

Relaxation for an Open System of Interacting Spins

Draft



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ABSTRACT

The preface pretty much says it all.

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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 different notation so that the type of an expression may be inferred if the reader is confused.

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

The text uses **Planck units** where $\hbar = c = G = k_B = 1$.

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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

¹That 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.

²On 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.

1.2 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. $I(p) \geq 0$: 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:

$$H = \langle I \rangle \tag{1.2}$$

$$= - \sum_i p_i \log p_i, \tag{1.3}$$

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

³This 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.

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

where $0 \log 0 := \lim_{p \rightarrow 0} p \log p = 0$. 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.

1.3 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 postulate 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.

1.4 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 1.3, 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 $0 \leq E \leq 1$.⁶

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

1. $0 \leq P(E) \leq 1$ for all effects E ,
2. $P(1) = 1$,
3. $P(E_1 + E_2 + \dots) = P(E_1) + P(E_2) + \dots$ for any sequence of events with $E_1 + E_2 + \dots \leq 1$.

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

$$\left(\sum_i p_i P_i \right)(E) = \sum_i p_i P_i(E). \quad (1.4)$$

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**

$$P(E) = \text{tr}(\rho E), \quad (1.5)$$

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

⁵Since a quantum system is identified only by its dimension d , we may wonder which d -dimensional Hilbert space to assign. However, all finite d -dimensional (separable) complex Hilbert spaces are isometrically isomorphic to \mathbb{C}^d , and all infinite-dimensional separable Hilbert spaces are isometrically isomorphic to ℓ^2 (square-summable sequences) and to L^2 (square-integrable functions).

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

⁷The 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).

TODO: Hermitian operators.

We now describe how operations change states.

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

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

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

$$\text{tr } \mathcal{O}_m(\rho) = P(m) = \text{tr}(\rho E_m). \quad (1.7)$$

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

$$\rho' = \sum_m P(m) \rho'_m = \sum_m \mathcal{O}_m(\rho), \quad (1.8)$$

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

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

$$\frac{\mathcal{O}_m(\rho)}{\text{tr } \mathcal{O}_m(\rho)} = \sum_i P(i|m) \frac{\mathcal{O}_m(\rho_i)}{\text{tr } \mathcal{O}_m(\rho_i)} \quad (1.9)$$

By Bayes' theorem,

$$P(i|m) = \frac{P(i)P(m|i)}{P(m)} = \frac{p_i \text{tr } \mathcal{O}_m(\rho_i)}{\text{tr } \mathcal{O}_m(\rho)}. \quad (1.10)$$

Now eq. (1.9) becomes

$$\mathcal{O}_m \left(\sum_i p_i \rho_i \right) = \sum_i p_i \mathcal{O}_m(\rho_i). \quad (1.11)$$

Thus operations are convex linear.

1.5 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

$$\text{tr}(\rho f_i(E_i)) = \text{tr}(g_i(\rho) E_i) \quad (1.12)$$

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

$$\left(\sum_i \alpha_i \rho_i^A, \sum_j \beta_j \rho_j^B \right) \sim \sum_{ij} \alpha_i \beta_j (\rho_i^A, \rho_j^B) \quad (1.13)$$

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 $(\rho_A \otimes \rho_B)(E_A \otimes E_B) = \rho_A E_A \otimes \rho_B E_B$.

⁸For 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.

⁹Is 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].

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

$$\text{tr}(A \otimes B) = \text{tr } A \text{tr } B. \quad (1.14)$$

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

We now extend to non-product states, which are called **entangled** states. Consider a map f of the f_i and the countable sum of events $E = \sum_a E_a$. By eq. (1.12),

$$\text{tr} \left(\rho \sum_a f(E_a) \right) = \sum_a \text{tr} (\rho f(E_a)) \quad (1.15)$$

$$= \sum_a \text{tr} (g(\rho) E_a) \quad (1.16)$$

$$= \text{tr} \left(g(\rho) \sum_a E_a \right) \quad (1.17)$$

$$= \text{tr} \left(\rho f \left(\sum_a E_a \right) \right) \quad (1.18)$$

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

$$0 \leq \text{tr}(g(\rho)(E_2 - E_1)) \quad (1.19)$$

$$= \text{tr}(\rho f(E_2 - E_1)), \quad (1.20)$$

so $f(E_1) \leq f(E_2)$. 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

$$g_A(\rho) = \text{tr}_B(\rho_A \otimes \rho_B) \equiv \rho_A \text{tr } \rho_B = \rho_A, \quad (1.21)$$

and is extended linearly to combinations of product states.

1.6 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.

¹⁰The argument is the same as that for the real linearity of a probability measure on effects given in [4].

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. (1.11). Since the information in the state ρ cannot change, \mathcal{O} must be invertible. Kadison's theorem¹¹ states that all such operations have the form

$$\mathcal{O}\rho = U\rho U^\dagger, \quad (1.22)$$

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

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

$$\rho(t) = U(t)\rho(0)U^\dagger(t) \quad (1.23)$$

as a function of time. We expect that $U(t)$ changes continuously¹² and satisfies

$$U(t + t') = U(t)U(t') \quad (1.24)$$

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

$$U(t) = e^{-iHt}. \quad (1.25)$$

This allows us to differentiate eq. (1.23) to find

$$\dot{\rho} = \dot{U}(t)\rho(0)U^\dagger(t) + U(t)\rho(0)\dot{U}^\dagger(t) \quad (1.26)$$

$$= -iH(U(t)\rho(0)U^\dagger(t)) + (U(t)\rho(0)U^\dagger(t))iH \quad (1.27)$$

$$= -i[H, \rho], \quad (1.28)$$

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

¹¹Wigner'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].

¹²More precisely, $U(t)$ is **strongly continuous** if $\lim_{t \rightarrow t_0} U(t)|v\rangle = U(t_0)|v\rangle$ 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].

¹³Equation (1.28) is given in **Planck units** where $\hbar = c = G = k_B = 1$. Otherwise $\dot{\rho} = -i[H, \rho]/\hbar$.

Given an observable A , its expected value over time is

$$\langle A \rangle = \text{tr}(\rho(t)A) \quad (1.29)$$

$$= \text{tr}(U(t)\rho(0)U^\dagger(t)A) \quad (1.30)$$

$$= \text{tr}(\rho(0)U^\dagger(t)AU(t)). \quad (1.31)$$

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

$$A_H(t) = U^\dagger(t)AU(t). \quad (1.32)$$

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

$$\dot{A}_H = -i[A_H, H] \quad (1.33)$$

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

1.7 CANONICAL QUANTIZATION

The discussion of quantum theory thus far has been fully general. The Liouville equation (eq. (1.28)) specifies how a state ρ changes in time, given the Hilbert space for the system, the operator H , and the initial state $\rho(0)$. How does one determine these quantities for a particular physical system? We will only consider physical systems that can be modeled by nonrelativistic classical mechanics. Consider a classical system with generalized coordinates q_i and momenta p_i . If the system has classical Hamiltonian $H(\mathbf{q}, \mathbf{p})$, then Hamilton's equations of motion are

$$\dot{q}_i = \frac{\partial H}{\partial p_i} = \{q_i, H\} \quad (1.34)$$

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} = \{p_i, H\}, \quad (1.35)$$

in terms of the **Poisson bracket**

$$\{f, g\} = \sum_i \left(\frac{\partial f}{\partial q_i} \frac{\partial g}{\partial p_i} - \frac{\partial g}{\partial q_i} \frac{\partial f}{\partial p_i} \right). \quad (1.36)$$

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

$$\dot{q}_i = -i[q_i, H] \quad (1.37)$$

$$\dot{p}_i = -i[p_i, H], \quad (1.38)$$

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

$$Q(\{f, g\}) = -i[Q(f), Q(g)]. \quad (1.39)$$

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

$$[q_i, p_j] = i\delta_{ij}. \quad (1.40)$$

For the moment, consider a classical system with only one degree of freedom.¹⁴ One can show that the only possible quantization for polynomials in q and p with degree less than four is the **Weyl quantization**. This simply averages over all possible operator orders.¹⁵ For example,

$$Q(3qp^2) = qp^2 + pqp + p^2q. \quad (1.42)$$

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

$$q^2p^2 = \frac{1}{9}\{q^3, p^3\} = \frac{1}{3}\{q^2p, qp^2\}, \quad (1.43)$$

yet

$$\frac{1}{9}[Q(q^3), Q(p^3)] \neq \frac{1}{3}[Q(q^2p), Q(qp^2)], \quad (1.44)$$

so there is no quantization of q^2p^2 . This result on the nonexistence of a general quantization map is known as Groenewold's theorem [14, p. 272]. Luckily, we will only consider systems where the Weyl quantization satisfies eq. (1.39), and we may put the issue of quantization aside.

Now we know that q and p must satisfy the ccr. But what are they? Weyl showed that q and p must be operators on an infinite-dimensional Hilbert space [15]. The usual assignment for square-integrable functions f is $qf(q) = qf(q)$ and $pf(q) = -if'(q)$, which

¹⁴All the considerations to follow generalize naturally to many degrees of freedom.

