)\big/2, \tag{1.47}$$

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

$$\gamma_{\alpha\beta}(\omega) \equiv \int_{-\infty}^\infty \mathrm{d}s\, e^{\mathrm{i}\omega s} \left\langle B^\dagger_\alpha(t) B_\beta(t-s)\right\rangle_{\rho_B} \tag{1.48}$$

is positive.

With this setup, we may now move to the main derivation. It is helpful to consider the interaction picture time evolution ?? in the integral form

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

Applying ?? again and tracing out the environment gives the closed equation

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

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

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

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: $\langle B_\alpha(t)\rangle_{\rho_B} = 0$.

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:

$$\dot{\rho}_S = -\int_0^\infty \mathrm{d}s\, \mathrm{tr}_B\, [H_I(t), [H_I(t-s), \rho_S(t) \otimes \rho_B]]. \tag{1.49}$$

This is justified when the reservoir correlation functions in eq. (1.46) vanish quickly over a time τ_B that is smaller than the relaxation time τ_R (see ??). Substituting eq. (1.44) into eq. (1.49) and using eq. (1.46) gives

$$\dot{\rho}_S = 2\, \mathrm{He} \sum_{\alpha\beta\omega\omega'} e^{\mathrm{i}(\omega'-\omega)t} \Gamma_{\alpha\beta}(\omega) \Big(A_{\beta\omega} \rho_S A^\dagger_{\alpha\omega'} - A^\dagger_{\alpha\omega'} A_{\beta\omega} \rho_S \Big), \tag{1.50}$$

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

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

for system evolution are large compared to the relaxation time τ_R, then the contribution from the fast-oscillating terms of eq. (1.50) 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

$$\dot{\rho}_S = 2\,\mathrm{He} \sum_{\alpha\beta\omega} \Gamma_{\alpha\beta}(\omega)\Big(A_{\beta\omega}\rho_S A^{\dagger}_{\alpha\omega} - A^{\dagger}_{\alpha\omega}A_{\beta\omega}\rho_S\Big). \tag{1.51}$$

Now applying the decomposition eq. (1.47) gives the interaction picture Lindblad equation

$$\dot{\rho}_S = -\mathrm{i}[H_{LS}, \rho_S] + \mathcal{D}\rho_S, \tag{1.52}$$

where the **Lamb shift Hamiltonian** is

$$H_{LS} = \sum_{\alpha\beta\omega} S_{\alpha\beta}(\omega) A^{\dagger}_{\alpha\omega}A_{\beta\omega}, \tag{1.53}$$

and the *dissipator* is

$$\mathcal{D}\rho_S = \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}\Big(A_{\beta\omega}\rho_S A^{\dagger}_{\alpha\omega} - \frac{1}{2}\Big\{A^{\dagger}_{\alpha\omega}A_{\beta\omega}, \rho_S\Big\}\Big). \tag{1.54}$$

The Lamb shift (or environment renormalization) Hamiltonian commutes with the system Hamiltonian since eq. (1.42) implies that $[H_S, A^{\dagger}_{\alpha\omega}A_{\beta\omega}] = 0$. Adding the system's Hamiltonian H_S to H_{LS} and diagonalizing gives the Schrödinger picture Lindblad equation eq. (1.41).

1.4 Relaxation to thermal equilibrium

The system will generally relax from its initial configuration to a stationary solution of eq. (1.41) (see **??**). We expect that the thermal state

$$\rho_S = \frac{e^{-\beta H_S}}{Z} \quad \text{where} \quad Z = \mathrm{tr}\Big(e^{-\beta H_S}\Big)$$

would be the equilibrium state. This is true when the reservoir correlation functions obey the KMS condition [17, 18]

$$\Big\langle B^{\dagger}_{\alpha}(t)B_{\beta}(0)\Big\rangle_{\rho_B} = \Big\langle B_{\beta}(0)B^{\dagger}_{\alpha}(t+\mathrm{i}\beta)\Big\rangle_{\rho_B}, \tag{1.55}$$

which is true when the environment is in the thermal state $\rho_B = e^{-\beta H_B}/\mathrm{tr}\Big(e^{-\beta H_B}\Big)$.

Chapter 2

Density operator theory

2.1 Mathematical details

Definition 1 (Tensor product). Consider vector spaces $V(k)$, $W(k)$, and Z. For any bilinear map $h : V \times W \to Z$, the **tensor product** $V \otimes W$ and associated bilinear map $\phi : V \times W \to V \otimes W$ map have the property that there is a unique linear map $g : V \otimes W \to Z$ such that $h = g \circ \phi$. For tensor products of Hilbert spaces, the inner product is defined on each element of a product and then the space is completed. There is then a natural correspondence between the element $v \otimes f$ of the tensor product $V \otimes V^*$ and the linear map $T : V \to V$ defined by $Tx = f(x)v$.

This induces an extension of Dirac notation where all pairs $f \otimes x$ of dual and usual vectors from the same space are evaluated as $\langle f|x\rangle = f(x)$ and extended linearly. For example, given a linear operator $U : V \otimes W \to V \otimes W$ and a basis $|\phi_i\rangle$ for W, the partial trace over W may be expressed as $\mathrm{tr}_W\, U = \langle\phi_i|U|\phi_i\rangle$. This forms the justification of the step from eq. (1.27) to eq. (1.28) and of the manipulations in theorem 2.1.4.

Theorem 2.1.1 (Klein inequality). *For density operators ρ and ρ', $S(\rho\|\rho') \geq 0$, with equality if and only if $\rho = \rho'$.*

Proof. The case for equality is trivial, so we will consider $\rho \neq \rho'$. Let $\mathcal{F}\rho = \rho \ln \rho$, so that we may express the relative entropy as

$$S(\rho\|\rho') = \mathrm{tr}(\mathcal{F}\rho - \mathcal{F}\rho' - \delta\mathcal{F}'\rho'),$$

where $\delta = \rho - \rho'$. We then have for $0 < t < 1$ that

$$\rho' + t\delta = t\rho + (1-t)\rho'.$$

Now let $f(t) = \operatorname{tr}(\mathcal{F}(\rho' + t\delta))$. Since the trace is monotonic and convex, f is convex and $f(t) \leq f(0) + t(f(1) - f(0))$. Rearranging and taking the limit as $t \to 0^+$ gives

$$f'(0) \leq f(1) - f(0),$$

which evaluates to

$$\operatorname{tr}(\delta \mathcal{F}' \rho') \leq \operatorname{tr} \mathcal{F}\rho - \operatorname{tr} \mathcal{F}\rho'. \qquad \square$$

Theorem 2.1.2. *For a unitary operator U and density operators ρ and ρ',*

$$S(U\rho U^\dagger \| U\rho' U^\dagger) = S(\rho\|\rho').$$

Proof. Since we may cycle the traces, it suffices to show that

$$\ln\left(U\rho U^\dagger\right) = \ln \rho.$$

This follows from Jacobi's formula for invertible matrices when applied to the logarithm that takes us from a Lie group to its corresponding Lie algebra, giving $\operatorname{tr} \circ \det = \operatorname{tr} \circ \log$. $\square$

Theorem 2.1.3. *For density operators ρ and ρ',*

$$S(\operatorname{tr}_B \rho \| \operatorname{tr}_B \rho') \leq S(\rho\|\rho'),$$

with equality if and only if ρ or ρ' is uncorrelated.

Theorem 2.1.4 (Choi-Kraus representation [19]). *A superoperator $\mathcal{S}$ on a density operator ρ is completely positive and trace-preserving if and only if it may be represented as*

$$\rho = \sum_{k=1}^{K} M_k \rho M_k^\dagger, \quad \textit{where} \quad \sum_{k=1}^{K} M_k M_k^\dagger = 1.$$

2.2 THE BORN-MARKOV APPROXIMATION FOR THE ISING CHAIN IN A BATH

The bath Hamiltonian is

$$H_B = \sum_{\boldsymbol{k},\lambda} \hbar\omega_{\boldsymbol{k}} a_{\boldsymbol{k},\lambda}^\dagger a_{\boldsymbol{k},\lambda}. \tag{2.1}$$

The vacuum energy $\sum_{\boldsymbol{k},\lambda} \hbar\omega_{\boldsymbol{k}}/2$ is dropped, since it diverges in the continuum limit.

The interaction Hamiltonian for spin-s objects in a magnetic field is [1]

$$\begin{aligned} H_I &= -\int \mathrm{d}\boldsymbol{r}\, \boldsymbol{\mu}\cdot\boldsymbol{B} && (2.2)\\ &= -\int \mathrm{d}\boldsymbol{r} \sum_i \mu_e \delta(\boldsymbol{r}_i)\boldsymbol{\sigma}_i \\ &\cdot \mathrm{i}\sum_{\boldsymbol{k},\lambda}\sqrt{\frac{\hbar c^2\mu_0}{2V\omega_{\boldsymbol{k}}}}\Big((\boldsymbol{k}\times\boldsymbol{e}_{\boldsymbol{k},\lambda})e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}a_{\boldsymbol{k},\lambda} - \big(\boldsymbol{k}\times\boldsymbol{e}^*_{\boldsymbol{k},\lambda}\big)e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}}a^\dagger_{\boldsymbol{k},\lambda}\Big) && (2.3)\\ &= -\sum_{i,\mu}\sigma_i^\mu B_i^\mu, && (2.4)\end{aligned}$$

where we have defined the Hermitian operator

$$B_i^\mu = \mathrm{i}\mu_e\sum_{\boldsymbol{k},\lambda}\sqrt{\frac{\hbar c^2\mu_0}{2V\omega_{\boldsymbol{k}}}}\Big(\big(\boldsymbol{k}\times\boldsymbol{e}_{\boldsymbol{k},\lambda}\big)_\mu e^{\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_i}a_{\boldsymbol{k},\lambda} - \big(\boldsymbol{k}\times\boldsymbol{e}^*_{\boldsymbol{k},\lambda}\big)_\mu e^{-\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{r}_i}a^\dagger_{\boldsymbol{k},\lambda}\Big). \quad (2.5)$$

This magnetic field operator includes the electron's magnetic moment so that the final rate γ (eq. (2.36)) carries the dimensions of frequency in the dissipator (eq. (1.54)).

The composite Hamiltonian we consider is

$$\begin{aligned} H &= H_S\otimes 1 + 1\otimes H_B + H_I && (2.6)\\ &= -J(g)\sum_{i\in\mathbb{Z}_N}\big(f(1-g)\sigma_i^x\sigma_{i+1}^x + f(g)\sigma_i^z\big)\otimes 1 \\ &+ 1\otimes\sum_{\boldsymbol{k},\lambda}\hbar\omega_{\boldsymbol{k}}a^\dagger_{\boldsymbol{k},\lambda}a_{\boldsymbol{k},\lambda} - \sum_{i,\mu}\sigma_i^\mu\otimes B_i^\mu, && (2.7)\end{aligned}$$

where

- $J(g) > 0\,\mathrm{J}$ 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. (2.22),
- The spin positions in eq. (2.5) are $\boldsymbol{r}_i = ai\hat{z}$ for some spacing a,
- The dipole approximation is valid. This requires that $a \ll c/\omega_{\boldsymbol{k}}$ for $\omega_{\boldsymbol{k}}$ up to the largest transition energy possible for H_S. A bound is $\omega_{\boldsymbol{k}} \leqslant 2NJ(1)/\hbar$ for constant J.

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

We will 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. (1.52)) are per the system timescale $\tau_S = \hbar/J(g)$.

In the interaction picture:

$$B_i^\mu(t) = e^{\mathrm{i}H_B t/\hbar} B_i^\mu e^{-\mathrm{i}H_B t/\hbar} \tag{2.8}$$

$$= \mathrm{i}\mu_e \sum_{\boldsymbol{k},\lambda} \sqrt{\frac{\hbar c^2 \mu_0}{2V\omega_{\boldsymbol{k}}}} \Big(\left(\boldsymbol{k} \times \boldsymbol{e}_{\boldsymbol{k},\lambda}\right)_\mu e^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}_i - \omega_{\boldsymbol{k}} t)} a_{\boldsymbol{k},\lambda} - \left(\boldsymbol{k} \times \boldsymbol{e}^*_{\boldsymbol{k},\lambda}\right)_\mu e^{-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}_i - \omega_{\boldsymbol{k}} t)} a^\dagger_{\boldsymbol{k},\lambda} \Big). \tag{2.9}$$

The spectral correlation tensor is then

$$\Gamma_{i\mu,j\nu}(\omega) = \frac{\mu_e^2}{\hbar^2} \int_0^\infty \mathrm{d}s\, e^{\mathrm{i}\omega s} \left\langle B_i^\mu(t)^\dagger B_j^\nu(t-s) \right\rangle \tag{2.10}$$

$$\begin{aligned} &= -\frac{\mu_e^2}{\hbar^2} \frac{\hbar c^2 \mu_0}{2V} \int_0^\infty \mathrm{d}s \sum_{\boldsymbol{k},\boldsymbol{k}',\lambda,\lambda'} \sqrt{\frac{1}{\omega_{\boldsymbol{k}}\omega_{\boldsymbol{k}'}}} \; : \\ &\left(\boldsymbol{k} \times \boldsymbol{e}_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k}' \times \boldsymbol{e}_{\boldsymbol{k}',\lambda'}\right)_\nu e^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}_i - \omega_{\boldsymbol{k}} t + \boldsymbol{k}'\cdot\boldsymbol{r}_j - \omega_{\boldsymbol{k}'}(t-s) + \omega s)} \left\langle a_{\boldsymbol{k},\lambda} a_{\boldsymbol{k}',\lambda'} \right\rangle \\ &- \left(\boldsymbol{k} \times \boldsymbol{e}_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k}' \times \boldsymbol{e}^*_{\boldsymbol{k}',\lambda'}\right)_\nu e^{\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}_i - \omega_{\boldsymbol{k}} t - \boldsymbol{k}'\cdot\boldsymbol{r}_j + \omega_{\boldsymbol{k}'}(t-s) + \omega s)} \left\langle a_{\boldsymbol{k},\lambda} a^\dagger_{\boldsymbol{k}',\lambda'} \right\rangle \\ &- \left(\boldsymbol{k} \times \boldsymbol{e}^*_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k}' \times \boldsymbol{e}_{\boldsymbol{k}',\lambda'}\right)_\nu e^{-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}_i - \omega_{\boldsymbol{k}} t - \boldsymbol{k}'\cdot\boldsymbol{r}_j + \omega_{\boldsymbol{k}'}(t-s) - \omega s)} \left\langle a^\dagger_{\boldsymbol{k},\lambda} a_{\boldsymbol{k}',\lambda'} \right\rangle \\ &+ \left(\boldsymbol{k} \times \boldsymbol{e}^*_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k} \times \boldsymbol{e}^*_{\boldsymbol{k}',\lambda'}\right)_\nu e^{-\mathrm{i}(\boldsymbol{k}\cdot\boldsymbol{r}_i - \omega_{\boldsymbol{k}} t + \boldsymbol{k}'\cdot\boldsymbol{r}_j - \omega_{\boldsymbol{k}'}(t-s) - \omega s)} \left\langle a^\dagger_{\boldsymbol{k},\lambda} a^\dagger_{\boldsymbol{k}',\lambda'} \right\rangle . \end{aligned} \tag{2.11}$$

In the thermal state

$$\rho_B = \frac{e^{-\beta H_B}}{\operatorname{tr} e^{-\beta H_B}} = \prod_{\boldsymbol{k},\lambda} \left(1 - e^{-\beta\hbar\omega_{\boldsymbol{k}}}\right) e^{-\beta\hbar\omega_{\boldsymbol{k}} a^\dagger_{\boldsymbol{k},\lambda} a_{\boldsymbol{k},\lambda}} \tag{2.12}$$

Since $\left[a_{\boldsymbol{k},\lambda}, a^\dagger_{\boldsymbol{k}',\lambda'}\right] = \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'} 1$,

$$\left\langle a^\dagger_{\boldsymbol{k},\lambda} a_{\boldsymbol{k}',\lambda'} \right\rangle = \operatorname{tr}\left(e^{-\beta H_B}\right)^{-1} \operatorname{tr}\left(e^{-\beta H_B} a^\dagger_{\boldsymbol{k},\lambda} a_{\boldsymbol{k}',\lambda'}\right) \tag{2.13}$$

$$= \operatorname{tr}\left(e^{-\beta H_B}\right)^{-1} \operatorname{tr}\left(e^{-\beta H_B} a_{\boldsymbol{k}',\lambda'} a^\dagger_{\boldsymbol{k},\lambda}\right) - \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'} \tag{2.14}$$

$$= \operatorname{tr}\left(e^{-\beta H_B}\right)^{-1} \operatorname{tr}\left(e^{\beta\hbar\omega_{\boldsymbol{k}}} a_{\boldsymbol{k}',\lambda'} e^{-\beta H_B} a^\dagger_{\boldsymbol{k},\lambda}\right) - \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'} \tag{2.15}$$

$$= e^{\beta\hbar\omega_{\boldsymbol{k}}} \left\langle a^\dagger_{\boldsymbol{k},\lambda} a_{\boldsymbol{k}',\lambda'} \right\rangle - \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'} \tag{2.16}$$

$$= \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'} n_B(\omega_{\boldsymbol{k}}), \tag{2.17}$$

where

$$n_B(\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}. \tag{2.18}$$

Similarly,

$$\left\langle a_{\boldsymbol{k},\lambda} a_{\boldsymbol{k}',\lambda'} \right\rangle = \left\langle a^\dagger_{\boldsymbol{k},\lambda} a^\dagger_{\boldsymbol{k}',\lambda'} \right\rangle = 0 \tag{2.19}$$

$$\left\langle a_{\boldsymbol{k},\lambda} a^\dagger_{\boldsymbol{k}',\lambda'} \right\rangle = \delta_{\boldsymbol{k}\boldsymbol{k}'}\delta_{\lambda\lambda'}(1 + n_B(\omega_{\boldsymbol{k}})). \tag{2.20}$$

Then for a thermal bath, the spectral correlation tensor becomes

$$\begin{aligned} \Gamma_{i\mu,j\nu}(\omega) = \frac{\mu_e^2 c^2 \mu_0}{2\hbar V} \int_0^\infty \mathrm{d}s \sum_{\boldsymbol{k},\,\lambda} \frac{1}{\omega_{\boldsymbol{k}}} :& \\ \left(\boldsymbol{k}\times\boldsymbol{e}_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k}\times\boldsymbol{e}^*_{\boldsymbol{k},\lambda}\right)_\nu e^{\mathrm{i}(\boldsymbol{k}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)+s(\omega-\omega_{\boldsymbol{k}}))}(1+n_B(\omega_{\boldsymbol{k}}))& \\ + \left(\boldsymbol{k}\times\boldsymbol{e}^*_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k}\times\boldsymbol{e}_{\boldsymbol{k},\lambda}\right)_\nu e^{-\mathrm{i}(\boldsymbol{k}\cdot(\boldsymbol{r}_i-\boldsymbol{r}_j)-s(\omega+\omega_{\boldsymbol{k}}))} n_B(\omega_{\boldsymbol{k}}).& \end{aligned} \tag{2.21}$$

To evaluate eq. (2.21), we now consider a chain of N spins along the z-axis, so that $\boldsymbol{r}_i = r_i\hat{\boldsymbol{z}}$.[2] Then $\boldsymbol{k}\cdot(\boldsymbol{r}_i - \boldsymbol{r}_j) = k_z \Delta r_{ij}$.

In the continuum limit,

$$\frac{1}{V}\sum_{\boldsymbol{k}} \mapsto \int \frac{\mathrm{d}\boldsymbol{k}}{(2\pi)^3} = \frac{1}{(2\pi c)^3}\int_0^\infty \mathrm{d}\omega_k\, \omega_k^2 \int \mathrm{d}\Omega\,, \tag{2.22}$$

where the integral over solid angle is

$$\int \mathrm{d}\Omega = \int \mathrm{d}\phi \int \mathrm{d}\theta \sin\theta. \tag{2.23}$$

To apply this limit to eq. (2.21), we first note that

$$\sum_\lambda \left(\boldsymbol{k}\times\boldsymbol{e}_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k}\times\boldsymbol{e}^*_{\boldsymbol{k},\lambda}\right)_\nu = \sum_{abcd} \varepsilon_{\mu ab}\varepsilon_{\nu cd} k^a k^c \sum_\lambda e^b_{\boldsymbol{k},\lambda}\left(e^d_{\boldsymbol{k},\lambda}\right)^* \tag{2.24}$$

$$= \sum_{abcd} \varepsilon_{\mu ab}\varepsilon_{\nu cd} k^a k^c \left(\delta_{bd} - \frac{k^b k^d}{k^2}\right) \tag{2.25}$$

$$= \sum_{abc} \varepsilon_{\mu ab}\varepsilon_{\nu cb} k^a k^c \tag{2.26}$$

$$= \sum_{ac} \left(\delta_{\mu\nu}\delta_{ac} - \delta_{\mu c}\delta_{a\nu}\right) k^a k^c \tag{2.27}$$

$$= k^2 \delta_{\mu\nu} - k^\mu k^\nu. \tag{2.28}$$

Thus

$$\int \mathrm{d}\Omega\, e^{\pm \mathrm{i} k_z \Delta r_{ij}} \sum_\lambda \left(\boldsymbol{k}\times\boldsymbol{e}_{\boldsymbol{k},\lambda}\right)_\mu \left(\boldsymbol{k}\times\boldsymbol{e}^*_{\boldsymbol{k},\lambda}\right)_\nu = \frac{8\pi\omega_k^2}{3c^2}\delta_{\mu\nu} G_\nu\left(\frac{\omega_k \Delta r_{ij}}{c}\right), \tag{2.29}$$

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

where

$$G_\nu(u) = \left(\delta_{\nu z} - \frac{\delta_{\nu x} + \delta_{\nu y}}{2}\right)\frac{\operatorname{sinc} u - \cos u}{u^2} + \frac{\delta_{\nu x} + \delta_{\nu y}}{2} \operatorname{sinc} u. \tag{2.30}$$

Note that in the dipole approximation

$$\lim_{u\to 0} G_\nu(u) = \left(\delta_{\nu z} - \frac{\delta_{\nu x} + \delta_{\nu y}}{2}\right)\frac{1}{3} + \frac{\delta_{\nu x} + \delta_{\nu y}}{2} = \frac{1}{3}. \tag{2.31}$$

Now eq. (2.29) gives that the continuum limit of the spectral correlation tensor for the spin chain is

$$\begin{aligned} \Gamma_{i\mu,j\nu}(\omega) = \delta_{\mu\nu} \frac{\mu_0}{6\pi^2 \mu_e^2 \hbar c^3} \int_0^\infty \mathrm{d}\omega_k \, \omega_k^3 G_\nu\left(\frac{\omega_k \Delta r_{ij}}{c}\right) : \\ (1 + n_B(\omega_k)) \int_0^\infty \mathrm{d}s \, e^{\mathrm{i}s(\omega-\omega_k)} + n_B(\omega_k) \int_0^\infty \mathrm{d}s \, e^{\mathrm{i}s(\omega+\omega_k)}. \end{aligned} \tag{2.32}$$

We now use that

$$n_B(-\omega) = -(1 + n_B(\omega)) \tag{2.33}$$

and

$$\int_0^\infty \mathrm{d}s \, e^{-\mathrm{i}\omega s} = \pi\delta(\omega) - \mathrm{i}\mathcal{P}\frac{1}{\omega}, \tag{2.34}$$

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

$$\Gamma_{i\mu,j\nu}(\omega) = \frac{1}{2}\gamma_{i\mu,j\nu}(\omega) + \mathrm{i}S_{i\mu,j\nu}(\omega), \tag{2.35}$$

where

$$\gamma_{i\mu,j\nu}(\omega) = \delta_{\mu\nu} \frac{\mu_e^2 \mu_0 \omega^3}{3\pi\hbar c^3} G_\nu\left(\frac{|\omega| \Delta r_{ij}}{c}\right)(1 + n_B(\omega)) \tag{2.36}$$

$$S_{i\mu,j\nu}(\omega) = \delta_{\mu\nu} \frac{\mu_e^2 \mu_0}{6\pi^2 \hbar c^3} \mathcal{P} \int_0^\infty \mathrm{d}\omega_k \, \omega_k^3 G_\nu\left(\frac{\omega_k \Delta r_{ij}}{c}\right)\left(\frac{1 + n_B(\omega_k)}{\omega - \omega_k} + \frac{n_B(\omega_k)}{\omega + \omega_k}\right). \tag{2.37}$$

The principal value integral in eq. (2.37) diverges to $-\infty$ when $i = j$ but vanishes otherwise. The net contribution to the Lamb shift Hamiltonian (eq. (1.53)) is effectively an infinite negative offset that may be neglected just like we neglect the zero-point energy of the bath. The unitary part of the reduced dynamics exactly matches that of the closed system, and $\mathcal{L} = \mathcal{D}$ in the interaction picture.

The dipole approximation then leaves

$$\gamma(\omega) = \frac{\mu_e^2 \mu_0 \omega^3}{9\pi\hbar c^3}(1 + n_B(\omega)) \tag{2.38}$$

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

$$\tilde{\gamma}(\tilde{\omega}) = \left(\frac{\tau_0}{\tau_S}\right)^2 \tilde{\omega}^3 \left(1 + \frac{1}{e^{\tau_B\tilde{\omega}/\tau_S} - 1}\right) \tag{2.39}$$

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

$$\tau_0 = \sqrt{\frac{\mu_e^2\mu_0}{9\pi\hbar c^3}} = 3.67 \times 10^{-23}\,\mathrm{s} \cong 56\,\mathrm{GeV}^{-1}. \tag{2.40}$$

If $\tau_B\tilde{\omega}/\tau_S \ll 1$, then

$$\tilde{\gamma}(\tilde{\omega}) \approx \frac{\tau_0^2}{\tau_B\tau_S}\tilde{\omega}^2. \tag{2.41}$$

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

$$\tilde{S}(\tilde{\omega}) = \frac{1}{2\pi}\left(\frac{\tau_0}{\tau_S}\right)^2 \mathcal{P}\int_0^\infty \mathrm{d}\tilde{\omega}_k\, \tilde{\omega}_k^3 \left(\frac{1 + \tilde{n}_B(\tilde{\omega}_k)}{\tilde{\omega} - \tilde{\omega}_k} + \frac{\tilde{n}_B(\tilde{\omega}_k)}{\tilde{\omega} + \tilde{\omega}_k}\right), \tag{2.42}$$

where

$$\tilde{n}_B(\tilde{\omega}) = \frac{1}{e^{\tau_B\tilde{\omega}/\tau_S} - 1}. \tag{2.43}$$

To avoid the divergence of eq. (2.42), we introduce an upper frequency cutoff $\tilde{\Omega}$. Physically, one expects the coupling to high-frequcency modes of the bath to weaken.[3] 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. In the limit where $\tau_B\tilde{\Omega}/\tau_S \ll 1$, $\tilde{S}$ now simplifies to

$$\begin{aligned}
\tilde{S}(\tilde{\omega}) &\approx \frac{1}{2\pi}\frac{\tau_0^2}{\tau_B\tau_S}\mathcal{P}\int_0^{\tilde{\Omega}} \mathrm{d}\tilde{\omega}_k\, \tilde{\omega}_k^2 \left(\frac{1}{\tilde{\omega} - \tilde{\omega}_k} + \frac{1}{\tilde{\omega} + \tilde{\omega}_k}\right) && (2.44)\\
&= \frac{\tau_0^2}{\tau_B\tau_S}\frac{\tilde{\omega}}{\pi}\left(\tilde{\omega}\,\mathrm{atanh}\left(\frac{\tilde{\omega}}{\tilde{\Omega}}\right) - \tilde{\Omega}\right) && (2.45)\\
&\approx -\frac{\tau_0^2}{\tau_B\tau_S}\frac{\tilde{\Omega}}{\pi}\tilde{\omega}, && (2.46)
\end{aligned}$$

where we have set the frequency cutoff $\tilde{\Omega} \gg \tilde{\omega}$ to be far above any system frequency.

[3] 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.

2.3 SUPEROPERATORS IN COORDINATES

Consider an orthonormal basis $|i\rangle$ for $\mathcal{H}$ and thus $\mathcal{L}$. This induces a basis for superoperators by pre and post-multiplication.

The superoperator matrix element for left-multiplication is

$$\langle ab|A_L|cd\rangle = \sum_{ef} \langle ab|A_{ef}|ef\rangle\,|cd\rangle \tag{2.47}$$
$$= \sum_{ef} \delta_{fc}\,\langle ab|A_{ef}|ed\rangle \tag{2.48}$$
$$= \sum_{ef} \delta_{fc}\delta_{ae}\delta_{bd}A_{ef} \tag{2.49}$$
$$= \delta_{db}A_{ac}, \tag{2.50}$$

while that for right-multiplication is

$$\langle ab|A_R|cd\rangle = \sum_{ef} \langle ab|A_{ef}|cd\rangle\,|ef\rangle \tag{2.51}$$
$$= \sum_{ef} \delta_{de}\,\langle ab|A_{ef}|cf\rangle \tag{2.52}$$
$$= \sum_{ef} \delta_{de}\delta_{ac}\delta_{bf}A_{ef} \tag{2.53}$$
$$= \delta_{ac}A_{db}. \tag{2.54}$$

Thus for both multiplications, we have that

$$\langle ab|A_LB_R|cd\rangle = \sum_{ef} \langle ab|A_L|ef\rangle\,\langle ef|B_R|cd\rangle \tag{2.55}$$
$$= \sum_{ef} \delta_{fb}\delta_{ec}A_{ae}B_{df} \tag{2.56}$$
$$= A_{ac}B_{db}. \tag{2.57}$$

In particular, if $B = A^\dagger$, this is $A_{ac}A^*_{bd}$, so that the trace of the superoperator is $\|A\|^2$.