¹⁵In general, the Weyl quantization of f is

$$Q(f) = \exp\left(\frac{1}{2i} \sum_i \frac{\partial^2}{\partial q_i \partial p_i}\right) \hat{f}(\mathbf{q}, \mathbf{p}), \quad (1.41)$$

where \hat{f} is f in the normal form where q_i always precedes p_i [13].

satisfies the CCR. How do we know that this is the right assignment? What if one should assign a different Hilbert space \mathcal{H} with other position and momentum operators q' and p' ? By Stone's theorem, there are unitary operators $U(t) = e^{itq'}$ and $V(s) = e^{isp'}$. Then a formal application of the Baker-Campbell-Hausdorff (BCH) formula¹⁶ gives that

$$U(t)V(s) = e^{-ist}V(s)U(t), \quad (1.46)$$

which is known as the Weyl relation [14, p. 281].¹⁷ The Stone-von Neumann theorem¹⁸ is that there is a unitary operator $T : L^2(\mathbb{R}) \rightarrow \mathcal{H}$ such that

$$T^\dagger U(t) T = e^{itq} \quad (1.47)$$

$$T^\dagger V(s) T = e^{isp}. \quad (1.48)$$

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

$$T^\dagger q' T = q \quad (1.49)$$

$$T^\dagger p' T = p. \quad (1.50)$$

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

$$\text{tr}(\rho' q') = \text{tr}(\rho q) \quad (1.51)$$

$$\text{tr}(\rho' p') = \text{tr}(\rho p), \quad (1.52)$$

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

1.8 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

¹⁶Namely that if $[A, [A, B]] = [B, [A, B]] = 0$, then

$$e^A e^B = e^{A+B+[A,B]/2}. \quad (1.45)$$

¹⁷Since the Weyl relation was derived through a merely formal procedure, not all operators satisfying the CCR satisfy the Weyl relation. The usual q and p do satisfy the Weyl relation, so we may as well stipulate that any putative operators q' and p' must satisfy it as well.

¹⁸The Stone-von Neumann theorem was also used to prove the equivalence between the Schrödinger equation and Heisenberg's matrix mechanics.

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

1. The state ρ_0 is promoted to a state of the composite system according to an **assignment map** $\mathcal{A}(\rho_0)$. A consistent assignment map should have the following intuitive properties: [16]
 - (a) \mathcal{A} is convex,
 - (b) $\text{tr}_B \mathcal{A}(\rho_0) = \rho_0$,
 - (c) $\mathcal{A}(\rho_0)$ is a density operator.
2. The assigned composite state becomes $\rho(t) = U(t)\mathcal{A}(\rho_0)U^\dagger(t)$ as usual for a closed system.
3. The state $\rho(t)$ is reduced to give the open system state $\rho_S(t) = \text{tr}_B \rho(t)$.

In summary, the state at time t is

$$\rho_S(t) = \text{tr}_B(U(t)\mathcal{A}(\rho_0)U^\dagger(t)), \quad (1.53)$$

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

One can show that the only consistent assignment maps for a two-dimensional system are of the form $\mathcal{A}(\rho_0) = \rho_0 \otimes \rho_B$, where ρ_B is a constant density operator on \mathcal{H}_B [17]. We will consider ρ_B to be a stationary state of the bath, such as a thermal state at some temperature. Why do we not require that the composite state $\rho(t)$ is always assignable, remaining within the image of \mathcal{A} ? This would make \mathcal{V} satisfy that

$$\mathcal{V}(t+s) = \mathcal{V}(t)\mathcal{V}(s). \quad (1.54)$$

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

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

effectively stationary. Thus $\rho(t)$ is approximately assignable if we only aim to consider the coarse-grained system dynamics. The notion of reduced dynamics only makes sense on system timescales, and requires several conditions on eq. (1.53) for the coarse-graining to be possible. Since the system must be weakly coupled to the bath for the bath to remain approximately stationary, these simplifications are collectively called the **weak-coupling limit**.

This process will lead to a differential equation (eq. (1.81)) for ρ_S . It is worth mentioning that this equation, known as the Lindblad equation, is in the general form for any map $\mathcal{V}(t)$ on density matrices that satisfies eq. (1.54), with the technical condition that it is also completely positive.¹⁹ On these grounds, it is often asserted that all reduced dynamics must be completely positive. This is not the case if the initial condition of the composite system is not a product state, and we have argued that the notion of reduced dynamics does not make sense outside of the weak-coupling limit. The debate concerning complete positivity remains a contentious issue [17, 19, 20].

1.9 THE WEAK-COUPPLING LIMIT

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

$$H = H_0 + H_I \tag{1.55}$$

$$= H_S \otimes 1 + 1 \otimes H_B + H_I, \tag{1.56}$$

where H_S is the Hamiltonian of the system, H_B is the Hamiltonian of the bath, and H_I is the interaction Hamiltonian between the system and the bath. First, we will recast the dynamics of the composite system into a convenient form. Recall the Heisenberg picture from section 1.6. Given eq. (1.55), we may similarly decompose the expected value of an observable A for the composite system. If we let

$$U_0(t) = e^{-iH_0 t} \tag{1.57}$$

$$U_I(t) = U_0^\dagger(t)U(t), \tag{1.58}$$

¹⁹For any Hilbert space \mathcal{H}' , define the combined operation $\mathcal{V}(t) \otimes \mathbb{1}$ by $(\mathcal{V}(t) \otimes \mathbb{1})(A \otimes B) = \mathcal{V}(t)A \otimes B$ and extending linearly. We say that $\mathcal{V}(t)$ is **completely positive** if $(\mathcal{V}(t) \otimes \mathbb{1})(C)$ is positive for every positive operator C on $\mathcal{H}_S \otimes \mathcal{H}'$ [18, p. 89].

then we may decompose the expected value as

$$\langle A \rangle = \text{tr}(AU(t)\rho(0)U^\dagger(t)) \quad (1.59)$$

$$= \text{tr}(U_0^\dagger(t)AU_0(t)U_I(t)\rho(0)U_I^\dagger(t)). \quad (1.60)$$

This suggests that we define the time-dependent operators

$$A_I(t) = U_0^\dagger(t)AU_0(t) \quad (1.61)$$

$$\rho_I(t) = U_I(t)\rho(0)U_I^\dagger(t). \quad (1.62)$$

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

$$\dot{\rho}_I = -i[H_I, \rho_I]. \quad (1.63)$$

We will use eq. (1.63) in its integral form

$$\rho_I(t) = \rho_I(0) - i \int_0^t ds [H_I(s), \rho_I(s)]. \quad (1.64)$$

It will also be helpful to relate the interaction Hamiltonian to transition frequencies of the system as follows.²⁰ First, we write a general interaction Hamiltonian as

$$H_I = \sum_{\alpha} A_{\alpha} \otimes B_{\alpha}. \quad (1.65)$$

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

$$A_{\alpha}(\omega) = \sum_{E'-E=\omega} \Pi(E)A_{\alpha}\Pi(E'). \quad (1.66)$$

By the completeness of the energy projectors,

$$\sum_{\omega} A_{\alpha}(\omega) = \sum_{\omega} \sum_{E'-E=\omega} \Pi(E)A_{\alpha}\Pi(E') \quad (1.67)$$

$$= \sum_{E_1, E_2} \Pi(E_1)A_{\alpha}\Pi(E_2) \quad (1.68)$$

$$= A_{\alpha}. \quad (1.69)$$

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

$$[H_S, A_{\alpha}(\omega)] = -\omega A_{\alpha}(\omega). \quad (1.70)$$

²⁰This decomposition requires that the spectrum of H_S is discrete.

Using eq. (1.70) to commute past the exponential in eq. (1.61) establishes that the corresponding interaction picture operators are

$$A_\alpha^I(\omega) = e^{-i\omega t} A_\alpha(\omega). \quad (1.71)$$

Thus the interaction Hamiltonian in the interaction picture is

$$H_I(t) = \sum_{\alpha\omega} e^{-i\omega t} A_\alpha(\omega) \otimes B_\alpha^I(t), \quad (1.72)$$

where by eq. (1.61)

$$B_\alpha^I(t) = e^{iH_B t} B_\alpha e^{-iH_B t}. \quad (1.73)$$

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

$$\langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle \quad (1.74)$$

and their one-sided Fourier transform

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty ds e^{i\omega s} \langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle \quad (1.75)$$

$$\equiv iS_{\alpha\beta}(\omega) + \gamma_{\alpha\beta}(\omega)/2, \quad (1.76)$$

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

$$\gamma_{\alpha\beta}(\omega) \equiv \int_{-\infty}^\infty ds e^{i\omega s} \langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle \quad (1.77)$$

is positive.

With this setup, we may now move to the main derivation. Applying eq. (1.63) to eq. (1.64) and tracing out the environment gives the closed equation

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

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

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

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: $\langle B_\alpha(t) \rangle = 0$.