Given A, we have the commutator superoperator $[A] = A_L - A_R$ and the anticommutator superoperator $\{A\} = A_L + A_R$. We then see that

$$\frac{1}{2}\,\langle ab|\{A^\dagger A\}|cd\rangle = \frac{1}{2}\sum_k \left(\delta_{db}A_{ak}A^*_{ck} + \delta_{ac}A_{dk}A^*_{bk}\right), \tag{2.58}$$

so the elements for the dissipator $\mathcal{D} = \sum_i \gamma_i \Big(A_L A_R^\dagger - \{A^\dagger A\}/2 \Big)$ are

$$\langle ab|\mathcal{D}|cd\rangle = \sum_i \gamma_i \left(A_{ac} A_{bd}^* - \frac{1}{2} \sum_k \left(\delta_{db} A_{ak} A_{ck}^* + \delta_{ac} A_{dk} A_{bk}^* \right) \right) \tag{2.59}$$

Chapter 3

Computing jump operators

```
using SymPy;
include("TransverseIsingModels.jl")
using .TransverseIsingModels
TIM = TransverseIsingModels;
```

3.1 Computation of jump operators

```
⊗ₖ(a, b) = kron(b, a);
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];

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;

function symeigen(H)
    symeig = H.eigenvects()
    vals, vecs = eltype(H)[], []
    for (λ, _, vs) in symeig
        for v in vs
            push!(vals, λ)
            push!(vecs, vec(v))
        end
    end
    vals, vecs
```

```
end;

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;

firstvalue(i, (x, y)) = x
lastvalue(i, (x, y)) = y
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;

TIM.sumprojector(A) = sum(a * a' for a in A);

function incentry!(dict, key; isequal=isequal)
    for k in keys(dict)
        if isequal(k, key)
            dict[k] += 1
            return dict
        end
    end
    dict[key] = 1
    dict
end;

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

function jumps(vals, vecs, As; combine=true, isequal=isequal)
    eigendict = dictby(zip(vals, vecs))
    ωs = dictby(((E2 - E1, (E1, E2)) for E1 in keys(eigendict) for E2 in keys(eigendict)),
     ↪  isequal=isequal)
    Πs = TIM.projectors(eigendict)
    Jωs = dictmap(ΔEs -> filter(x -> !isequal(x, zero(x)), [simplify.(sum(Πs[E1]*A*Πs[E2]
     ↪  for (E1, E2) in ΔEs)) for A in As]), ωs)
    combine ? dictmap(combinejumps, Jωs) : Jωs
```

```
end
spindim(v) = Int(log2(length(v)))
dipole_interactions(n) = vcat(map(A -> [siteop(A, i, n) for i in 1:n], [σx, σy, σz])...)
dipolejumps(vals, vecs; kwargs...) = jumps(vals, vecs,
    dipole_interactions(spindim(first(vecs)));
    kwargs...);

@vars s1p=>"σ₁⁺" s1m=>"σ₁⁻" commutative=false
@vars s2p=>"σ₂⁺" s2m=>"σ₂⁻" commutative=false
@vars s1x=>"σ₁ˣ" s2x=>"σ₂ˣ" commutative=false
@vars s1y=>"σ₁ʸ" s2y=>"σ₂ʸ" commutative=false
@vars s1z=>"σ₁ᶻ" s2z=>"σ₂ᶻ" commutative=false
@vars n1 =>"n₁"   n2=>"n₂"  commutative=false
@vars g d real=true;

spinops = [s1p, s1m, s2p, s2m, s1x, s2x, s1y, s2y, s1z, s2z, n1, n2];
_symspinop = cat([n1 s1p; s1m (1 - n1)], [n2 s2p; s2m (1 - n2)], dims=3)
_dummy_spinop = Dict(s => sympy.Dummy(s.name) for s in spinops);
site_collect_ops(siteops) = push!([_dummy_spinop[op] for op in siteops], 1)
_collect_ops = [a * b for a in site_collect_ops([s1p, s1m, n1]) for b in
 ↪  site_collect_ops([s2p, s2m, n2])];

u, v, w = Wild(:u), Wild(:v), Wild(:w);

symspinop(l, r, i) = _symspinop[l+1, r+1, i];
function jumpsimplify(J)
    s = mapreduce(+, CartesianIndices(J)[J .!= 0]) do I
        x = J[I]
        i, j = Tuple(I - CartesianIndex(1, 1))
        x * symspinop(i÷2, j÷2, 1) * symspinop(i%2, j%2, 2)
    end
    s = subs(expand(s), √(g^2 + 1) => d)
    s = s.simplify()
    s = s.xreplace(_dummy_spinop)
    for op in _collect_ops
        s = s.collect(op)
    end
    s.simplify()
end;

=>ₛ(a, b) = _dummy_spinop[a] => b
thesis_latex(J) = sympy.latex(J,
        imaginary_unit = "\\im",
        symbol_names = Dict(
            g   =>  "g",
            d   =>  "d",
            n1  =>ₛ "\\opr{n}_1",
            n2  =>ₛ "\\opr{n}_2",
            s1p =>ₛ "\\pauli_1^+",
            s2p =>ₛ "\\pauli_2^+",
            s1m =>ₛ "\\pauli_1^-",
            s2m =>ₛ "\\pauli_2^-",
        ));

function save_jump_latex(path, sJωs)
    open(path, "w") do file
```

```
        for (ω, Js) in sJωs
            sω = factor(subs(expand(ω), √(g^2 + 1) => d))
            println(file, thesis_latex(sω))
            println(file, " \\\\")
            for J in Js
                println(file, thesis_latex(J))
                println(file, " \\\\")
            end
            println(file, " \\\\")
        end
    end
end;
```

3.1.1 Nondegenerate jump operators

```
H = -2*(σx ⊗ₖ σx) - g*(σz ⊗ₖ σ0 + σ0 ⊗ₖ σz)
```

$$\begin{bmatrix} -2g & 0 & 0 & -2 \\ 0 & 0 & -2 & 0 \\ 0 & -2 & 0 & 0 \\ -2 & 0 & 0 & 2g \end{bmatrix}$$

```
sJωs = dictmap(Js -> jumpsimplify.(Js), dipolejumps(symeigen(H)...; combine=true))
save_jump_latex("nondegen-jumps.tex", sJωs)
```

3.1.2 Degenerate jump operators

```
H0 = subs.(-2*(σx ⊗ₖ σx) - g*(σz ⊗ₖ σ0 + σ0 ⊗ₖ σz), g => 0)
```

$$\begin{bmatrix} 0 & 0 & 0 & -2 \\ 0 & 0 & -2 & 0 \\ 0 & -2 & 0 & 0 \\ -2 & 0 & 0 & 0 \end{bmatrix}$$

```
sJωs0 = dictmap(Js -> jumpsimplify.(Js), dipolejumps(symeigen(H0)...; combine=true))
save_jump_latex("degen-jumps.tex", sJωs0)
```

3.2 Dissipator eigenvalue plots

```
leftmul(A)  = one(A) ⊗ₖ A
rightmul(A) = permutedims(A) ⊗ₖ one(A)
```

```
comm(A, B) = A*B - B*A
acomm(A, B) = A*B + B*A
commwith(A) = leftmul(A) - rightmul(A)
acommwith(A) = leftmul(A) + rightmul(A);

nB(ω, β) = 1 / (exp(β*ω) - 1)
γdiv(ω; β) = isapprox(ω, 0, atol=1e-9) ? 0 : ω^3 * (nB(ω, β) + 1)
# γdiv(ω; β) = isapprox(ω, 0, atol=1e-9) ? 0 : ω^2 # High temperature approx.
ℋLSterm(J, S) = S * commwith(J' * J)
ℋLS(Jωs, S; params...) = -im * sum(ℋLSterm(J, S(ω; params...)) for (ω, Js) in Jωs for J in
↪  Js)
𝒟term(J, γ) = γ * (leftmul(J) * rightmul(J') - acommwith(J' * J) / 2)
𝒟(Jωs, γ; params...) = sum(𝒟term(J, γ(ω; params...)) for (ω, Js) in Jωs for J in Js);
𝒟LRterm(J, γ) = γ * (leftmul(J) * rightmul(J'))
𝒟LR(Jωs, γ; params...) = sum(𝒟LRterm(J, γ(ω; params...)) for (ω, Js) in Jωs for J in Js);
𝒟Aterm(J, γ) = γ * (- acommwith(J' * J) / 2)
𝒟A(Jωs, γ; params...) = sum(𝒟Aterm(J, γ(ω; params...)) for (ω, Js) in Jωs for J in Js);

function numeigen(H)
    vals, vecs = eigen(H)
    vals, eachcol(vecs)
end

isequalto(atol=1e-9) = (x, y) -> isapprox(x, y, atol=atol)

function unitary_rates(H, dict, γ; params...)
    Jωs = dipolejumps(numeigen(N.(subs.(H, dict)))...;
        combine=true, isequal=isequalto())
    lambham = (x -> isequalto()(x, zero(x)) ? zero(x) : x).(ℋLS(Jωs, γ; params...))
    eigvals(lambham)
end

function dissipation_rates(H, dict, γ; params...)
    Jωs = dipolejumps(numeigen(N.(subs.(H, dict)))...;
        combine=true, isequal=isequalto())
    dissipator = (x -> isequalto()(x, zero(x)) ? zero(x) : x).(𝒟(Jωs, γ; params...))
    eigvals(dissipator)
end;

function dissipation_rates(H, γ; params...)
    Jωs = dipolejumps(numeigen(H)...; combine=true, isequal=isequalto())
    dissipator = (x -> isequalto()(x, zero(x)) ? zero(x) : x).(𝒟(Jωs, γ; params...))
    eigvals(dissipator)
end;

rubric = RGB(0.7, 0.05, 0.0);

function ηenergyvariance(H, η)
    Es = eigvals(H) / η
    Z = sum(exp(-E) for E in Es)
    Ps = [exp(-E) / Z for E in Es]
    H1 = sum(E * P for (E, P) in zip(Es, Ps))
    H2 = sum(E^2 * P for (E, P) in zip(Es, Ps))
    H2 - H1^2
end;
```

We map $E \mapsto E/\eta$ so that η is a dimensionless inverse temperature β.

```
using Roots

trnorm(A) = √(tr(A'*A))
trnormalize(A) = A / trnorm(A)
∠(A, B) = acos(trnorm(trnormalize(A)' * trnormalize(B)))
function slerp(A, B, g)
    θ = ∠(A, B)
    (sin((1-g)*θ)*A + sin(g*θ)*B) / sin(θ)
end

# Requirement: `normslerp` must not change the reference Hamiltonian.
function normslerp(A, B, g)
    C = slerp(A, B, g)
    C /= trnorm(C)
end

Ainvar(g, H0) = find_zero(A -> ηenergyvariance(H0(0), 1) - ηenergyvariance(H0(g), 1/A), 1)
function Hinterp(H1, H2)
    H0(g) = normslerp(trnormalize(H1), trnormalize(H2), g)
    g -> Ainvar(g, H0) * H0(g)
end

function plot_interp_rates(H1, H2, g0s; kwargs...)
    β = 1.0
    H = Hinterp(H1, H2)
    rates_ising = [real(dissipation_rates(H(g), γdiv, β = β)) for g in g0s]
    rates_free_ising = real(dissipation_rates(H(0), γdiv, β = β));
    rates_free_trans = real(dissipation_rates(H(1), γdiv, β = β));

    plot(g0s, -hcat(rates_ising...)',
        xlabel=L"Relative angle $g$",
        ylabel="Relative dissipator eigenvalues (negated)",
        color=:black,
        alpha=0.25,
        key=false;
        kwargs...)

    scatter!(repeat([g0s[1] - 2e-2], length(rates_free_ising)), -rates_free_ising,
        marker=(:rtriangle, 2, rubric),
        markerstrokecolor=rubric
    )
    scatter!(repeat([g0s[end] + 2e-2], length(rates_free_trans)), -rates_free_trans,
        marker=(:ltriangle, 2, rubric),
        markerstrokecolor=rubric
    )
end;

η0s = 10 .^ range(-1, 1.5, length=128)
βs = [1e-1, 2e-1, 5e-1, 1e0, 2e0, 5e0, 1e1, 2e1, 5e1];
```

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);
```

Convenient slerp:

```
plot_interp_rates(Hx(2), Hz(2), range(1e-3, 1-1e-3, length=64))
```

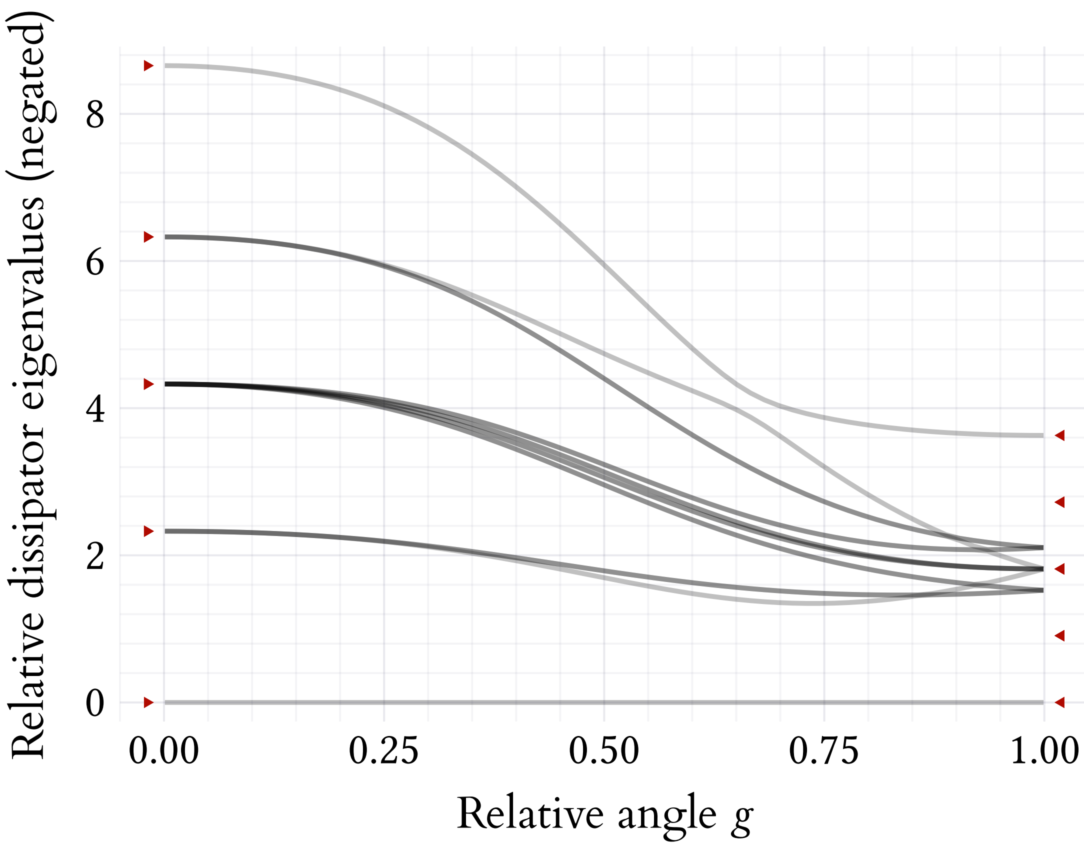

Figure 3.1