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

$$\dot{\rho}_S = - \int_0^\infty ds \operatorname{tr}_B [H_I(t), [H_I(t-s), \rho_S(t) \otimes \rho_B]]. \quad (1.78)$$

This is justified when the reservoir correlation functions in eq. (1.75) vanish quickly over a time τ_C that is smaller than the relaxation time τ_R . Substituting eq. (1.72) into eq. (1.78) and using eq. (1.75) gives

$$\dot{\rho}_S = 2 \operatorname{He} \sum_{\alpha\beta\omega\omega'} e^{i(\omega' - \omega)t} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_S A_\alpha^\dagger(\omega') - A_\alpha^\dagger(\omega') A_\beta(\omega) \rho_S \right), \quad (1.79)$$

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

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

for system evolution are small compared to the relaxation time τ_R , then the contribution from the fast-oscillating terms of eq. (1.79) 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

$$\dot{\rho}_S = 2 \operatorname{He} \sum_{\alpha\beta\omega} \Gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_S A_\alpha^\dagger(\omega) - A_\alpha^\dagger(\omega) A_\beta(\omega) \rho_S \right). \quad (1.80)$$

Now applying the decomposition eq. (1.76) gives the interaction picture **Lindblad equation**

$$\dot{\rho}_S = -i[H_{LS}, \rho_S] + \mathcal{D}(\rho_S), \quad (1.81)$$

where the **Lamb shift Hamiltonian** is

$$H_{LS} = \sum_{\alpha\beta\omega} S_{\alpha\beta}(\omega) A_\alpha^\dagger(\omega) A_\beta(\omega), \quad (1.82)$$

and the **dissipator** is

$$\mathcal{D}(\rho_S) = \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega) \rho_S A_\alpha^\dagger(\omega) - \frac{1}{2} \{ A_\alpha^\dagger(\omega) A_\beta(\omega), \rho_S \} \right). \quad (1.83)$$

To transform back to the Schrödinger picture, one only needs to add the system Hamiltonian H_S to H_{LS} . One may then diagonalize $\gamma_{\alpha\beta}$ to put eq. (1.81) into the standard form of eq. (A.17). In our examples $\gamma_{\alpha\beta}$ will already be diagonal. In this case, we call the operators defined by eq. (1.70) in the dissipator the **jump operators** of the open system.

1.10 RELAXATION TO THERMAL EQUILIBRIUM

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

$$\rho_B = \frac{e^{-\beta H_B}}{\text{tr } e^{-\beta H_B}}, \quad (1.84)$$

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

$$\rho_{\text{th}} = \frac{e^{-\beta H_S}}{\text{tr } e^{-\beta H_S}}. \quad (1.85)$$

We will now prove that ρ_{th} is a stationary state. First, we see that the Lamb shift Hamiltonian commutes with the system Hamiltonian, since eq. (1.70) implies that

$$[H_S, A_\alpha^\dagger(\omega)A_\beta(\omega)] = 0. \quad (1.86)$$

Thus ρ_{th} is unchanged by the unitary part of \mathcal{L} , and may turn our attention towards showing that $\mathcal{D}(\rho_{\text{th}}) = 0$. We may also use eq. (1.70) to find that

$$\rho_{\text{th}}A_\alpha(\omega) = e^{\beta\omega}A_\alpha(\omega)\rho_{\text{th}} \quad (1.87)$$

$$\rho_{\text{th}}A_\alpha^\dagger(\omega) = e^{-\beta\omega}A_\alpha^\dagger(\omega)\rho_{\text{th}}. \quad (1.88)$$

The reservoir correlation functions obey the **kms condition** [21, 22]

$$\langle B_\alpha^\dagger(t)B_\beta(0) \rangle = \langle B_\beta(0)B_\alpha^\dagger(t + i\beta) \rangle. \quad (1.89)$$

From eq. (1.89) it follows that

$$\gamma_{\alpha\beta}(-\omega) = e^{-\beta\omega}\gamma_{\beta\alpha}(\omega). \quad (1.90)$$

We may then use eqs. (1.87), (1.88) and (1.90) to compute that the dissipator is

$$\mathcal{D}(\rho_{\text{th}}) = \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega) \left(A_\beta(\omega)\rho_{\text{th}}A_\alpha^\dagger(\omega) - \frac{1}{2}\{A_\alpha^\dagger(\omega)A_\beta(\omega), \rho_{\text{th}}\} \right) \quad (1.91)$$

$$= \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega) \left(e^{-\beta\omega}A_\beta(\omega)A_\alpha^\dagger(\omega) - \frac{1}{2}A_\alpha^\dagger(\omega)A_\beta(\omega) - \frac{1}{2}A_\alpha^\dagger(\omega)A_\beta(\omega) \right) \rho_{\text{th}} \quad (1.92)$$

$$= \left(\sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega)e^{-\beta\omega}A_\beta(\omega)A_\alpha^\dagger(\omega) - \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}(\omega)A_\alpha^\dagger(\omega)A_\beta(\omega) \right) \rho_{\text{th}} \quad (1.93)$$

$$= 0. \quad (1.94)$$

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

CHAPTER 2

APPLICATION TO INTERACTING SPINS

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

2.1 THE CLOSED TWO-DIMENSIONAL SYSTEM

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

$$[\sigma^a, \sigma^b] = 2i\epsilon_{abc}\sigma^c, \quad (2.1)$$

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

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

The expectation values of the Pauli operators are $\langle \boldsymbol{\sigma} \rangle = \mathbf{v}$, so it suffices to determine the time evolution of \mathbf{v} . A similar vector $\boldsymbol{\omega}$ determines the general Hamiltonian¹

$$H = \frac{1}{2}\boldsymbol{\omega} \cdot \boldsymbol{\sigma}. \quad (2.3)$$

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

The Liouville equation (eq. (1.28)) is then

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

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

so the Bloch vector follows the differential equation

$$\dot{\boldsymbol{v}} = \boldsymbol{\omega} \times \boldsymbol{v}. \quad (2.6)$$

The solution of this equation is

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

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

$$[L^a, L^b] = \varepsilon_{abc} L^c. \quad (2.8)$$

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

2.2 RELAXATION OF THE TWO-DIMENSIONAL SYSTEM

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

$$H_S = \frac{\omega}{2} \sigma^z, \quad (2.9)$$

where ω is the frequency of light emitted from the transition. The weak-coupling limit for the electric dipole interaction with the bath is similar to that for the magnetic dipole interaction considered later in section 2.3, so will simply state the results here and focus on investigating the dynamics.² To focus on the relaxation of the system, we ignore the Lamb shift and consider only the effect of the dissipator. The jump operators are

$$\sigma^\pm = \frac{\sigma^x \pm i\sigma^y}{2} \quad (2.10)$$

²A full derivation is given in [18, pp. 141–149].

and the Lindblad equation is

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

where

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

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

$$\dot{v}_x = -\frac{\gamma}{2} v_x, \quad (2.13)$$

$$\dot{v}_y = -\frac{\gamma}{2} v_y, \quad (2.14)$$

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

where the total transition rate is

$$\gamma = \gamma_0(2N+1). \quad (2.16)$$

The equilibrium solution is seen to be

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

so the stationary population of the excited state is

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

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

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

2.3 THE WEAK-COUPPLING LIMIT FOR THE ISING CHAIN

The bath Hamiltonian is

$$H_B = \sum_{\mathbf{k}, \lambda} \hbar \omega_{\mathbf{k}} a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}, \lambda}. \quad (2.20)$$

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

The interaction Hamiltonian for spin- s objects in a magnetic field is³

$$H_I = - \int d\mathbf{r} \, \boldsymbol{\mu} \cdot \mathbf{B} \quad (2.21)$$

$$= - \int d\mathbf{r} \sum_i \mu_e \delta(\mathbf{r}_i) \boldsymbol{\sigma}_i \quad (2.22)$$

$$\cdot i \sum_{\mathbf{k}, \lambda} \sqrt{\frac{\hbar c^2 \mu_0}{2V \omega_{\mathbf{k}}}} \left((\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda}) e^{i\mathbf{k} \cdot \mathbf{r}} a_{\mathbf{k}, \lambda} - (\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda}^*) e^{-i\mathbf{k} \cdot \mathbf{r}} a_{\mathbf{k}, \lambda}^\dagger \right) \quad (2.23)$$

$$= - \sum_{i, \mu} \sigma_i^\mu B_i^\mu, \quad (2.23)$$

where the components of the **magnetic field operator** evaluated at \mathbf{r}_i are⁴

$$B_i^\mu = i\mu_e \sum_{\mathbf{k}, \lambda} \sqrt{\frac{\hbar c^2 \mu_0}{2V \omega_{\mathbf{k}}}} \left((\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda})_\mu e^{i\mathbf{k} \cdot \mathbf{r}_i} a_{\mathbf{k}, \lambda} - (\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda}^*)_\mu e^{-i\mathbf{k} \cdot \mathbf{r}_i} a_{\mathbf{k}, \lambda}^\dagger \right). \quad (2.24)$$

This magnetic field operator includes the electron's magnetic moment so that the final rate γ (eq. (2.55)) carries the dimensions of frequency in the dissipator (eq. (1.83)).

The composite Hamiltonian we consider is

$$H = H_S \otimes 1 + 1 \otimes H_B + H_I \quad (2.25)$$

$$= -J(g) \sum_{i \in \mathbb{Z}_N} (f(1-g) \sigma_i^x \sigma_{i+1}^x + f(g) \sigma_i^z) \otimes 1 \quad (2.26)$$

$$+ 1 \otimes \sum_{\mathbf{k}, \lambda} \hbar \omega_{\mathbf{k}} a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}, \lambda} - \sum_{i, \mu} \sigma_i^\mu \otimes B_i^\mu,$$

where

- $J(g) > 0$ for $0 \leq g \leq 1$,
- $f(g)$ is monotonic for $0 \leq g \leq 1$, $f(0) = 0$, and $f(1) = 1$, like for $f(g) = g$,
- The bath is a 3D continuum of modes according to eq. (2.41),
- The spin positions in eq. (2.24) are $\mathbf{r}_i = ai\hat{z}$ for some spacing a ,

³An 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 $a_{\mathbf{k}, \lambda}$, and the prefactor is chosen so that these operators are dimensionless, but \mathbf{B} is not.

⁴This operator arises from quantizing the electromagnetic field. See the discussion of field quantization in [23, p. 506] for more details.

- The dipole approximation is valid. This requires that $a \ll c/\omega_{\mathbf{k}}$ for $\omega_{\mathbf{k}}$ up to the largest transition energy possible for H_S . A bound is $\omega_{\mathbf{k}} \leq 2NJ(1)/\hbar$ for constant J .

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

In the interaction picture:

$$B_i^\mu(t) = e^{iH_B t/\hbar} B_i^\mu e^{-iH_B t/\hbar} \quad (2.27)$$

$$= i\mu_e \sum_{\mathbf{k}, \lambda} \sqrt{\frac{\hbar c^2 \mu_0}{2V \omega_{\mathbf{k}}}} \left((\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda})_\mu e^{i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k}} t)} a_{\mathbf{k}, \lambda} - (\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda}^*)_\mu e^{-i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k}} t)} a_{\mathbf{k}, \lambda}^\dagger \right). \quad (2.28)$$

The spectral correlation tensor is then

$$\begin{aligned} \Gamma_{i\mu, j\nu}(\omega) &= \frac{1}{\hbar^2} \int_0^\infty ds e^{i\omega s} \langle B_i^\mu(t)^\dagger B_j^\nu(t-s) \rangle \\ &= -\frac{\mu_e^2}{\hbar^2} \frac{\hbar c^2 \mu_0}{2V} \int_0^\infty ds \sum_{\mathbf{k}, \mathbf{k}', \lambda, \lambda'} \sqrt{\frac{1}{\omega_{\mathbf{k}} \omega_{\mathbf{k}'}}} : \\ &\quad (\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda})_\mu (\mathbf{k}' \times \mathbf{e}_{\mathbf{k}', \lambda'})_\nu e^{i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k}} t + \mathbf{k}' \cdot \mathbf{r}_j - \omega_{\mathbf{k}'}(t-s) + \omega s)} \langle a_{\mathbf{k}, \lambda} a_{\mathbf{k}', \lambda'} \rangle \\ &\quad - (\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda})_\mu (\mathbf{k}' \times \mathbf{e}_{\mathbf{k}', \lambda'}^*)_\nu e^{i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k}} t - \mathbf{k}' \cdot \mathbf{r}_j + \omega_{\mathbf{k}'}(t-s) + \omega s)} \langle a_{\mathbf{k}, \lambda} a_{\mathbf{k}', \lambda'}^\dagger \rangle \\ &\quad - (\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda}^*)_\mu (\mathbf{k}' \times \mathbf{e}_{\mathbf{k}', \lambda'})_\nu e^{-i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k}} t - \mathbf{k}' \cdot \mathbf{r}_j + \omega_{\mathbf{k}'}(t-s) - \omega s)} \langle a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}', \lambda'} \rangle \\ &\quad + (\mathbf{k} \times \mathbf{e}_{\mathbf{k}, \lambda}^*)_\mu (\mathbf{k}' \times \mathbf{e}_{\mathbf{k}', \lambda'}^*)_\nu e^{-i(\mathbf{k} \cdot \mathbf{r}_i - \omega_{\mathbf{k}} t + \mathbf{k}' \cdot \mathbf{r}_j - \omega_{\mathbf{k}'}(t-s) - \omega s)} \langle a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}', \lambda'}^\dagger \rangle. \end{aligned} \quad (2.30)$$

In the thermal state

$$\rho_B = \frac{e^{-\beta H_B}}{\text{tr } e^{-\beta H_B}} = \prod_{\mathbf{k}, \lambda} (1 - e^{-\beta \hbar \omega_{\mathbf{k}}}) e^{-\beta \hbar \omega_{\mathbf{k}} a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}, \lambda}} \quad (2.31)$$

Since $[a_{\mathbf{k}, \lambda}, a_{\mathbf{k}', \lambda'}^\dagger] = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'} 1$,

$$\langle a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}', \lambda'} \rangle = \text{tr}(e^{-\beta H_B})^{-1} \text{tr}(e^{-\beta H_B} a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}', \lambda'}) \quad (2.32)$$

$$= \text{tr}(e^{-\beta H_B})^{-1} \text{tr}(e^{-\beta H_B} a_{\mathbf{k}', \lambda'} a_{\mathbf{k}, \lambda}^\dagger) - \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'} \quad (2.33)$$

$$= \text{tr}(e^{-\beta H_B})^{-1} \text{tr}(e^{\beta \hbar \omega_{\mathbf{k}}} a_{\mathbf{k}', \lambda'} e^{-\beta H_B} a_{\mathbf{k}, \lambda}^\dagger) - \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'} \quad (2.34)$$

$$= e^{\beta \hbar \omega_{\mathbf{k}}} \langle a_{\mathbf{k}, \lambda}^\dagger a_{\mathbf{k}', \lambda'} \rangle - \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'} \quad (2.35)$$

$$= \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'} n_B(\omega_{\mathbf{k}}), \quad (2.36)$$

where

$$n_B(\omega) = \frac{1}{e^{\beta\hbar\omega} - 1}. \quad (2.37)$$

Similarly,

$$\langle a_{\mathbf{k},\lambda} a_{\mathbf{k}',\lambda'}^\dagger \rangle = \langle a_{\mathbf{k},\lambda}^\dagger a_{\mathbf{k}',\lambda'}^\dagger \rangle = 0 \quad (2.38)$$

$$\langle a_{\mathbf{k},\lambda} a_{\mathbf{k}',\lambda'}^\dagger \rangle = \delta_{\mathbf{k}\mathbf{k}'} \delta_{\lambda\lambda'} (1 + n_B(\omega_{\mathbf{k}})). \quad (2.39)$$

Then for a thermal bath, the spectral correlation tensor becomes

$$\begin{aligned} \Gamma_{i\mu,j\nu}(\omega) &= \frac{\mu_e^2 c^2 \mu_0}{2\hbar V} \int_0^\infty ds \sum_{\mathbf{k},\lambda} \frac{1}{\omega_{\mathbf{k}}} : \\ &\quad (\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda})_\mu (\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda}^*)_\nu e^{i(\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j) + s(\omega - \omega_{\mathbf{k}}))} (1 + n_B(\omega_{\mathbf{k}})) \\ &\quad + (\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda}^*)_\mu (\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda})_\nu e^{-i(\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j) - s(\omega + \omega_{\mathbf{k}}))} n_B(\omega_{\mathbf{k}}). \end{aligned} \quad (2.40)$$

To evaluate eq. (2.40), we now consider a chain of N spins along the z -axis, so that $\mathbf{r}_i = r_i \hat{\mathbf{z}}$.⁵

Then $\mathbf{k} \cdot (\mathbf{r}_i - \mathbf{r}_j) = k_z \Delta r_{ij}$.

In the continuum limit,

$$\frac{1}{V} \sum_{\mathbf{k}} \mapsto \int \frac{d\mathbf{k}}{(2\pi)^3} = \frac{1}{(2\pi c)^3} \int_0^\infty d\omega_k \omega_k^2 \int d\Omega, \quad (2.41)$$

where the integral over solid angle is

$$\int d\Omega = \int d\phi \int d\theta \sin \theta. \quad (2.42)$$

To apply this limit to eq. (2.40), we first note that

$$\sum_{\lambda} (\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda})_\mu (\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda}^*)_\nu = \sum_{abcd} \varepsilon_{\mu ab} \varepsilon_{\nu cd} k^a k^c \sum_{\lambda} e_{\mathbf{k},\lambda}^b (e_{\mathbf{k},\lambda}^d)^* \quad (2.43)$$

$$= \sum_{abcd} \varepsilon_{\mu ab} \varepsilon_{\nu cd} k^a k^c \left(\delta_{bd} - \frac{k^b k^d}{k^2} \right) \quad (2.44)$$

$$= \sum_{abc} \varepsilon_{\mu ab} \varepsilon_{\nu cb} k^a k^c \quad (2.45)$$

$$= \sum_{ac} (\delta_{\mu\nu} \delta_{ac} - \delta_{\mu c} \delta_{a\nu}) k^a k^c \quad (2.46)$$

$$= k^2 \delta_{\mu\nu} - k^\mu k^\nu. \quad (2.47)$$

⁵We could consider any axis given the spherical symmetry, but the z -axis is the simplest to evaluate.