```
plot_interp_rates(Hx(3), Hz(3), range(1e-3, 1-1e-3, length=64))
```

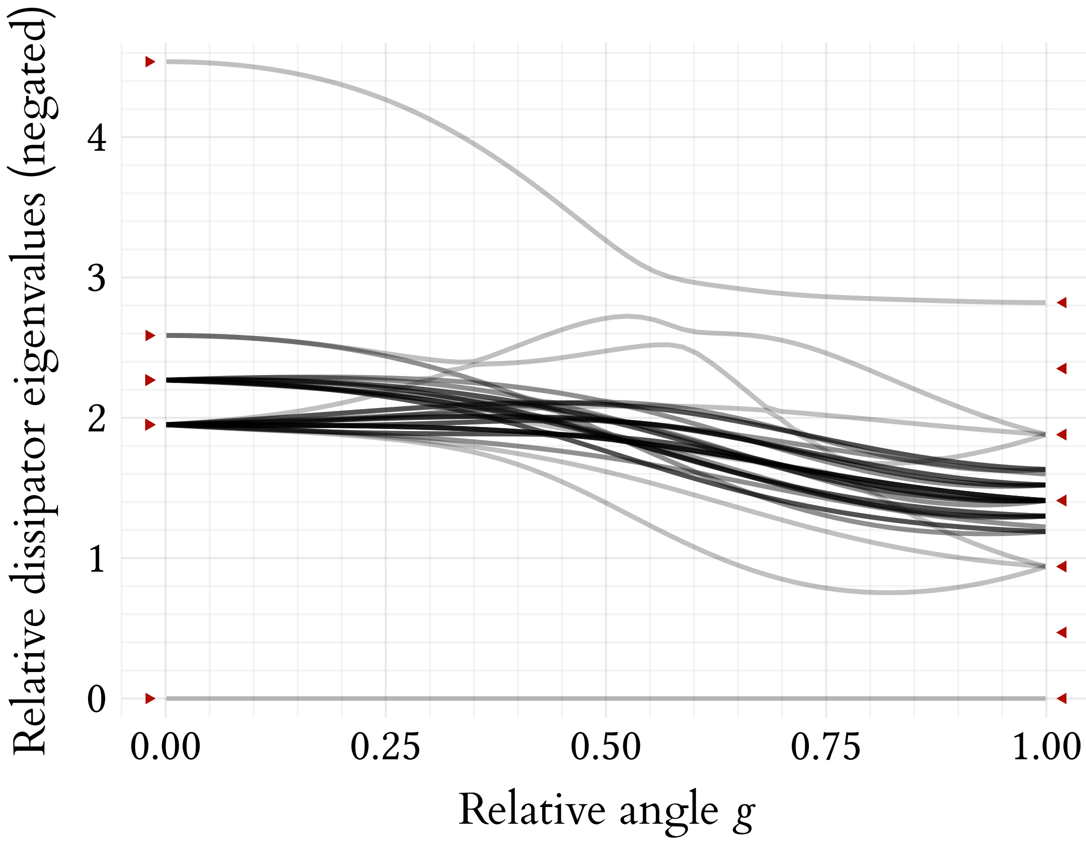

Figure 3.2

```
Hp = Hinterp(Hx(6), Hz(6));
```

```
lgs = range(1e-3, 1-1e-3, length=64)
energies = [eigvals(Hp(g)) for g in lgs]
Hnorms = [trnorm(Hp(g))^2 for g in lgs]
energydifferences = [[x - y for (x, y) in Iterators.product(Es, Es)] for Es in energies];
```

```
plot(lgs, hcat(energies...)', color=:black, alpha=0.25, key=false, xlabel=L"g", ylabel=L"E")
```

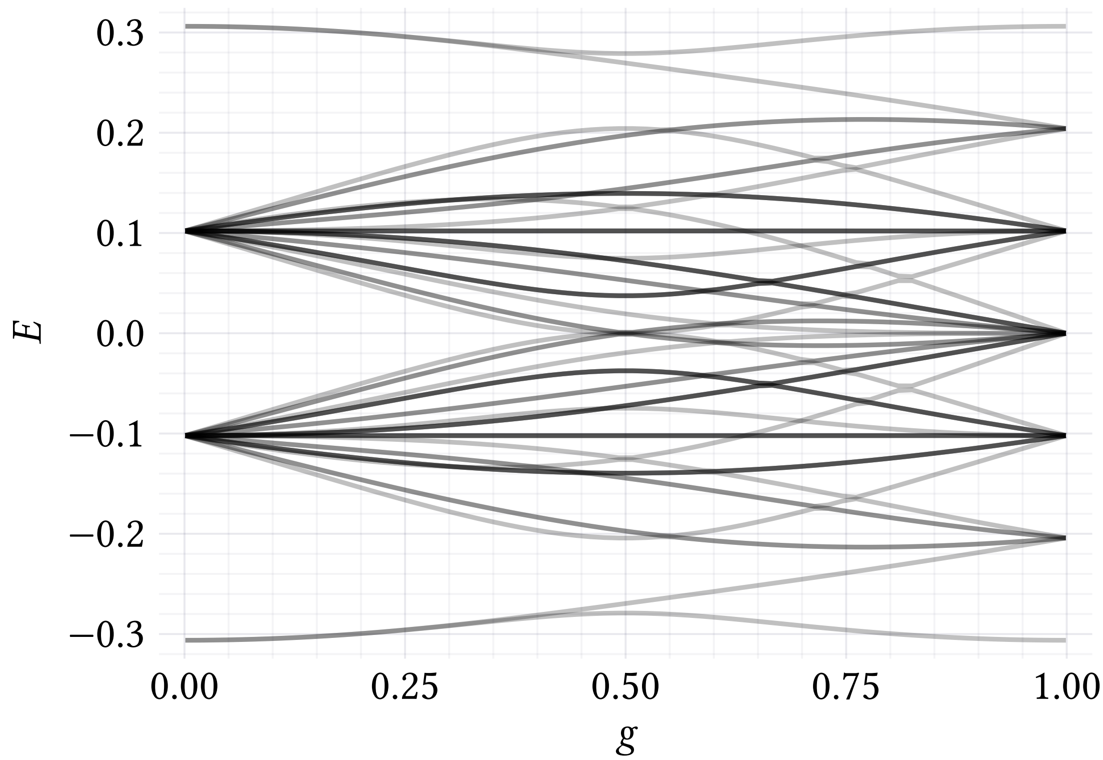

Figure 3.3

3.3 PLOTS FOR SEMINAR

```
σ2zs(n) = -1 / (2n + 1)
σ2z(τ, n) = (1 - σ2zs(n))*exp(-τ) + σ2zs(n)
nH = 0
plot(τ -> (1 - σ2z(τ, nH))/2, label="Ground state",
    color=:black,
    xlim=(0, 5),
    ylim=(-0.01, 1),
    xlabel=L"Time ($\gamma t$)",
    ylabel="Populations",
    title="Decay from the excited state in vacuum",
)
plot!(τ -> (1 + σ2z(τ, nH))/2, xlim=(0, 5), label="Excited state", linestyle=:dash,
 ↪  color=:black)
scatter!(5 * [1, 1], [1 + σ2zs(nH), 1 - σ2zs(nH)] / 2, label="Equilibrium value",
    marker=(:ltriangle, 4, rubric),
    markerstrokecolor=rubric)
```

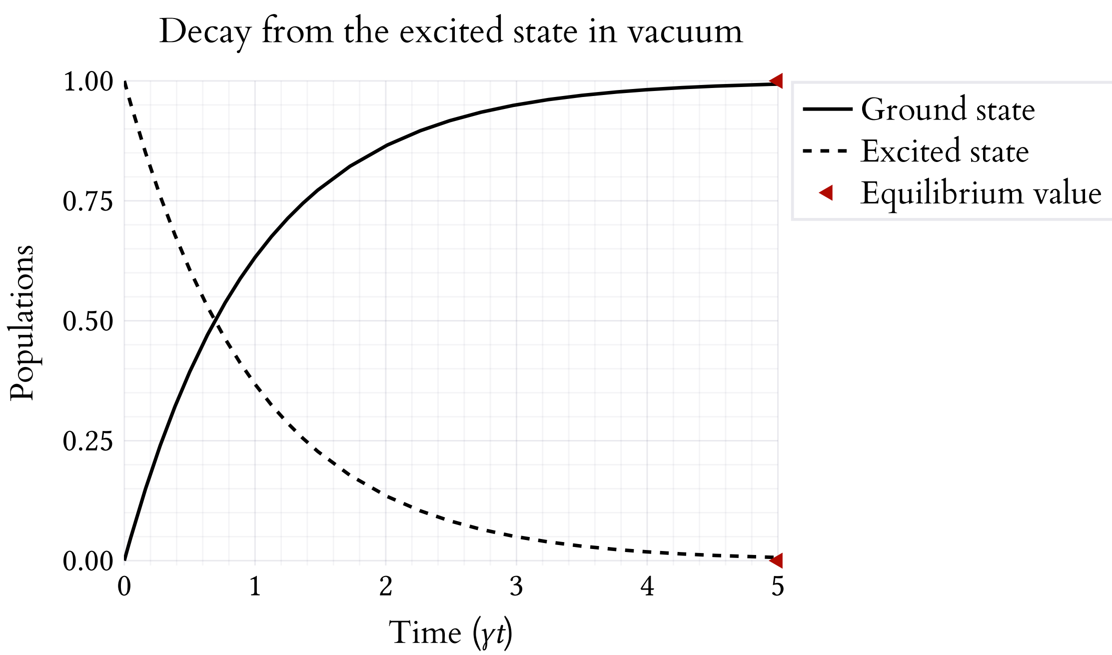

Figure 3.4

```
savefig("populations.pdf")
```

3.4 EXPLICIT SIMULATION

```
g = 0.25
n = 4
Hsys = Hinterp(Hx(n), Hz(n))(g)
Jωs = dipolejumps(numeigen(Hsys)...; combine=true, isequal=isequalto());
```

QuantumOptics simulation

```
b = SpinBasis(1//2)
sys = ⊗(repeat([b], n)...);
jumpops, rates = [], Float64[]
α = 1e-2 # Modifies amplitudes of γ and S due to vacuum timescale. α = τ0 / τB τS.
Ω = 1e1 * maximum(keys(Jωs))
for (ω, Js) in Jωs
    for J in Js
        push!(rates, α * ω^2)
        push!(jumpops, DenseOperator(sys, J))
    end
end
lambham = -α * (Ω / π) * sum(ω * J' * J for (ω, Js) in Jωs for J in Js);
```

```
σzm = dense(embed(sys, 1, sigmaz(b)))
function fout(t, ρ)
```

```
    ρ = normalize(ρ)
    real(expect(σzm, ρ))
end
Hspin = DenseOperator(sys, Hsys)
Hopen = DenseOperator(sys, Hsys + lambham)
σzth = fout(0.0, thermalstate(Hspin, 1e0))
tf = 5e2
ts = range(0.0, tf, length=501);

up = spinup(b)
ψ0 = ⊗(repeat([up], n)...)
ρ0 = projector(ψ0)
_, fouts0 = timeevolution.schroedinger(ts, ψ0, Hspin; fout=fout)
_, fouts1 = timeevolution.schroedinger(ts, ψ0, Hopen; fout=fout)
_, fouts = timeevolution.master(ts, ρ0, Hopen, jumpops; rates=rates, fout=fout)
_, foutsd = timeevolution.master(ts, ρ0, 0*Hspin, jumpops; rates=rates, fout=fout);

plot(
    title=L"ODE solutions for $N = %$n$",
    xlabel=L"Time ($s$)",
    ylabel=L"\ev{\pauli_1^z}",
)
plot!(ts, [fouts0 fouts1 fouts foutsd], label=["Closed" L"Closed (with $\ham_{LS}$)" "Open"
 ↪  "Dissipator"])
```

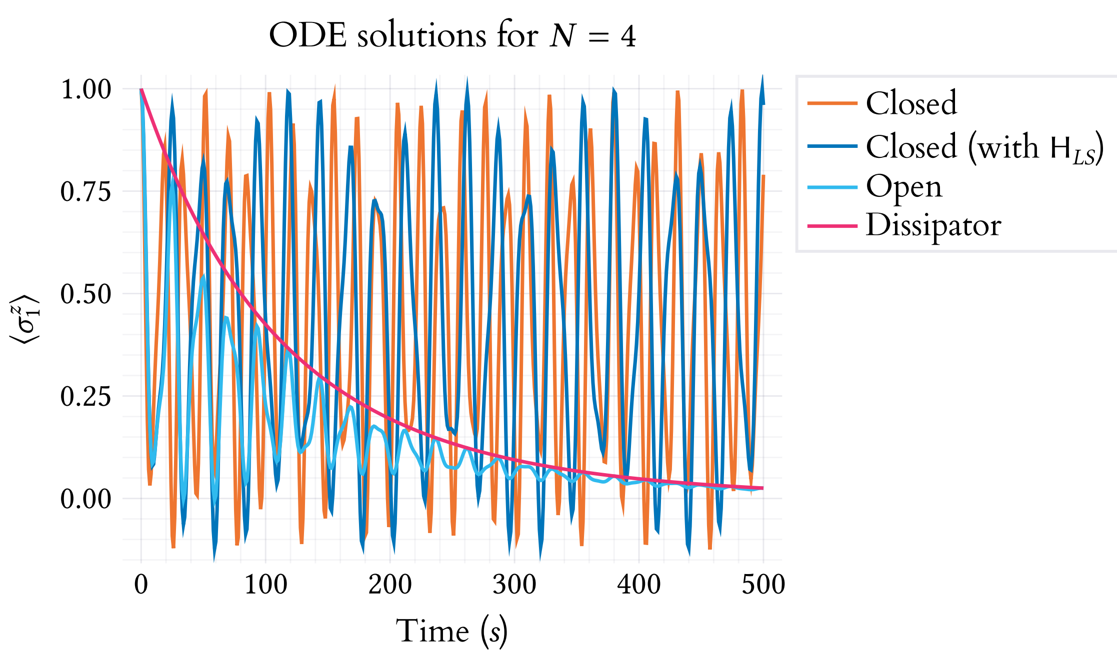

Figure 3.5

```
ℒ = steadystate.liouvillian(Hopen, jumpops; rates=rates);
```

The adjoint Liouvillian can be found by taking the adjoint of the matrix for $\mathcal{L}$. This has the same spectrum as $\mathcal{L}$.

```
ℒspectrum = steadystate.liouvillianspectrum(ℒ;
↪  nev=length(ℒ.basis_r[1])*length(ℒ.basis_r[2]))
𝒟rates = real(ℒspectrum[1])
```

```
256-element Vector{Float64}:
 -2.5477339636199218e-17
 -0.0006899863086337092
 -0.00473864459256778
 -0.00498818926598614
 -0.0050570716724551565
 -0.005069450295544094
 -0.005069450295544111
 -0.00506945029554412
 -0.005069450295544128
 -0.005069450295544132
 -0.005069450295544136
 -0.005069450295544139
 -0.005069450295544156
  ⋮
 -0.01057924890753321
 -0.01057924890753345
 -0.012783168352329045
 -0.012783168352329058
 -0.017995282447441342
 -0.017995282447441863
 -0.017943931696574933
 -0.01794393169657464
 -0.017943931696574836
 -0.017943931696574822
 -0.017892580945707892
 -0.017892580945708003
```

```
mean(𝒟rates)
```

```
-0.009477289185135535
```

```
coeffs = hcat([vec(V.data) for V in ℒspectrum[2]]...) \ vec(ρ0.data)
```

```
256-element Vector{ComplexF64}:
      0.2500000000000043 + 8.842846366035223e-15im
     -0.0748149646405942 + 1.9234759328589347e-15im
   1.5277735603797055e-15 - 8.34878837203075e-15im
     -0.1669218556306542 - 4.51370315198793le-15im
    1.300600042830515e-14 - 2.595043724748l774e-14im
    9.887770645641099e-15 + 1.613192747617552e-15im
    3.583973702173136e-15 + 3.366424278058229e-14im
   2.5697176775342834e-14 + 1.169572072782087e-14im
   -2.935805273568061e-14 - 1.2646162494917541e-14im
    3.161686283305576e-14 + 1.6029279509312884e-14im
    3.759884170332577e-15 + 2.6302949391241534e-14im
   -3.196220865838927e-14 - 8.503063271940365e-15im
    5.827524737741796e-14 + 3.890624031327461e-14im
                         ⋮
     -0.1918540363051984 + 3.457658251967246e-16im
    -0.19185403630520037 - 5.55964033525093e-15im
     0.07903486836634614 - 1.143696749786896e-15im
      0.0790348683663434 - 2.982185948284355e-15im
  -4.3113667435224516e-17 - 6.821359964983261e-17im
    3.481983938458291e-17 - 1.8379346772733038e-16im
   -5.393032090618151e-17 - 2.066833272533412e-17im
   5.2960120012542536e-17 - 1.5723047460740617e-16im
   -8.491028488113494e-17 - 9.518092876799662e-17im
   -3.061298708459077e-16 - 7.907292010401243e-17im
     0.12361525154468493 - 1.613251271582742e-16im
     0.12361525154468506 + 2.1709844684430279e-16im
```

```
eigenexpectations = [tr(σzm * V) for V in ℒspectrum[2]];

contributors = @. (abs(eigenexpectations) > 1e-9) & (abs(coeffs) > 1e-9);

weightedrate = -real(sum(@. abs2(coeffs) * ℒspectrum[1]) ./ sum(abs2, coeffs))
```

```
0.008912199413846697
```

Note that the eigenoperators are not orthogonal.

```
sum(abs, [tr(V1' * V2) for V1 in ℒspectrum[2], V2 in ℒspectrum[2]] - Matrix(1.0I, 256, 256))
```

```
46.495885713019845
```

```
using LsqFit

# @. decay_exponential(x, p) = (p[1]*exp(-x*p[2]) + p[3]*exp(-x*p[4])) / 2
# p0 = [1.0, 1e-4, 1.0, 1e-4]
@. decay_exponential(x, p) = p[1]*exp(-x*p[2])
p0 = [1.0, 1e-4]
fit = curve_fit(decay_exponential, ts, foutsd, p0)
plot(ts, (foutsd .- decay_exponential(ts, fit.param)) .^ 2)
```

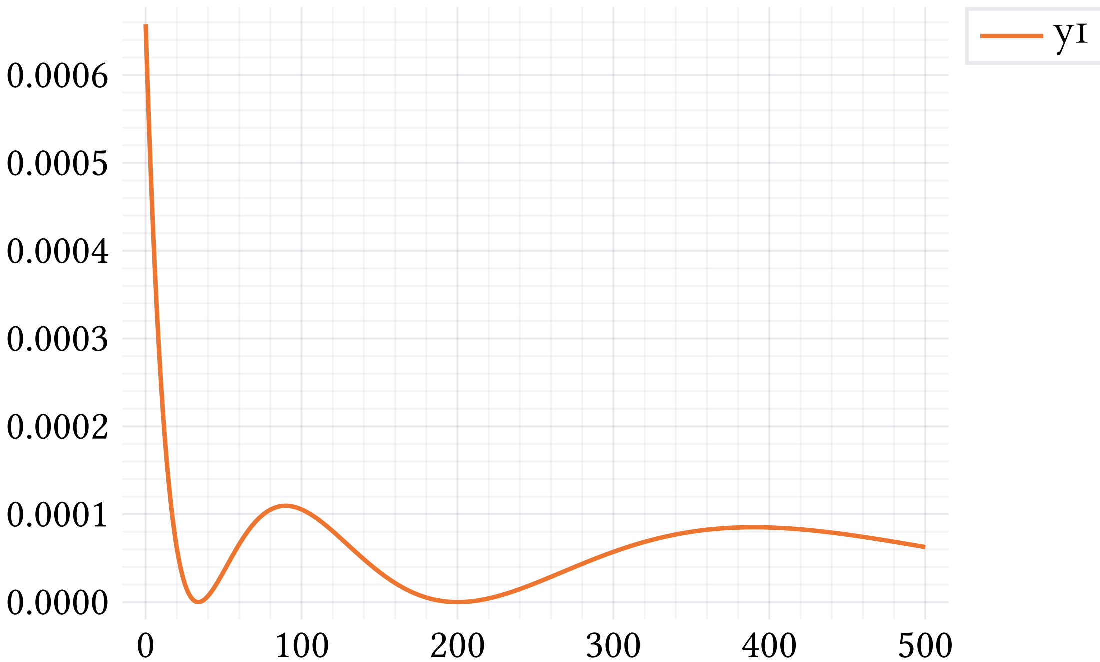

Figure 3.6

```
plot(ts, [foutsd decay_exponential(ts, fit.param) decay_exponential(ts, [1.0,
 ↪  weightedrate])])
```

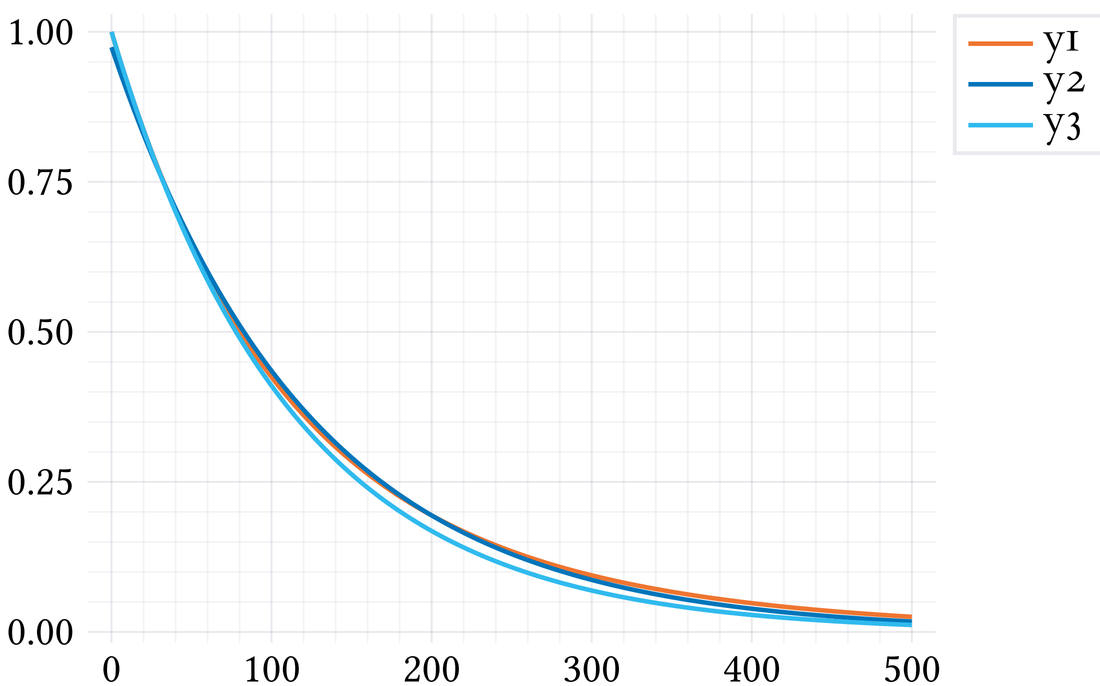

Figure 3.7