Thus

$$\int d\Omega e^{\pm i k_z \Delta r_{ij}} \sum_{\lambda} (\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda})_{\mu} (\mathbf{k} \times \mathbf{e}_{\mathbf{k},\lambda}^*)_{\nu} = \frac{8\pi\omega_k^2}{3c^2} \delta_{\mu\nu} G_{\nu} \left(\frac{\omega_k \Delta r_{ij}}{c} \right), \quad (2.48)$$

where

$$G_{\nu}(u) = \left(\delta_{\nu z} - \frac{\delta_{\nu x} + \delta_{\nu y}}{2} \right) \frac{\text{sinc } u - \cos u}{u^2} + \frac{\delta_{\nu x} + \delta_{\nu y}}{2} \text{sinc } u. \quad (2.49)$$

Note that in the dipole approximation

$$\lim_{u \rightarrow 0} G_{\nu}(u) = \left(\delta_{\nu z} - \frac{\delta_{\nu x} + \delta_{\nu y}}{2} \right) \frac{1}{3} + \frac{\delta_{\nu x} + \delta_{\nu y}}{2} = \frac{1}{3}. \quad (2.50)$$

Now eq. (2.48) gives that the continuum limit of the spectral correlation tensor for the spin chain is

$$\begin{aligned} \Gamma_{i\mu,j\nu}(\omega) &= \delta_{\mu\nu} \frac{\mu_0}{6\pi^2 \mu_e^2 \hbar c^3} \int_0^{\infty} d\omega_k \omega_k^3 G_{\nu} \left(\frac{\omega_k \Delta r_{ij}}{c} \right) : \\ &\quad (1 + n_B(\omega_k)) \int_0^{\infty} ds e^{is(\omega - \omega_k)} + n_B(\omega_k) \int_0^{\infty} ds e^{is(\omega + \omega_k)}. \end{aligned} \quad (2.51)$$

We now use that

$$n_B(-\omega) = -(1 + n_B(\omega)) \quad (2.52)$$

and

$$\int_0^{\infty} ds e^{-i\omega s} = \pi \delta(\omega) - i \mathcal{P} \frac{1}{\omega}, \quad (2.53)$$

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

$$\Gamma_{i\mu,j\nu}(\omega) = \frac{1}{2} \gamma_{i\mu,j\nu}(\omega) + i S_{i\mu,j\nu}(\omega), \quad (2.54)$$

where

$$\gamma_{i\mu,j\nu}(\omega) = \delta_{\mu\nu} \frac{\mu_e^2 \mu_0 \omega^3}{3\pi \hbar c^3} G_{\nu} \left(\frac{|\omega| \Delta r_{ij}}{c} \right) (1 + n_B(\omega)) \quad (2.55)$$

$$S_{i\mu,j\nu}(\omega) = \delta_{\mu\nu} \frac{\mu_e^2 \mu_0}{6\pi^2 \hbar c^3} \mathcal{P} \int_0^{\infty} d\omega_k \omega_k^3 G_{\nu} \left(\frac{\omega_k \Delta r_{ij}}{c} \right) \left(\frac{1 + n_B(\omega_k)}{\omega - \omega_k} + \frac{n_B(\omega_k)}{\omega + \omega_k} \right). \quad (2.56)$$

The principal value integral in eq. (2.56) diverges to $-\infty$ when $i = j$ but vanishes otherwise. The net contribution to the Lamb shift Hamiltonian (eq. (1.82)) 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

$$\gamma(\omega) = \frac{\mu_e^2 \mu_0 \omega^3}{9\pi \hbar c^3} (1 + n_B(\omega)) \quad (2.57)$$

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

$$\tilde{\gamma}(\tilde{\omega}) = \left(\frac{\tau_0}{\tau_S}\right)^2 \tilde{\omega}^3 \left(1 + \frac{1}{e^{\tau_B \tilde{\omega} / \tau_S} - 1}\right) \quad (2.58)$$

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

$$\tau_0 = \sqrt{\frac{\mu_e^2 \mu_0}{9\pi \hbar c^3}} = 3.67 \times 10^{-23} \text{ s} \cong 56 \text{ GeV}^{-1}. \quad (2.59)$$

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

$$\tilde{\gamma}(\tilde{\omega}) \approx \frac{\tau_0^2}{\tau_B \tau_S} \tilde{\omega}^2. \quad (2.60)$$

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

$$\tilde{\gamma}_0 = \lim_{\tau_B \rightarrow \infty} \tilde{\gamma}(1) = \left(\frac{\tau_0}{\tau_S}\right)^2. \quad (2.61)$$

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

$$\tilde{S}(\tilde{\omega}) = \frac{1}{2\pi} \left(\frac{\tau_0}{\tau_S}\right)^2 \mathcal{P} \int_0^\infty d\tilde{\omega}_k \tilde{\omega}_k^3 \left(\frac{1 + \tilde{n}_B(\tilde{\omega}_k)}{\tilde{\omega} - \tilde{\omega}_k} + \frac{\tilde{n}_B(\tilde{\omega}_k)}{\tilde{\omega} + \tilde{\omega}_k} \right), \quad (2.62)$$

where

$$\tilde{n}_B(\tilde{\omega}) = \frac{1}{e^{\tau_B \tilde{\omega} / \tau_S} - 1}. \quad (2.63)$$

To avoid the divergence of eq. (2.62), we introduce an upper frequency cutoff $\tilde{\Omega}$. Physically, one expects the coupling to high-frequency modes of the bath to weaken.⁶ For simplicity, we just set the upper limit of the integral to $\tilde{\Omega}$, though other cutoffs like $e^{-\tilde{\omega}_k / \tilde{\Omega}}$ are common. As we will see, the exact functional form does not matter. If we set the frequency cutoff $\tilde{\Omega} \gg \tilde{\omega}$ to be far above any system frequency, we have the following limits.

⁶This 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.

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

$$\tilde{S}(\tilde{\omega}) \approx \frac{1}{2\pi} \frac{\tau_0^2}{\tau_B \tau_S} \mathcal{P} \int_0^{\tilde{\Omega}} d\tilde{\omega}_k \tilde{\omega}_k^2 \left(\frac{1}{\tilde{\omega} - \tilde{\omega}_k} + \frac{1}{\tilde{\omega} + \tilde{\omega}_k} \right) \quad (2.64)$$

$$= \frac{\tau_0^2}{\tau_B \tau_S} \frac{\tilde{\omega}}{\pi} \left(\tilde{\omega} \operatorname{atanh} \left(\frac{\tilde{\omega}}{\tilde{\Omega}} \right) - \tilde{\Omega} \right) \quad (2.65)$$

$$\approx -\frac{\tau_0^2}{\tau_B \tau_S} \frac{\tilde{\Omega}}{\pi} \tilde{\omega}. \quad (2.66)$$

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

$$\tilde{S}(\tilde{\omega}) \approx \frac{1}{2\pi} \left(\frac{\tau_0}{\tau_S} \right)^2 \mathcal{P} \int_0^{\tilde{\Omega}} d\tilde{\omega}_k \frac{\tilde{\omega}_k^2}{\tilde{\omega} - \tilde{\omega}_k} \quad (2.67)$$

$$= -\frac{1}{2\pi} \left(\frac{\tau_0}{\tau_S} \right)^2 \left(\frac{\tilde{\Omega}^2}{2} + \tilde{\Omega} \tilde{\omega} - \tilde{\omega}^2 \log \left(\frac{\tilde{\omega}}{\tilde{\Omega} - \tilde{\omega}} \right) \right) \quad (2.68)$$

$$\approx -\frac{1}{2\pi} \left(\frac{\tau_0}{\tau_S} \right)^2 \left(\frac{\tilde{\Omega}^2}{2} + \tilde{\Omega} \tilde{\omega} \right). \quad (2.69)$$

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

We may verify that the reservoir correlation functions do decay over a time scale that is much less than the relaxation time τ_R .⁷ Recall that the rate $\gamma(\omega)$ is given by the Fourier transform of the reservoir correlation functions $\langle B_i^\mu(t)^\dagger B_j^\nu(t-s) \rangle$, which are constant in t and the same for all sites and polarizations. The correlation functions are then the inverse Fourier transform of γ :

$$\frac{1}{\hbar^2} \langle B_i^\mu(t)^\dagger B_j^\nu(t-s) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega e^{-i\omega s} \gamma(\omega). \quad (2.70)$$

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

$$\frac{1}{\hbar^2 \tau_S^2} \langle B_i^\mu(\tilde{s})^\dagger B_j^\nu(0) \rangle = \frac{1}{2\pi} \int_{-\infty}^{\infty} d\tilde{\omega} e^{-i\tilde{\omega} \tilde{s}} \tilde{\gamma}(\tilde{\omega}) \quad (2.71)$$

$$= \left(\frac{\tau_0}{\tau_S} \right)^2 \frac{\pi^3}{\eta^4} \sinh \left(\frac{\pi \tilde{s}}{\eta} \right)^{-4} \left(1 + 2 \cosh \left(\frac{\pi \tilde{s}}{\eta} \right)^2 \right). \quad (2.72)$$

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

$$\frac{1}{\hbar^2 \tau_S^2} \langle B_i^\mu(\tilde{s})^\dagger B_j^\nu(0) \rangle = \left(\frac{\tau_0}{\tau_S} \right)^2 \frac{3}{\pi \tilde{s}^4}, \quad (2.73)$$

⁷Analogous results for the electric field are given in [18, p. 574].