```
fit.param
```

```
2-element Vector{Float64}:
 0.9743534083163763
 0.008065309064495676
```

3.5 Two-spin degenerate jump operators

(Divided by 2.)

For $\omega = 0$:

$$2\sigma_1^x \tag{3.1}$$

$$2\sigma_2^x \tag{3.2}$$

For $\omega = -4$:

$$\sigma_1^y - \mathrm{i}\sigma_1^z\sigma_2^x \tag{3.3}$$

$$\mathrm{i}\sigma_1^y\sigma_2^x + \sigma_1^z \tag{3.4}$$

$$-\mathrm{i}\sigma_1^x\sigma_2^z + \sigma_2^y \tag{3.5}$$

$$\mathrm{i}\sigma_1^x\sigma_2^y + \sigma_2^z \tag{3.6}$$

For $\omega = 4$:

$$\sigma_1^y + \mathrm{i}\sigma_1^z\sigma_2^x \tag{3.7}$$

$$-\mathrm{i}\sigma_1^y\sigma_2^x + \sigma_1^z \tag{3.8}$$

$$\mathrm{i}\sigma_1^x\sigma_2^z + \sigma_2^y \tag{3.9}$$

$$-\mathrm{i}\sigma_1^x\sigma_2^y + \sigma_2^z \tag{3.10}$$

3.6 Two-spin nondegenerate jump operators

Simplify further: better operators and collecting noncommutative terms as usual.

See figs. 3.8 and 3.9.

Let $d = \sqrt{g^2 + 1}$.

For $\omega = -4d$:

$$-\sqrt{2}g\sigma_1^x\sigma_2^x + \sqrt{2}g\sigma_1^y\sigma_2^y + \sqrt{2}\mathrm{i}d\sigma_1^x\sigma_2^y + \sqrt{2}\mathrm{i}d\sigma_1^y\sigma_2^x + \sqrt{2}\sigma_1^z + \sqrt{2}\sigma_2^z \tag{3.70}$$

For $\omega = -2d - 2$:

$$-\mathrm{i}g^2\sigma_1^x - \mathrm{i}g^2\sigma_1^x\sigma_2^z + g^2\sigma_1^z\sigma_2^y + g^2\sigma_2^y - gd\sigma_1^y - gd\sigma_1^y\sigma_2^z + \mathrm{i}gd\sigma_1^z\sigma_2^x + \mathrm{i}gd\sigma_2^x - g\sigma_1^y + \mathrm{i}g\sigma_1^z\sigma_2^x - \mathrm{i}d\sigma_1^x\sigma_2^z + d\sigma_2^y - \mathrm{i}\sigma_1^x\sigma_2^z + \sigma_2^y \tag{3.71}$$

$$g^2\sigma_1^x + g^2\sigma_1^x\sigma_2^z + \mathrm{i}g^2\sigma_1^z\sigma_2^y + \mathrm{i}g^2\sigma_2^y - \mathrm{i}gd\sigma_1^y - \mathrm{i}gd\sigma_1^y\sigma_2^z - gd\sigma_1^z\sigma_2^x - gd\sigma_2^x + \mathrm{i}g\sigma_1^y\sigma_2^z + g\sigma_2^x - d\sigma_1^x - \mathrm{i}d\sigma_1^z\sigma_2^y + \sigma_1^x + \mathrm{i}\sigma_1^z\sigma_2^y \tag{3.72}$$

$$\mathrm{i}g^2\sigma_1^y + \mathrm{i}g^2\sigma_1^y\sigma_2^z + g^2\sigma_1^z\sigma_2^x + g^2\sigma_2^x - gd\sigma_1^x - gd\sigma_1^x\sigma_2^z - \mathrm{i}gd\sigma_1^z\sigma_2^y - \mathrm{i}gd\sigma_2^y + g\sigma_1^x + \mathrm{i}g\sigma_1^z\sigma_2^y - \mathrm{i}d\sigma_1^y\sigma_2^z - d\sigma_2^x + \mathrm{i}\sigma_1^y\sigma_2^z + \sigma_2^x \tag{3.73}$$

$$g^2\sigma_1^y + g^2\sigma_1^y\sigma_2^z - \mathrm{i}g^2\sigma_1^z\sigma_2^x - \mathrm{i}g^2\sigma_2^x + \mathrm{i}gd\sigma_1^x + \mathrm{i}gd\sigma_1^x\sigma_2^z - gd\sigma_1^z\sigma_2^y - gd\sigma_2^y + \mathrm{i}g\sigma_1^x\sigma_2^z - g\sigma_2^y + d\sigma_1^y - \mathrm{i}d\sigma_1^z\sigma_2^x + \sigma_1^y - \mathrm{i}\sigma_1^z\sigma_2^x \tag{3.74}$$

For $\omega = 2d + 2$:

$$\mathrm{i}g^2\sigma_1^x + \mathrm{i}g^2\sigma_1^x\sigma_2^z + g^2\sigma_1^z\sigma_2^y + g^2\sigma_2^y - gd\sigma_1^y - gd\sigma_1^y\sigma_2^z - \mathrm{i}gd\sigma_1^z\sigma_2^x - \mathrm{i}gd\sigma_2^x - g\sigma_1^y - \mathrm{i}g\sigma_1^z\sigma_2^x + \mathrm{i}d\sigma_1^x\sigma_2^z + d\sigma_2^y + \mathrm{i}\sigma_1^x\sigma_2^z + \sigma_2^y \tag{3.75}$$
$$-\mathrm{i}g^2\sigma_1^y - \mathrm{i}g^2\sigma_1^y\sigma_2^z + g^2\sigma_1^z\sigma_2^x + g^2\sigma_2^x - gd\sigma_1^x - gd\sigma_1^x\sigma_2^z + \mathrm{i}gd\sigma_1^z\sigma_2^y + \mathrm{i}gd\sigma_2^y + g\sigma_1^x - \mathrm{i}g\sigma_1^z\sigma_2^y + \mathrm{i}d\sigma_1^y\sigma_2^z - d\sigma_2^x - \mathrm{i}\sigma_1^y\sigma_2^z + \sigma_2^x \tag{3.76}$$
$$g^2\sigma_1^y + g^2\sigma_1^y\sigma_2^z + \mathrm{i}g^2\sigma_1^z\sigma_2^x + \mathrm{i}g^2\sigma_2^x - \mathrm{i}gd\sigma_1^x - \mathrm{i}gd\sigma_1^x\sigma_2^z - gd\sigma_1^z\sigma_2^y - gd\sigma_2^y - \mathrm{i}g\sigma_1^x\sigma_2^z - g\sigma_2^y + d\sigma_1^y + \mathrm{i}d\sigma_1^z\sigma_2^x + \sigma_1^y + \mathrm{i}\sigma_1^z\sigma_2^x \tag{3.77}$$
$$g^2\sigma_1^x + g^2\sigma_1^x\sigma_2^z - \mathrm{i}g^2\sigma_1^z\sigma_2^y - \mathrm{i}g^2\sigma_2^y + \mathrm{i}gd\sigma_1^y + \mathrm{i}gd\sigma_1^y\sigma_2^z - gd\sigma_1^z\sigma_2^x - gd\sigma_2^x - \mathrm{i}g\sigma_1^y\sigma_2^z + g\sigma_2^x - d\sigma_1^x + \mathrm{i}d\sigma_1^z\sigma_2^y + \sigma_1^x - \mathrm{i}\sigma_1^z\sigma_2^y \tag{3.78}$$

For $\omega = 0$:

$$4\sqrt{2}g^4 + 4\sqrt{2}g^4\sigma_1^z + 4\sqrt{2}g^4\sigma_1^z\sigma_2^z + 4\sqrt{2}g^4\sigma_2^z + 4\sqrt{2}g^3\sigma_1^x\sigma_2^x - 4\sqrt{2}g^3\sigma_1^y\sigma_2^y + 4\sqrt{2}g^2 + 2\sqrt{2}g^2\sigma_1^z + 4\sqrt{2}g^2\sigma_1^z\sigma_2^z + 2\sqrt{2}g^2\sigma_2^z + 2\sqrt{2}g\sigma_1^x\sigma_2^x - 2\sqrt{2}g\sigma_1^y\sigma_2^y \tag{3.79}$$

For $\omega = 2 - 2d$:

$$\mathrm{i}g^2\sigma_1^x + \mathrm{i}g^2\sigma_1^x\sigma_2^z + g^2\sigma_1^z\sigma_2^y + g^2\sigma_2^y + gd\sigma_1^y + gd\sigma_1^y\sigma_2^z + \mathrm{i}gd\sigma_1^z\sigma_2^x + \mathrm{i}gd\sigma_2^x - g\sigma_1^y - \mathrm{i}g\sigma_1^z\sigma_2^x - \mathrm{i}d\sigma_1^x\sigma_2^z - d\sigma_2^y + \mathrm{i}\sigma_1^x\sigma_2^z + \sigma_2^y \tag{3.80}$$
$$g^2\sigma_1^y + g^2\sigma_1^y\sigma_2^z + \mathrm{i}g^2\sigma_1^z\sigma_2^x + \mathrm{i}g^2\sigma_2^x + \mathrm{i}gd\sigma_1^x + \mathrm{i}gd\sigma_1^x\sigma_2^z + gd\sigma_1^z\sigma_2^y + gd\sigma_2^y - \mathrm{i}g\sigma_1^x\sigma_2^z - g\sigma_2^y - d\sigma_1^y - \mathrm{i}d\sigma_1^z\sigma_2^x + \sigma_1^y + \mathrm{i}\sigma_1^z\sigma_2^x \tag{3.81}$$
$$g^2\sigma_1^x + g^2\sigma_1^x\sigma_2^z - \mathrm{i}g^2\sigma_1^z\sigma_2^y - \mathrm{i}g^2\sigma_2^y - \mathrm{i}gd\sigma_1^y - \mathrm{i}gd\sigma_1^y\sigma_2^z + gd\sigma_1^z\sigma_2^x + gd\sigma_2^x - \mathrm{i}g\sigma_1^y\sigma_2^z + g\sigma_2^x + d\sigma_1^x - \mathrm{i}d\sigma_1^z\sigma_2^y + \sigma_1^x - \mathrm{i}\sigma_1^z\sigma_2^y \tag{3.82}$$
$$-\mathrm{i}g^2\sigma_1^y - \mathrm{i}g^2\sigma_1^y\sigma_2^z + g^2\sigma_1^z\sigma_2^x + g^2\sigma_2^x + gd\sigma_1^x + gd\sigma_1^x\sigma_2^z - \mathrm{i}gd\sigma_1^z\sigma_2^y - \mathrm{i}gd\sigma_2^y + g\sigma_1^x - \mathrm{i}g\sigma_1^z\sigma_2^y - \mathrm{i}d\sigma_1^y\sigma_2^z + d\sigma_2^x - \mathrm{i}\sigma_1^y\sigma_2^z + \sigma_2^x \tag{3.83}$$

For $\omega = 2d - 2$:

$$g^2\sigma_1^y + g^2\sigma_1^y\sigma_2^z - \mathrm{i}g^2\sigma_1^z\sigma_2^x - \mathrm{i}g^2\sigma_2^x - \mathrm{i}gd\sigma_1^x - \mathrm{i}gd\sigma_1^x\sigma_2^z + gd\sigma_1^z\sigma_2^y + gd\sigma_2^y + \mathrm{i}g\sigma_1^x\sigma_2^z - g\sigma_2^y - d\sigma_1^y + \mathrm{i}d\sigma_1^z\sigma_2^x + \sigma_1^y - \mathrm{i}\sigma_1^z\sigma_2^x \tag{3.84}$$
$$g^2\sigma_1^x + g^2\sigma_1^x\sigma_2^z + \mathrm{i}g^2\sigma_1^z\sigma_2^y + \mathrm{i}g^2\sigma_2^y + \mathrm{i}gd\sigma_1^y + \mathrm{i}gd\sigma_1^y\sigma_2^z + gd\sigma_1^z\sigma_2^x + gd\sigma_2^x + \mathrm{i}g\sigma_1^y\sigma_2^z + g\sigma_2^x + d\sigma_1^x + \mathrm{i}d\sigma_1^z\sigma_2^y + \sigma_1^x + \mathrm{i}\sigma_1^z\sigma_2^y \tag{3.85}$$
$$-\mathrm{i}g^2\sigma_1^x - \mathrm{i}g^2\sigma_1^x\sigma_2^z + g^2\sigma_1^z\sigma_2^y + g^2\sigma_2^y + gd\sigma_1^y + gd\sigma_1^y\sigma_2^z - \mathrm{i}gd\sigma_1^z\sigma_2^x - \mathrm{i}gd\sigma_2^x - g\sigma_1^y + \mathrm{i}g\sigma_1^z\sigma_2^x + \mathrm{i}d\sigma_1^x\sigma_2^z - d\sigma_2^y - \mathrm{i}\sigma_1^x\sigma_2^z + \sigma_2^y \tag{3.86}$$
$$\mathrm{i}g^2\sigma_1^y + \mathrm{i}g^2\sigma_1^y\sigma_2^z + g^2\sigma_1^z\sigma_2^x + g^2\sigma_2^x + gd\sigma_1^x + gd\sigma_1^x\sigma_2^z + \mathrm{i}gd\sigma_1^z\sigma_2^y + \mathrm{i}gd\sigma_2^y + g\sigma_1^x + \mathrm{i}g\sigma_1^z\sigma_2^y + \mathrm{i}d\sigma_1^y\sigma_2^z + d\sigma_2^x + \mathrm{i}\sigma_1^y\sigma_2^z + \sigma_2^x \tag{3.87}$$

For $\omega = 4d$:

$$-\sqrt{2}g\sigma_1^x\sigma_2^x + \sqrt{2}g\sigma_1^y\sigma_2^y - \sqrt{2}\mathrm{i}d\sigma_1^x\sigma_2^y - \sqrt{2}\mathrm{i}d\sigma_1^y\sigma_2^x + \sqrt{2}\sigma_1^z + \sqrt{2}\sigma_2^z \tag{3.88}$$

For $\omega = 4$:

$$-\mathrm{i}\sigma_1^x\sigma_2^y + \mathrm{i}\sigma_1^y\sigma_2^x - \sigma_1^z + \sigma_2^z \tag{3.89}$$
$$\mathrm{i}\sigma_1^x\sigma_2^y - \mathrm{i}\sigma_1^y\sigma_2^x + \sigma_1^z - \sigma_2^z \tag{3.90}$$

For $\omega = -4$:

$$\mathrm{i}\sigma_1^x\sigma_2^y - \mathrm{i}\sigma_1^y\sigma_2^x - \sigma_1^z + \sigma_2^z \tag{3.91}$$
$$-\mathrm{i}\sigma_1^x\sigma_2^y + \mathrm{i}\sigma_1^y\sigma_2^x + \sigma_1^z - \sigma_2^z \tag{3.92}$$

$$-4 \tag{3.11}$$

$$-2n_1 + 2n_2 - 2\sigma_1^+\sigma_2^- + 2\sigma_1^-\sigma_2^+ \tag{3.12}$$

$$2n_1 - 2n_2 + 2\sigma_1^+\sigma_2^- - 2\sigma_1^-\sigma_2^+ \tag{3.13}$$

$$\tag{3.14}$$

$$4d \tag{3.15}$$

$$2\sqrt{2}\,(n_1 + n_2 - \sigma_1^+\sigma_2^+ (d+g) + \sigma_1^-\sigma_2^- (d-g) - 1) \tag{3.16}$$

$$\tag{3.17}$$

$$-2(d-1) \tag{3.18}$$

$$-2n_1 g\,(\sigma_2^+ (d-g+1) - \sigma_2^- (d+g+1)) + \sigma_1^+ (-2n_2 (-dg+d+g^2+1) + d+g+1) + \sigma_1^- (2n_2 (dg+d+g^2+1) - d+g-1) + \sigma_2^+ (d+g+1) + \sigma_2^- (d-g+1) \tag{3.19}$$

$$\mathrm{i}\,(-2n_1 g\,(\sigma_2^+ (-d+g+1) - \sigma_2^- (d+g-1)) - \sigma_1^+ (2n_2 (dg+d-g^2-1) - d-g+1) + \sigma_1^- (2n_2 (dg-d+g^2+1) + d-g-1) + \sigma_2^+ (d+g-1) + \sigma_2^- (-d+g+1)) \tag{3.20}$$

$$-2n_1 (\sigma_2^+ (-dg+d+g^2+1) - \sigma_2^- (dg+d+g^2+1)) + \sigma_1^+ (-2n_2 g\,(d-g+1) + d+g+1) + \sigma_1^- (2n_2 g\,(d+g+1) + d-g+1) + \sigma_2^+ (d+g+1) - \sigma_2^- (d-g+1) \tag{3.21}$$

$$\mathrm{i}\,(-2n_1 (\sigma_2^+ (dg+d-g^2-1) - \sigma_2^- (dg-d+g^2+1)) - \sigma_1^+ (2n_2 g\,(-d+g+1) - d-g+1) + \sigma_1^- (2n_2 g\,(d+g-1) - d+g+1) + \sigma_2^+ (d+g-1) - \sigma_2^- (-d+g+1)) \tag{3.22}$$

$$\tag{3.23}$$

$$-2(d+1) \tag{3.24}$$

$$2n_1 g\,(\sigma_2^+ (-d+g+1) + \sigma_2^- (d+g-1)) - \sigma_1^+ (2n_2 (dg+d-g^2-1) - d-g+1) - \sigma_1^- (2n_2 (dg-d+g^2+1) + d-g-1) - \sigma_2^+ (d+g-1) + \sigma_2^- (-d+g+1) \tag{3.25}$$

$$\mathrm{i}\,(-2n_1 (\sigma_2^+ (-dg+d+g^2+1) + \sigma_2^- (dg+d+g^2+1)) - \sigma_1^+ (-2n_2 g\,(d-g+1) + d+g+1) + \sigma_1^- (2n_2 g\,(d+g+1) + d-g+1) + \sigma_2^+ (d+g+1) + \sigma_2^- (d-g+1)) \tag{3.26}$$

$$\mathrm{i}\,(2n_1 g\,(\sigma_2^+ (d-g+1) + \sigma_2^- (d+g+1)) + \sigma_1^+ (-2n_2 (-dg+d+g^2+1) + d+g+1) - \sigma_1^- (2n_2 (dg+d+g^2+1) - d+g-1) - \sigma_2^+ (d+g+1) + \sigma_2^- (d-g+1)) \tag{3.27}$$

$$-2n_1 (\sigma_2^+ (dg+d-g^2-1) + \sigma_2^- (dg-d+g^2+1)) + \sigma_1^+ (2n_2 g\,(-d+g+1) - d-g+1) + \sigma_1^- (2n_2 g\,(d+g-1) - d+g+1) + \sigma_2^+ (d+g-1) + \sigma_2^- (-d+g+1) \tag{3.28}$$

$$\tag{3.29}$$

$$-4d \tag{3.30}$$

$$2\sqrt{2}\,(n_1 + n_2 + \sigma_1^+\sigma_2^+ (d-g) - \sigma_1^-\sigma_2^- (d+g) - 1) \tag{3.31}$$

$$\tag{3.32}$$

$$0 \tag{3.33}$$

$$4\sqrt{2}g\,(n_1 g\,(4n_2 (g^2+1) - 1) - n_2 g + \sigma_1^+\sigma_2^+ (2g^2+1) + \sigma_1^-\sigma_2^- (2g^2+1) + g) \tag{3.34}$$

$$\tag{3.35}$$

$$4 \tag{3.36}$$

$$2n_1 - 2n_2 - 2\sigma_1^+\sigma_2^- + 2\sigma_1^-\sigma_2^+ \tag{3.37}$$

$$-2n_1 + 2n_2 + 2\sigma_1^+\sigma_2^- - 2\sigma_1^-\sigma_2^+ \tag{3.38}$$

$$\tag{3.39}$$

$$2(d+1) \tag{3.40}$$

$$-2n_1 (\sigma_2^+ (dg-d+g^2+1) + \sigma_2^- (dg+d-g^2-1)) + \sigma_1^+ (2n_2 g\,(d+g-1) - d+g+1) + \sigma_1^- (2n_2 g\,(-d+g+1) - d-g+1) + \sigma_2^+ (-d+g+1) + \sigma_2^- (d+g-1) \tag{3.41}$$

$$2n_1 g\,(\sigma_2^+ (d+g-1) + \sigma_2^- (-d+g+1)) - \sigma_1^+ (2n_2 (dg-d+g^2+1) + d-g-1) - \sigma_1^- (2n_2 (dg+d-g^2-1) - d-g+1) + \sigma_2^+ (-d+g+1) - \sigma_2^- (d+g-1) \tag{3.42}$$

$$\mathrm{i}\,(-2n_1 g\,(\sigma_2^+ (d+g+1) + \sigma_2^- (d-g+1)) + \sigma_1^+ (2n_2 (dg+d+g^2+1) - d+g-1) - \sigma_1^- (-2n_2 (-dg+d+g^2+1) + d+g+1) - \sigma_2^+ (d-g+1) + \sigma_2^- (d+g+1)) \tag{3.43}$$

$$\mathrm{i}\,(2n_1 (\sigma_2^+ (dg+d+g^2+1) + \sigma_2^- (-dg+d+g^2+1)) - \sigma_1^+ (2n_2 g\,(d+g+1) + d-g+1) + \sigma_1^- (-2n_2 g\,(d-g+1) + d+g+1) - \sigma_2^+ (d-g+1) - \sigma_2^- (d+g+1)) \tag{3.44}$$

$$\tag{3.45}$$

$$2(d-1) \tag{3.46}$$

$$2n_1 g\,(\sigma_2^+ (d+g+1) - \sigma_2^- (d-g+1)) + \sigma_1^+ (2n_2 (dg+d+g^2+1) - d+g-1) + \sigma_1^- (-2n_2 (-dg+d+g^2+1) + d+g+1) + \sigma_2^+ (d-g+1) + \sigma_2^- (d+g+1) \tag{3.47}$$

$$\mathrm{i}\,(-2n_1 g\,(\sigma_2^+ (d+g-1) - \sigma_2^- (-d+g+1)) - \sigma_1^+ (2n_2 (dg-d+g^2+1) + d-g-1) + \sigma_1^- (2n_2 (dg+d-g^2-1) - d-g+1) - \sigma_2^+ (-d+g+1) - \sigma_2^- (d+g-1)) \tag{3.48}$$

$$2n_1 (\sigma_2^+ (dg+d+g^2+1) - \sigma_2^- (-dg+d+g^2+1)) + \sigma_1^+ (2n_2 g\,(d+g+1) + d-g+1) + \sigma_1^- (-2n_2 g\,(d-g+1) + d+g+1) - \sigma_2^+ (d-g+1) + \sigma_2^- (d+g+1) \tag{3.49}$$

$$\mathrm{i}\,(-2n_1 (\sigma_2^+ (dg-d+g^2+1) - \sigma_2^- (dg+d-g^2-1)) - \sigma_1^+ (2n_2 g\,(d+g-1) - d+g+1) + \sigma_1^- (2n_2 g\,(-d+g+1) - d-g+1) + \sigma_2^+ (-d+g+1) - \sigma_2^- (d+g-1)) \tag{3.50}$$

$$\tag{3.51}$$

$$\tag{3.52}$$

Figure 3.8: The jump operators for the nondegenerate case ($g \neq 0$).

$$-4 \tag{3.53}$$

$$2\mathrm{i}\left(-2n_1\left(\sigma_2^+ + \sigma_2^-\right) - \sigma_1^+ + \sigma_1^- + \sigma_2^+ + \sigma_2^-\right) \tag{3.54}$$

$$2\mathrm{i}\left(-\sigma_1^+\left(2n_2 - 1\right) - \sigma_1^-\left(2n_2 - 1\right) - \sigma_2^+ + \sigma_2^-\right) \tag{3.55}$$

$$4n_1 + 2\sigma_1^+\left(\sigma_2^+ + \sigma_2^-\right) - 2\sigma_1^-\left(\sigma_2^+ + \sigma_2^-\right) - 2 \tag{3.56}$$

$$4n_2 + 2\sigma_1^+\left(\sigma_2^+ - \sigma_2^-\right) + 2\sigma_1^-\left(\sigma_2^+ - \sigma_2^-\right) - 2 \tag{3.57}$$

$$\tag{3.58}$$

$$0 \tag{3.59}$$

$$4\sigma_2^+ + 4\sigma_2^- \tag{3.60}$$

$$4\sigma_1^+ + 4\sigma_1^- \tag{3.61}$$

$$\tag{3.62}$$

$$4 \tag{3.63}$$

$$2\mathrm{i}\left(\sigma_1^+\left(2n_2 - 1\right) + \sigma_1^-\left(2n_2 - 1\right) - \sigma_2^+ + \sigma_2^-\right) \tag{3.64}$$

$$4n_1 - 2\sigma_1^+\left(\sigma_2^+ + \sigma_2^-\right) + 2\sigma_1^-\left(\sigma_2^+ + \sigma_2^-\right) - 2 \tag{3.65}$$

$$4n_2 - 2\sigma_1^+\left(\sigma_2^+ - \sigma_2^-\right) - 2\sigma_1^-\left(\sigma_2^+ - \sigma_2^-\right) - 2 \tag{3.66}$$

$$2\mathrm{i}\left(2n_1\left(\sigma_2^+ + \sigma_2^-\right) - \sigma_1^+ + \sigma_1^- - \sigma_2^+ - \sigma_2^-\right) \tag{3.67}$$

$$\tag{3.68}$$

$$\tag{3.69}$$

Figure 3.9: The jump operators for the degenerate case ($g = 0$).

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 transverse-field Ising model

We would like to solve the Hamiltonian

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

which we nondimensionalize as

$$\frac{4}{J} H = -\sum_{i\in\mathbb{Z}_N} \left(\sigma_i^x \sigma_{i+1}^x + g\sigma_i^z\right) \tag{A.2}$$

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

$$\sigma_i^\pm = \frac{\sigma_i^x \pm \mathrm{i}\sigma_i^y}{2} \tag{A.3}$$

satisfy

$$\sigma_i^z = 2\sigma_i^+\sigma_i^- - 1 \tag{A.4}$$

and have commutators

$$\begin{aligned}
\left[\sigma_i^+, \sigma_j^-\right] &= \frac{1}{4}\left[\sigma_i^x + \mathrm{i}\sigma_i^y, \sigma_j^x - \mathrm{i}\sigma_j^y\right] && \text{(A.5)}\\
&= \frac{1}{4}\left(\left[\sigma_i^x, \sigma_j^x\right] + \left[\sigma_i^y, \sigma_j^y\right] + \mathrm{i}\left[\sigma_i^y, \sigma_j^x\right] - \mathrm{i}\left[\sigma_i^x, \sigma_j^y\right]\right) && \text{(A.6)}\\
&= \delta_{ij}\sigma_i^z. && \text{(A.7)}
\end{aligned}$$

Thus their anticommutators are

$$\begin{aligned}
\left\{\sigma_i^+, \sigma_j^-\right\} &= 2\sigma_i^+\sigma_j^- - \left[\sigma_i^+, \sigma_j^-\right] && \text{(A.8)}\\
&= 2\sigma_i^+\sigma_j^- - \delta_{ij}\sigma_i^z && \text{(A.9)}\\
&= \delta_{ij}1 + 2\sigma_i^+\sigma_j^-(1 - \delta_{ij}). && \text{(A.10)}
\end{aligned}$$

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

$$|\boldsymbol{n}\rangle = \prod_{i\in\mathbb{Z}_N} \left(c_i^\dagger\right)^{n_i} |\boldsymbol{0}\rangle\,, \tag{A.11}$$

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

$$c_i\,|\boldsymbol{n}\rangle = -n_i(-1)^{n_{<i}}\,|\boldsymbol{n}_{i\leftarrow 0}\rangle \tag{A.12}$$

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

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

$$c_i^\dagger c_i\,|\boldsymbol{n}\rangle = (1-0)(-1)^{n_{<i}} n_i(-1)^{n_{<i}}\,|\boldsymbol{n}_{i\leftarrow 1}\rangle \tag{A.14}$$

$$= n_i\,|\boldsymbol{n}\rangle\,. \tag{A.15}$$

This leads us to consider

$$c_i = -\left(\prod_{j<i} -\sigma_j^z\right)\sigma_i^- \tag{A.16}$$

acting on the states

$$|\boldsymbol{n}\rangle = \prod_{i\in\mathbb{Z}_N} \left(\sigma_i^+\right)^{n_i} |\boldsymbol{0}\rangle\,, \tag{A.17}$$

where $|\boldsymbol{0}\rangle = |\uparrow\rangle^{\otimes N}$ is the state with all z-spins up, or all zero qubits. This gives the same result as eq. (A.12), 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

$$\sigma_i^+\sigma_i^- = c_i^\dagger c_i \tag{A.18}$$

$$\sigma_i^z = 2c_i^\dagger c_i - 1 \tag{A.19}$$

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

$$\sigma_i^y = \mathrm{i}\left(\prod_{j<i}\left(1-2c_j^\dagger c_j\right)\right)\left(c_i^\dagger - c_i\right). \tag{A.21}$$

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

$$\sigma_i^x \sigma_{i+1}^x = \left(\prod_{j<i} \left(2c_j^\dagger c_j - 1\right)\right)\left(c_i^\dagger + c_i\right)\left(\prod_{j<i+1} \left(2c_j^\dagger c_j - 1\right)\right)\left(c_{i+1}^\dagger + c_{i+1}\right) \tag{A.22}$$

$$= \left(c_i^\dagger + c_i\right)\left(1 - 2c_i^\dagger c_i\right)\left(c_{i+1}^\dagger + c_{i+1}\right) \tag{A.23}$$

$$= \left(c_i^\dagger - c_i\right)\left(c_{i+1}^\dagger + c_{i+1}\right), \tag{A.24}$$

and for $i = N-1$,

$$\sigma_{N-1}^x \sigma_0^x = \left(\prod_{j<N-1} \left(2c_j^\dagger c_j - 1\right)\right)\left(c_{N-1}^\dagger + c_{N-1}\right)\left(c_0^\dagger + c_0\right). \tag{A.25}$$

We may now perform the Jordan-Wigner transformation of eq. (A.2) to obtain

$$\begin{aligned} H = &\sum_i \left(c_i - c_i^\dagger\right)\left(c_{i+1}^\dagger + c_{i+1}\right) - g\sum_i 2c_i^\dagger c_i + gN1 \\ &- \left(1 - \prod_{j<N-1} \left(2c_j^\dagger c_j - 1\right)\right)\left(c_{N-1} - c_{N-1}^\dagger\right)\left(c_0^\dagger + c_0\right). \end{aligned} \tag{A.26}$$

We now Fourier transform with

$$c_i = \frac{1}{\sqrt{N}} \sum_k e^{\mathrm{i}ki} C_k \tag{A.27a}$$

$$C_k = \frac{1}{\sqrt{N}} \sum_i e^{-\mathrm{i}ki} c_i \tag{A.27b}$$

and

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-\mathrm{i}ki} C_k^\dagger \tag{A.27c}$$

$$C_k^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{\mathrm{i}ki} c_i^\dagger. \tag{A.27d}$$

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

$$c_0 = \frac{1}{\sqrt{N}} \sum_k C_k \tag{A.28}$$

$$c_N = \frac{1}{\sqrt{N}} \sum_k e^{\mathrm{i}kN} C_k. \tag{A.29}$$

We then must require that

$$kN \equiv 0 \pmod{2\pi} \tag{A.30}$$

$$k = \frac{2\pi n}{N} - \frac{N - [N \text{ odd}]}{N}\pi, \quad n \in \mathbb{Z}_N. \tag{A.31}$$

For N odd, what is C_π?

$$C_\pi = \frac{1}{\sqrt{N}} \sum_i e^{-\mathrm{i}\pi i} c_i. \tag{A.32}$$

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

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 $\boldsymbol{U}$. We may change bases with

$$C_k^\dagger = \sum_i U_{ik} c_i^\dagger. \tag{A.33}$$

Then

$$\begin{aligned}
\left\{C_k, C_{k'}^\dagger\right\} &= \sum_{ij} U_{ik}^* U_{jk'} \left\{c_i, c_j^\dagger\right\} && \text{(A.34)}\\
&= \sum_i U_{ik}^* U_{ik'} && \text{(A.35)}\\
&= \left(\boldsymbol{U}^\dagger \boldsymbol{U}\right)_{kk'} && \text{(A.36)}\\
&= \delta_{kk'}, && \text{(A.37)}
\end{aligned}$$

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

For the Fourier transform,

$$F_{ik} = \frac{1}{\sqrt{N}} e^{\mathrm{i}ki}. \tag{A.38}$$

We may then confirm that

$$\begin{aligned}
\left(\boldsymbol{F}^\dagger \boldsymbol{F}\right)_{kk'} &= \sum_i \frac{1}{N} e^{\mathrm{i}(k'-k)i} && \text{(A.39)}\\
&= \delta_{kk'}. && \text{(A.40)}
\end{aligned}$$

Thus the Fourier transform is unitary. □

We are now equipped to Fourier transform eq. (A.26) as follows. Since

$$\frac{1}{N}\sum_{i\in\mathbb{Z}_N} e^{\mathrm{i}(k'-k)i} = \delta_{kk'}, \tag{A.41}$$

and also

$$\begin{aligned} C_{-k} &= C_k^* && \text{(A.42)}\\ &= \frac{1}{\sqrt{N}}\sum_i e^{-\mathrm{i}(-k)i} c_i && \text{(A.43)}\\ &= \frac{1}{N}\sum_{ik'} e^{\mathrm{i}(k'+k)i} C_{k'}, && \text{(A.44)} \end{aligned}$$

we have that

$$\begin{aligned} \sum_i c_i^\dagger c_i &= \frac{1}{N}\sum_{ikk'} e^{\mathrm{i}(k'-k)i} C_k^\dagger C_{k'} && \text{(A.45)}\\ &= \sum_k C_k^\dagger C_k, && \text{(A.46)}\\ \sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right) &= \frac{1}{N}\sum_{ikk'} e^{\mathrm{i}(k'-k)i}\left(e^{\mathrm{i}k'} + e^{-\mathrm{i}k}\right) C_k^\dagger C_{k'} && \text{(A.47)}\\ &= \sum_k 2\cos k\; C_k^\dagger C_k, && \text{(A.48)}\\ \sum_i \left(c_{i+1} c_i + c_i^\dagger c_{i+1}^\dagger\right) &= \frac{1}{N}\sum_{ikk'} \left(e^{\mathrm{i}(k'+k)i} e^{\mathrm{i}k} C_k C_{k'} + e^{-\mathrm{i}(k'+k)i} e^{-\mathrm{i}k'} C_k^\dagger C_{k'}^\dagger\right) && \text{(A.49)}\\ &= \sum_k \left(e^{-\mathrm{i}k} C_{-k} C_k + e^{\mathrm{i}k} C_k^\dagger C_{-k}^\dagger\right). && \text{(A.50)} \end{aligned}$$

Thus eq. (A.26) is now

$$\begin{aligned} H &= -\sum_k 2\cos k\; C_k^\dagger C_k + \sum_k \left(e^{-\mathrm{i}k} C_{-k} C_k + e^{\mathrm{i}k} C_k^\dagger C_{-k}^\dagger\right) - \sum_k 2g C_k^\dagger C_k + gN1 && \text{(A.51)}\\ &= -\sum_k (g+\cos k)\left(C_k^\dagger C_k + C_{-k}^\dagger C_{-k}\right) + \sum_k \mathrm{i}\sin k\left(C_{-k} C_k - C_k^\dagger C_{-k}^\dagger\right) + gN1 && \text{(A.52)}\\ &= -\sum_k (g+\cos k)\left(C_k^\dagger C_k - C_{-k} C_{-k}^\dagger\right) + \sum_k \mathrm{i}\sin k\left(C_{-k} C_k - C_k^\dagger C_{-k}^\dagger\right) && \text{(A.53)}\\ &= \sum_k \boldsymbol{v}_k^\dagger \boldsymbol{H}_k \boldsymbol{v}_k, && \text{(A.54)} \end{aligned}$$

where

$$\begin{aligned} \boldsymbol{H}_k &= \begin{bmatrix} -(g+\cos k) & -\mathrm{i}\sin k \\ \mathrm{i}\sin k & g+\cos k \end{bmatrix}, && \text{(A.55)}\\ \boldsymbol{v}_k &= \begin{bmatrix} C_k \\ C_{-k}^\dagger \end{bmatrix}, && \text{(A.56)} \end{aligned}$$

and we have used that

$$\sum_k \cos k = 0. \tag{A.57}$$

Since the $\boldsymbol{H}_k$ are Hermitian, they may be diagonalized by a unitary transformation of the $\boldsymbol{v}_k$.[1] The $\boldsymbol{H}_k$ are traceless, so they have the eigenvalues

$$E_k^{\pm} = \pm\sqrt{-\det \boldsymbol{H}_k} \tag{A.63}$$

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

$$= \pm\sqrt{g^2 + 2g\cos k + 1}. \tag{A.65}$$

The eigenvectors are then

$$\boldsymbol{q}_k^{\pm} = \begin{bmatrix} -\mathrm{i}\sin k \\ E_k^{\pm} + g + \cos k \end{bmatrix}, \tag{A.66}$$

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

$$\boldsymbol{q}_k^{-} = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \boldsymbol{q}_k^{+} = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{A.67}$$

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

$$C_k = u f_k + v g_k^{\dagger} \tag{A.58a}$$

and

$$C_{-k} = -v f_k^{\dagger} + u g_k. \tag{A.58b}$$

For these transformations to preserve the CARs,

$$\left\{C_k^{\dagger}, C_k\right\} = |u|^2\left\{f_k^{\dagger}, f_k\right\} + |v|^2\left\{g_k, g_k^{\dagger}\right\} + u^* v\left\{f_k^{\dagger}, g_k^{\dagger}\right\} + v^* u\{g_k, f_k\} \tag{A.59}$$

$$= \left(|u|^2 + |v|^2\right)1, \tag{A.60}$$

so we must have

$$|u|^2 + |v|^2 = 1. \tag{A.61}$$

We may choose

$$u = e^{\mathrm{i}\phi_1}\cos\theta \tag{A.62a}$$

$$v = e^{\mathrm{i}\phi_2}\sin\theta \tag{A.62b}$$

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 $\boldsymbol{H}_{-\pi} = \boldsymbol{0}$. To construct the unitary transformation, we must normalize the $\boldsymbol{q}_k^{\pm}$. We find that

$$\begin{aligned}
\left\|\boldsymbol{q}_k^{\pm}\right\|^2 &= \left(E_k^{\pm} + g + \cos k\right)^2 + \sin^2 k && \text{(A.68)}\\
&= \left(E_k^{\pm}\right)^2 + g^2 + \cos^2 k + 2g\cos k + 2E_k^{\pm}(g + \cos k) + 1 - \cos^2 k && \text{(A.69)}\\
&= 2E_k^{\pm}\left(E_k^{\pm} + g + \cos k\right). && \text{(A.70)}
\end{aligned}$$

Now

$$\begin{aligned}
\frac{(\boldsymbol{q}_k^{\pm})_1}{\left\|\boldsymbol{q}_k^{\pm}\right\|} &= \frac{-\mathrm{i}\sin k}{\sqrt{2E_k^{\pm}\left(E_k^{\pm} + g + \cos k\right)}} && \text{(A.71)}\\
&= \frac{-\mathrm{i}\sin k}{\sqrt{2\left|E_k^{\pm}\right|\left(\left|E_k^{\pm}\right| \pm (g + \cos k)\right)}} && \text{(A.72)}
\end{aligned}$$

and

$$\begin{aligned}
\frac{(\boldsymbol{q}_k^{\pm})_2}{\left\|\boldsymbol{q}_k^{\pm}\right\|} &= \pm\sqrt{\frac{E_k^{\pm} + (g + \cos k)}{2E_k^{\pm}}} && \text{(A.73)}\\
&= \pm\sqrt{\frac{\left|E_k^{\pm}\right| \pm (g + \cos k)}{2\left|E_k^{\pm}\right|}} && \text{(A.74)}
\end{aligned}$$

$$\boldsymbol{U}_k^{\dagger} = \begin{bmatrix} \left(\hat{\boldsymbol{q}}_k^{-}\right)^{\dagger} \\ \left(\hat{\boldsymbol{q}}_k^{+}\right)^{\dagger} \end{bmatrix}. \tag{A.75}$$

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

$$\eta_k^{\pm} = \frac{\mathrm{i}\sin k}{\sqrt{2E_k(E_k \pm (g + \cos k))}} C_k \pm \sqrt{\frac{E_k \pm (g + \cos k)}{2E_k}} C_{-k}^{\dagger} \tag{A.76}$$

so that

$$\begin{aligned}
\left\{\left(\eta_k^{\pm}\right)^{\dagger}, \eta_k^{\pm}\right\} &= \frac{\sin^2 k}{2E_k(E_k \pm (g + \cos k))}\mathbb{1} + \frac{E_k \pm (g + \cos k)}{2E_k}\mathbb{1} && \text{(A.77)}\\
&= \mathbb{1} && \text{(A.78)}\\
\left\{\left(\eta_k^{\pm}\right)^{\dagger}, \eta_k^{\mp}\right\} &= \frac{\sin^2 k}{2E_k\sqrt{E_k \pm (g + \cos k)}\sqrt{E_k \mp (g + \cos k)}}\mathbb{1} \\
&\quad - \frac{\sqrt{E_k \pm (g + \cos k)}\sqrt{E_k \mp (g + \cos k)}}{2E_k}\mathbb{1} && \text{(A.79)}\\
&= 0. && \text{(A.80)}
\end{aligned}$$

Note that eq. (A.76) 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 (A.54) becomes

$$H = \sum_k E_k^+ \left(\eta_k^+\right)^\dagger \eta_k^+ + \sum_k E_k^- \left(\eta_k^-\right)^\dagger \eta_k^-. \tag{A.81}$$

Since

$$\left(\eta_{-k}^-\right)^\dagger = \eta_k^+ =: \eta_k \tag{A.82}$$

and $E_{-k}^\pm = E_k^\pm$, we may reduce eq. (A.81) to

$$H = \sum_k E_k \eta_k^\dagger \eta_k - \sum_k E_k \left(1 - \eta_k^\dagger \eta_k\right) \tag{A.83}$$

$$= \sum_k 2E_k \eta_k^\dagger \eta_k - 1 \sum_k E_k. \tag{A.84}$$

Appendix B

Computer details

B.1 Julia version information