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

$$\frac{1}{\hbar^2 \tau_S^2} \langle B_i^\mu(\tilde{s})^\dagger B_j^\nu(0) \rangle = \left(\frac{\tau_0}{\tau_S} \right)^2 \frac{8\pi^3}{\eta^4} e^{-2\pi\tilde{s}/\eta} \quad (2.74)$$

$$= \left(\frac{\tau_0^2}{\tau_B \tau_S} \right) \frac{8\pi^3}{\eta^3} e^{-2\pi\tilde{s}/\eta}. \quad (2.75)$$

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

CHAPTER 3

COMPUTING JUMP OPERATORS

Here we go.¹

3.1 INTERPOLATING HAMILTONIANS

```
function  $\eta$ energyvariance(H,  $\eta$ )  
    Es = eigvals(H)  
    Es .-= minimum(Es) # Shift energies for numerics  
    Z = sum(exp(- $\eta$ *E) for E in Es)  
    Ps = [exp(- $\eta$ *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 .

```
trnorm(A) =  $\sqrt{\text{tr}(A' * A)}$   
trnormalize(A) = A / trnorm(A)
```

¹A spaghetti diagram [24].

Spaghetti Diagrams



```

 $\angle(A, B) = \text{acos}(\text{trnorm}(\text{trnormalize}(A)' * \text{trnormalize}(B)))$ 
function slerp(A, B, g)
     $\theta = \angle(A, B)$ 
     $(\sin((1-g)*\theta)*A + \sin(g*\theta)*B) / \sin(\theta)$ 
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,  $\eta$ ) = find_zero(A  $\rightarrow$   $\eta$ energyvariance(H0(0.5),  $\eta$ ) -  $\eta$ energyvariance(A*H0(g),  $\eta$ ),
     $\hookrightarrow$  1.0)
function Hinterp(H1, H2,  $\eta=1.0$ )
    H0(g) = normslerp(trnormalize(H1), trnormalize(H2), g)
#     g  $\rightarrow$  Ainvar(g, H0,  $\eta$ ) * H0(g)
    H0
end;

```

The Ising interaction and transverse-field Hamiltonians are

```

Hx(n) = -sum(siteop( $\sigma_x$ , i, n) * siteop( $\sigma_x$ , i+1, n) for i in 1:n)
Hz(n) = -sum(siteop( $\sigma_z$ , i, n) for i in 1:n);

Hp = Hinterp(Hx(4), Hz(4));

 $\eta_0 = 1.5e1$ 
H0(g) = normslerp(trnormalize(Hx(4)), trnormalize(Hz(4)), g)
Hinvar = Hinterp(Hx(4), Hz(4),  $\eta_0$ )
plot(g  $\rightarrow$   $\eta$ energyvariance(H0(g),  $\eta_0$ ), xlim=(0.0, 1.0))

```

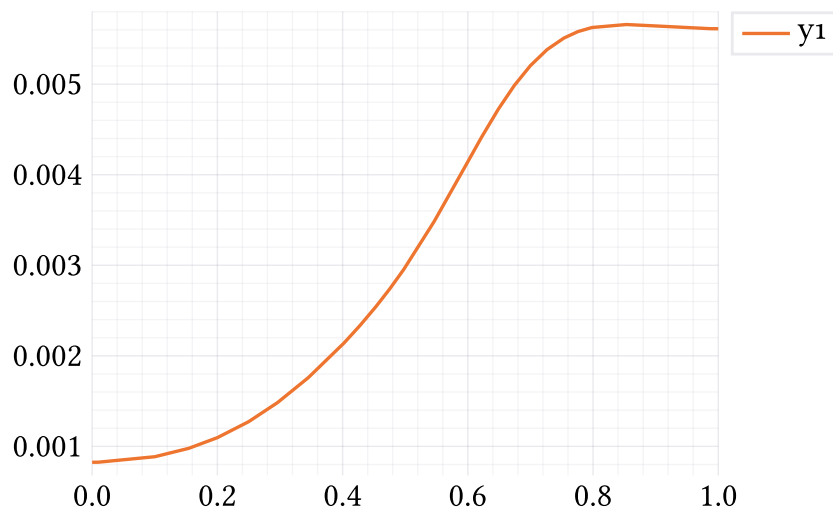


Figure 3.1

```

plot(g  $\rightarrow$  Ainvar(g, H0, 1.8e-1), xlim=(0.0, 1.0))

```

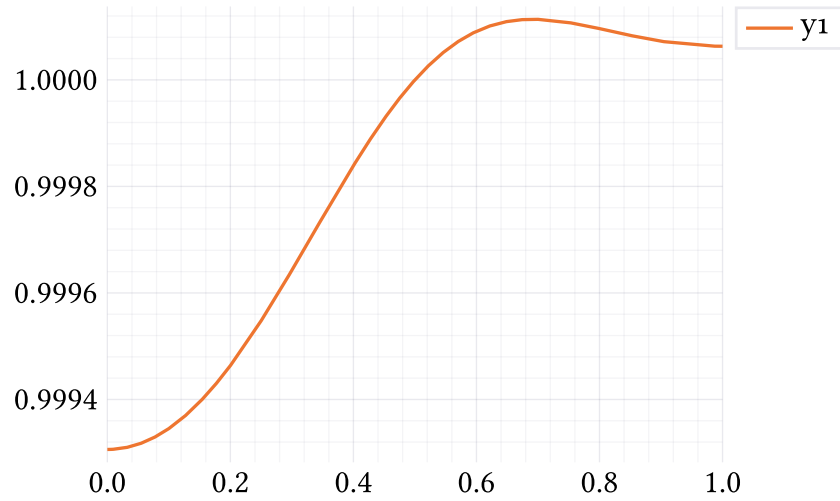


Figure 3.2

```

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")

```

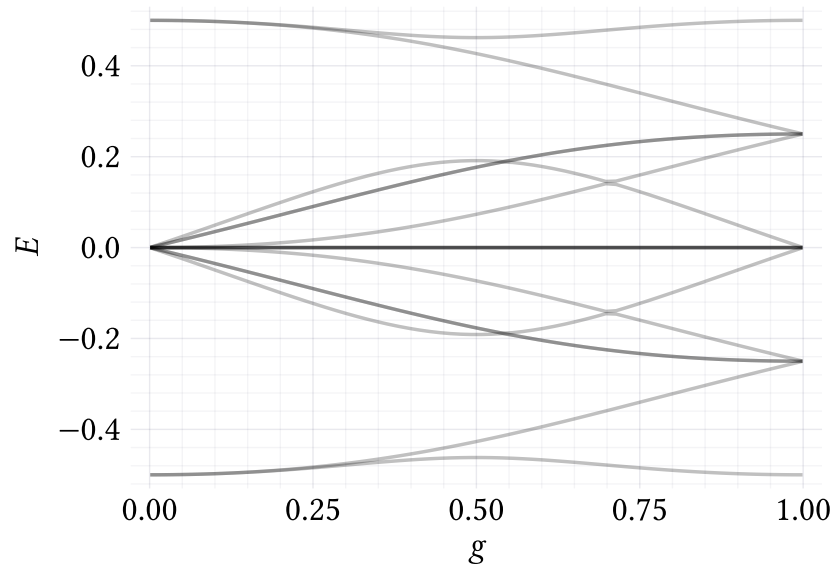


Figure 3.3

3.2 COMPUTATION OF JUMP OPERATORS

```

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

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

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

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

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

isequalto(atol=1e-9) = (x, y) → isapprox(x, y, atol=atol)
function jumps(vals, vecs, As; combine=true, isequal=isequalto())
    eigdict = dictby(zip(vals, vecs))
    ws = dictby(((E2 - E1, (E1, E2)) for E1 in keys(eigdict), E2 in keys(eigdict))),

```



```

    isequal=isequal)
  Πs = projectors(eigendict)
  Jws = dictmap(ws) do ΔEs
    filter(x → !isequal(x, zero(x)),
      [sum(Πs[E1]*A*Πs[E2] for (E1, E2) in ΔEs) for A in As])
  end
  combine ? dictmap(combinejumps, Jws) : Jws
end

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

```

3.3 NUMERICAL SOLUTION OF THE LINDBLAD EQUATION

```

g = 0.5
n = 5
b = SpinBasis(1//2)
sys = ⊗(repeat([b], n)...)
Hint = Hinterp(Hx(n), Hz(n))
Hsys = Hint(g)
Jws = dipolejumps(Hsys)
η = 1e1
α = 1e0 # Large α means that Lamb shift dominates. For relaxation illustration only.
Ω = 1e1
up = spinup(b)
ψ0 = ⊗(repeat([up], n)...)
ρ0 = projector(ψ0)
op = dense(embed(sys, 1, sigmaz(b)));

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

function fout(t, ρ)
  ρ = normalize(ρ)
  real(expect(op, ρ))
end

Hspin = DenseOperator(sys, Hsys)
Hopen = DenseOperator(sys, Hsys + lambham)
opth = fout(0.0, thermalstate(Hspin, 1e0))

```

```

tf = 2*n^2 / (α * γ(1.0, η))
ts = range(0.0, tf, length=501);