```
versioninfo()
```

```
Julia Version 1.4.0
Commit b8e9a9ecc6 (2020-03-21 16:36 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-8.0.1 (ORCJIT, haswell)
```

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

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

```
Pkg.status()
```

```
Status `~/drive/thesis/notebooks/Project.toml`
  [7d9fca2a] Arpack v0.4.0
  [b964fa9f] LaTeXStrings v1.2.0
  [eff96d63] Measurements v2.3.0
```

```
  [3b7a836e] PGFPlots v3.3.3
  [91a5bcdd] Plots v1.6.12
  [6e0679c1] QuantumOptics v0.8.2
  [1986cc42] Unitful v1.5.0
  [37e2e46d] LinearAlgebra
```

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

```
:mkl
```

B.2 Notebook Preamble

```
using Plots, LaTeXStrings
using Unitful, Measurements
using LinearAlgebra, Arpack, QuantumOptics

# import PGFPlots: pushPGFPlotsPreamble, popPGFPlotsPreamble
# popPGFPlotsPreamble() # If reevaluating, so no duplicates
# pushPGFPlotsPreamble("
#     \\usepackage{amsmath}
#     \\usepackage{physics}
#     \\usepackage{siunitx}
#     \\usepackage[full]{textcomp} % to get the right copyright, etc.
#     \\usepackage{libertinus-otf}
#     \\usepackage[scaled=.95,type1]{cabin} % sans serif in style of Gill Sans
#     \\usepackage[T1]{fontenc} % LY1 also works
#     \\setmainfont[Numbers={OldStyle,Proportional}]{fbb}
#     \\usepackage[supstfm=fbb-Regular-sup-t1]{superiors}
#     \\usepackage[cal=boondoxo,bb=boondox,frak=boondox]{mathalfa}
#     \\input{latexdefs}
#     ")
# pgfplots()

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{libertinus-otf}
    \\usepackage[scaled=.95,type1]{cabin} % sans serif in style of Gill Sans
    \\usepackage[T1]{fontenc} % LY1 also works
    \\setmainfont[Numbers={OldStyle,Proportional}]{fbb}
    \\usepackage[supstfm=fbb-Regular-sup-t1]{superiors}
    \\usepackage[cal=boondoxo,bb=boondox,frak=boondox]{mathalfa}
```

```
    \\input{$(pwd())/latexdefs.tex}
    ");
pgfplotsx()

using PlotThemes
theme(:vibrant,
    size=(400, 300),
    dpi=300,
    titlefontsize=12,
    tickfontsize=11,
    legendfontsize=11,
)
```

References

[1] C. E. Shannon. A mathematical theory of communication. *Bell Syst. Tech. J.*, 27(3): 379–423, July 1948. ISSN 0005-8580. doi: 10.1002/j.1538-7305.1948.tb01338.x. 1.1.1

[2] Lucien Hardy. Quantum Theory From Five Reasonable Axioms. *ArXivquant-Ph0101012*, September 2001. URL http://arxiv.org/abs/quant-ph/0101012. Comment: 34 pages. Version 4: Improved proofs of K=Nr̂ and D=DT̂. Discussion of state update rule after measurement added. Various clarifications in proofs Version 2: Axiom 2 modified and corresponding corrections made to proof in Sec. 8.1. Typos and minor errors fixed. 1.1.2

[3] P. Busch. Quantum States and Generalized Observables: A Simple Proof of Gleason's Theorem. *Phys. Rev. Lett.*, 91(12):120403, September 2003. doi: 10.1103/PhysRevLett.91.120403. URL https://link.aps.org/doi/10.1103/PhysRevLett.91.120403. 1.2, 10

[4] Paul Busch, Marian Grabowski, and Pekka J. Lahti. *Operational Quantum Physics*. Springer Science & Business Media, November 1997. ISBN 978-3-540-59358-4. 1.2

[5] Andrew M. Gleason. Measures on the Closed Subspaces of a Hilbert Space. In C. A. Hooker, editor, *The Logico-Algebraic Approach to Quantum Mechanics: Volume I: Historical Evolution*, The University of Western Ontario Series in Philosophy of Science, pages 123–133. Springer Netherlands, Dordrecht, 1975. ISBN 978-94-010-1795-4. doi: 10.1007/978-94-010-1795-4_7. URL https://doi.org/10.1007/978-94-010-1795-4_7. 7

[6] Raymond F. Streater and Arthur S. Wightman. *PCT, Spin and Statistics, and All That*. Princeton University Press, 1989. URL https://www.jstor.org/stable/j.ctt1cx3vcq. 9

[7] Valter Moretti. Mathematical Foundations of Quantum Mechanics: An Advanced Short Course. *Int. J. Geom. Methods Mod. Phys.*, 13(Supp. 1):1630011, October 2016. ISSN 0219-8878, 1793-6977. doi: 10.1142/S0219887816300117. URL http://arxiv.org/abs/

1508.06951. Comment: 103 pages, no figures. Some text corrections performed, to appear in Int. J. Geometrical Methods in Modern Physics. 1.2.2, 11

[8] Kan He, Qing Yuan, and Jinchuan Hou. Entropy-preserving maps on quantum states. *Linear Algebra and its Applications*, 467:243–253, February 2015. ISSN 0024-3795. doi: 10.1016/j.laa.2014.11.013. URL https://www.sciencedirect.com/science/article/pii/S002437951400737X. 11

[9] Lajos Molnár and Patrícia Szokol. Maps on states preserving the relative entropy II. *Linear Algebra and its Applications*, 432(12):3343–3350, July 2010. ISSN 0024-3795. doi: 10.1016/j.laa.2010.01.025. URL https://www.sciencedirect.com/science/article/pii/S0024379510000388. 11

[10] Ingemar Bengtsson and Karol Życzkowski. *Geometry of Quantum States: An Introduction to Quantum Entanglement.* Cambridge University Press, August 2017. ISBN 978-1-107-02625-4. 1.2.2

[11] J. v. Neumann. Uber Einen Satz Von Herrn M. H. Stone. *Ann. Math.*, 33(3):567–573, 1932. ISSN 0003-486X. doi: 10.2307/1968535. URL https://www.jstor.org/stable/1968535. 12

[12] M. H. Stone. On One-Parameter Unitary Groups in Hilbert Space. *Ann. Math.*, 33(3): 643–648, 1932. ISSN 0003-486X. doi: 10.2307/1968538. URL https://www.jstor.org/stable/1968538. 1.2.2

[13] Robert Alicki. Comment on "Reduced Dynamics Need Not Be Completely Positive". *Phys. Rev. Lett.*, 75(16):3020–3020, October 1995. doi: 10.1103/PhysRevLett.75.3020. URL https://link.aps.org/doi/10.1103/PhysRevLett.75.3020. 1.

[14] Philip Pechukas. Reduced Dynamics Need Not Be Completely Positive. *Phys. Rev. Lett.*, 73(8):1060–1062, August 1994. doi: 10.1103/PhysRevLett.73.1060. URL https://link.aps.org/doi/10.1103/PhysRevLett.73.1060. 1.2.3

[15] Anil Shaji and E. C. G. Sudarshan. Who's afraid of not completely positive maps? *Physics Letters A*, 341(1):48–54, June 2005. ISSN 0375-9601. doi: 10.1016/j.physleta.2005.04.029. URL https://www.sciencedirect.com/science/article/pii/S0375960105005748. 1.2.3

[16] Michael E. Cuffaro and Wayne C. Myrvold. On the Debate Concerning the Proper Characterization of Quantum Dynamical Evolution. *Philosophy of Science*, 80(5):1125–

1136, December 2013. ISSN 0031-8248. doi: 10.1086/673733. URL https://www.journals.uchicago.edu/doi/10.1086/673733. 1.2.3

[17] Ryogo Kubo. Statistical-mechanical theory of irreversible processes. I. General theory and simple applications to magnetic and conduction problems. *J. Phys. Soc. Jpn.*, 12(6):570–586, 1957. doi: 10.1143/JPSJ.12.570. 1.4

[18] Paul C. Martin and Julian Schwinger. Theory of many-particle systems. I. *Phys. Rev.*, 115(6):1342–1373, September 1959. doi: 10.1103/PhysRev.115.1342. URL https://link.aps.org/doi/10.1103/PhysRev.115.1342. 1.4

[19] Daniel Manzano. A short introduction to the Lindblad master equation. *AIP Adv.*, 10 (2):025106, 2020. doi: 10.1063/1.5115323. 2.1.4

Index