# _, 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"Solution for $N = %n$, $g = %g$, $\eta = %\eta$, $\alpha = %\alpha$, $\Omega = %\Omega$",
    ↪ "%Q$",
    xlabel=L"Time ($t / \tau_S$)",
    ylabel=L"$\langle \sigma_z \rangle$",
)
# plot!(ts, [fouts0 fouts1 fouts foutsd], label=["Closed" L"Closed (with $\ham_{LS}$)"
    ↪ "Open" "Dissipator"])
plot!(ts, [fouts foutsd], label=[L"$\dot{\rho} = \mathcal{L}\rho$" L"$\dot{\rho} = \mathcal{D}\rho$"])

```

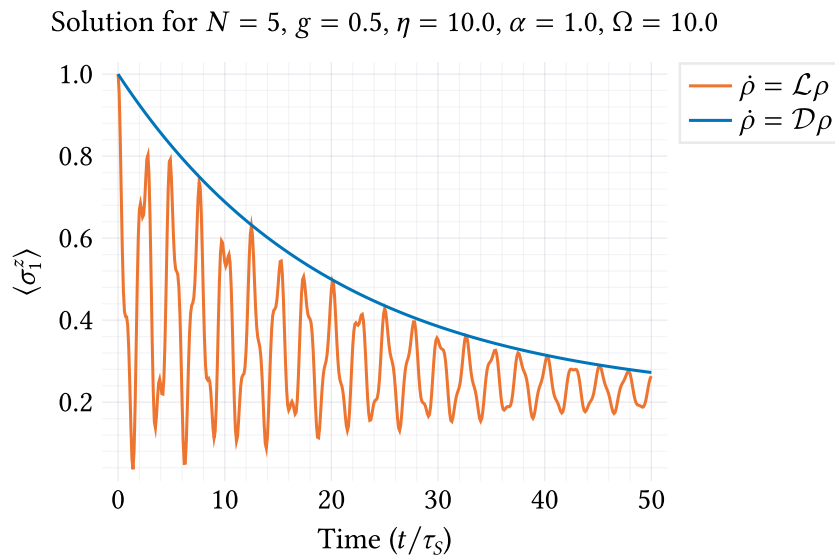


Figure 3.4

```
savefig("time-evolution-$(n).pdf")
```

```

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

```

```

2-element Vector{Float64}:
 0.7561465114487986
-0.06263476313864966

```

```

plot(ts, foutsd, label=L"$\dot{\rho} = \mathcal{D}\rho$",
    title="Exponential fit over short and medium times",

```

```

xlabel=L"Time ($t / \tau_S$)",
ylabel=L"\ev{\pauli_1^z}"
plot!(ts, decay_exponential(ts, coef(fit)), label=L"Fit: $Ae^{-s t} + \rightarrow \ev{\pauli_1^z}_{\text{eq}}$")

```

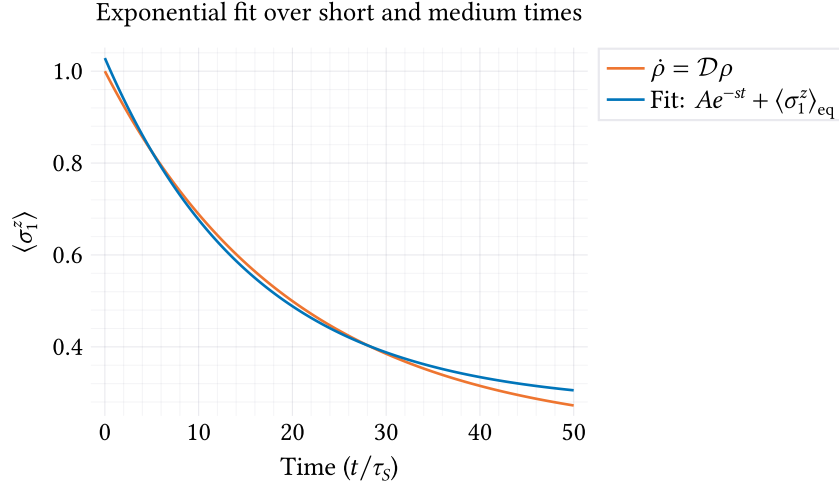


Figure 3.5

```

savefig("exponential-fit-$(n).pdf")

```

3.4 OBTAINING RELAXATION FROM SPAGHETTI (DIAGRAMS)

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

```

@. decay_exponential(x, p) = p[1]*exp(x*p[2])
function effective_rate(Lrates, Lops, ρ0, op, η)
    cs = hcat([vec(V.data) for V in Lops]...) \ vec(ρ0.data)
    V0s = [tr(op * V) for V in Lops]
    tf = 2 * op_to_spindim(ρ0)^2 / γ(1.0, η)
    ts = range(0, tf, length=501)
    ys = real(sum(@. c * V0 * exp(real(s)*ts) for (s, c, V0) in zip(Lrates, cs, V0s)))
    p0 = [1.0, -1.0 / η]
    yf = real(cs[1] * V0s[1])
    fit = curve_fit(decay_exponential, ts, ys .- yf, p0)
    fit.converged || error("Could not fit an effective exponential.")
    coef(fit)[2], stderror(fit)[2]
end

```

```

γ(ω, η) = (1e-1 < η*ω ? ω^3 * (1 + 1 / (exp(η*ω) - 1)) : ω^2 / η)

```

```

function  $\mathcal{D}$ _rates(H, n = op_to_spindim(H);  $\eta=1.0$ ,  $\rho_0$ , op)
    Jws = dipolejumps(H)
    sys =  $\rho_0$ .basis_r
    jumpops, rates = [], Float64[]
    for ( $\omega$ , Js) in Jws
        for J in Js
            push!(rates,  $\gamma(\omega, \eta)$ )
            push!(jumpops, DenseOperator(sys, J))
        end
    end
    # Just the dissipator suffices.
    L = steadystate.liouvillian(DenseOperator(sys), jumpops; rates=rates)
    Lrates, Lops = steadystate.liouvillianspectrum(L; nev=4^n)
    effrate = effective_rate(Lrates, Lops,  $\rho_0$ , op,  $\eta$ )
    sort(real(Lrates)), effrate...
end;

function plot_ $\mathcal{D}$ _rates(Hint;
    points=16,  $\eta=1.0$ ,  $\rho_0$ , op, onplot=false,
    spectrum=true, extremes=true, effective=true,
    kwargs...)
    g0s = range(1e-3, 1-1e-3, length=points)
    outs = map(g  $\rightarrow$   $\mathcal{D}$ _rates(Hint(g);  $\eta$ ,  $\rho_0$ , op), g0s)
    rates = [o[1] for o in outs]
    r0 = [o[2] for o in outs]
     $\sigma$ r0 = [o[3] for o in outs]

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

        if extremes
            rates0 =  $\mathcal{D}$ _rates(Hint(0);  $\eta$ ,  $\rho_0$ , op)[1]
            rates1 =  $\mathcal{D}$ _rates(Hint(1);  $\eta$ ,  $\rho_0$ , op)[1]
            scatter!(p, repeat([g0s[1] - 2e-2], length(rates0)), -rates0,
                marker=(:rtriangle, 2, rubric), markerstrokecolor=rubric, label=false)
            scatter!(p, repeat([g0s[end] + 2e-2], length(rates1)), -rates1,
                marker=(:ltriangle, 2, rubric), markerstrokecolor=rubric, label=false)
        end
    end
    if effective
        plot!(p, g0s, -r0, ribbon= $\sigma$ r0, label=L"%$(round(log10( $\eta$ ), digits=1))",
            color = (onplot == false) ? rubric : :auto)
    end
    p
end;

```

```
plot_D_rates(Hint; η, ρ0, op)
```

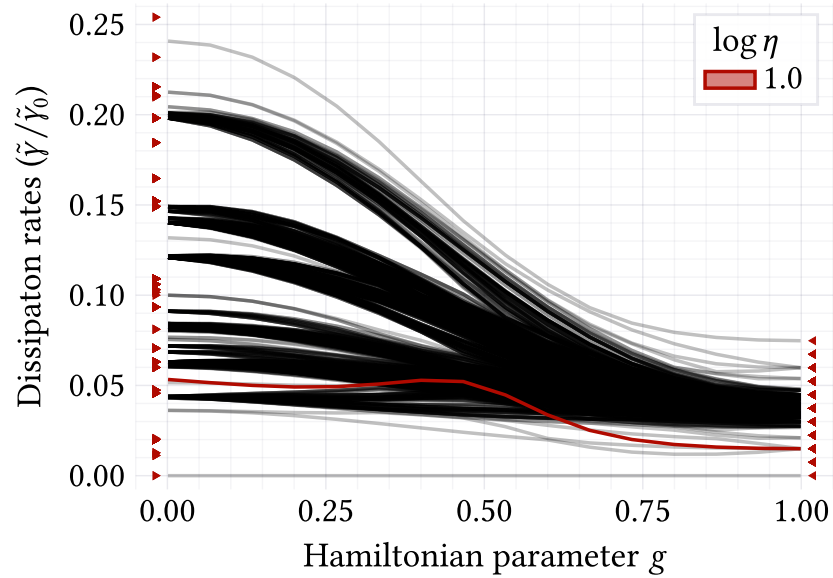


Figure 3.6

```
savefig("spin-spectrum-$(n).pdf")
```

```
plot([reduce((p, η) →
    plot_D_rates(Hint; η, ρ0, op, spectrum=false, onplot=p),
    10.^range(ln, ln + 1, length=4);
    init = plot(size=2.*(400, 300 * 3//2),
        xlabel=L"Hamiltonian parameter $g$",
        ylabel=L"Decay rates for $\text{pauli\_1}^z$ ($\tilde{\gamma} / \tilde{\gamma}_0$)",
        legend=:topright,
        legendtitle=L"\log\eta"))
    for ln in -2:3]...,
    layout=(3,2))
```

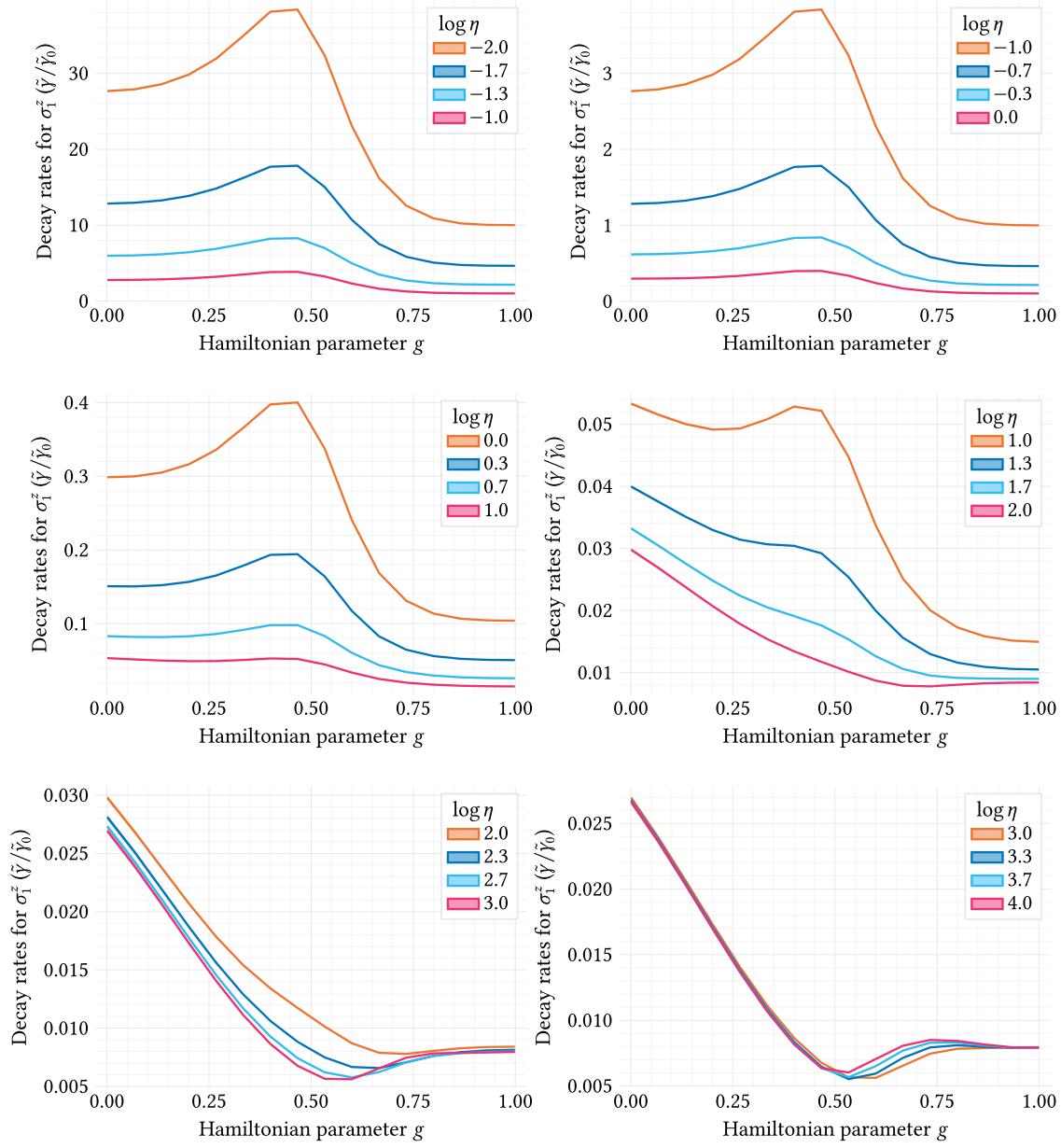


Figure 3.7: Single-spin relaxation rates in different temperature regimes.

```
savefig("spin-relaxations-$(n).pdf")
```

CONCLUSION

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

APPENDIX A

THE GENERATOR OF A QUANTUM DYNAMICAL SEMIGROUP

The contents of this appendix follow [18].

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

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

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

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

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

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

$$\dot{\rho} = \mathcal{L}\rho. \quad (\text{A.3})$$

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

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

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

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

where

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

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

$$a_{mn} \equiv \lim_{t \rightarrow 0^+} \frac{c_{mn}(t) - d\delta_{d^2} d^2}{t} \quad (\text{A.7})$$

and introduce the sum of Kraus operators

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

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

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

$$\dot{\rho} = \lim_{\Delta t \rightarrow 0^+} \frac{\mathcal{V}(\Delta t)\rho - \rho}{\Delta t} \quad (\text{A.10})$$

$$\begin{aligned} &= \lim_{\Delta t \rightarrow 0^+} \left(\frac{c_{d^2 d^2} - d}{d\Delta t} \rho + \sum_{m,n=1}^{d^2-1} \frac{c_{mn}(\Delta t)}{\Delta t} F_m \rho F_n^\dagger \right. \\ &\quad \left. + \frac{1}{\sqrt{d}} \sum_{n=1}^{d^2-1} \left(\frac{c_{nd^2}(\Delta t)}{\Delta t} F_n \rho + \frac{c_{d^2 n}(\Delta t)}{\Delta t} \rho F_n^\dagger \right) \right) \end{aligned} \quad (\text{A.11})$$

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

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

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

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

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

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

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

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

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

which is the diagonal form of the Lindblad equation.

It has been proven that that this is the most general generator for a quantum dynamical semigroup when the system is finite-dimensional [25] and when the system is infinite-dimensional but \mathcal{L} is bounded [26]. This is not much help, since the Hamiltonians for even simple infinite-dimensional systems like the harmonic oscillator are unbounded. Regardless, most examples where \mathcal{L} is unbounded may still be cast into Lindblad form with little or no modification.

APPENDIX B

THE TRANSVERSE-FIELD ISING MODEL

We would like to solve the Hamiltonian

$$H = -J \sum_{i \in \mathbb{Z}_N} (S_i^x S_{i+1}^x + g S_i^z) \quad (\text{B.1})$$

which we nondimensionalize as

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

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

$$\sigma_i^\pm = \frac{\sigma_i^x \pm i \sigma_i^y}{2} \quad (\text{B.3})$$

satisfy

$$\sigma_i^z = 2\sigma_i^+ \sigma_i^- - 1 \quad (\text{B.4})$$

and have commutators

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

$$= \frac{1}{4} ([\sigma_i^x, \sigma_j^x] + [\sigma_i^y, \sigma_j^y] + i [\sigma_i^y, \sigma_j^x] - i [\sigma_i^x, \sigma_j^y]) \quad (\text{B.6})$$

$$= \delta_{ij} \sigma_i^z. \quad (\text{B.7})$$

Thus their anticommutators are

$$\{\sigma_i^+, \sigma_j^-\} = 2\sigma_i^+ \sigma_j^- - [\sigma_i^+, \sigma_j^-] \quad (\text{B.8})$$

$$= 2\sigma_i^+ \sigma_j^- - \delta_{ij} \sigma_i^z \quad (\text{B.9})$$

$$= \delta_{ij} 1 + 2\sigma_i^+ \sigma_j^- (1 - \delta_{ij}). \quad (\text{B.10})$$

It could be helpful to think of the σ_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 $\mathbf{n} = (n_i)_{i \in \mathbb{Z}_N}$, we have the corresponding states

$$|\mathbf{n}\rangle = \prod_{i \in \mathbb{Z}_N} (c_i^\dagger)^{n_i} |\mathbf{0}\rangle, \quad (\text{B.11})$$

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

$$c_i |\mathbf{n}\rangle = -n_i (-1)^{n_{<i}} |\mathbf{n}_{i \leftarrow 0}\rangle \quad (\text{B.12})$$

$$c_i^\dagger |\mathbf{n}\rangle = -(1 - n_i) (-1)^{n_{<i}} |\mathbf{n}_{i \leftarrow 1}\rangle, \quad (\text{B.13})$$

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

Thus the number operator is

$$c_i^\dagger c_i |\mathbf{n}\rangle = (1 - 0) (-1)^{n_{<i}} n_i (-1)^{n_{<i}} |\mathbf{n}_{i \leftarrow 1}\rangle \quad (\text{B.14})$$

$$= n_i |\mathbf{n}\rangle. \quad (\text{B.15})$$

This leads us to consider

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

acting on the states

$$|\mathbf{n}\rangle = \prod_{i \in \mathbb{Z}_N} (\sigma_i^+)^{n_i} |\mathbf{0}\rangle, \quad (\text{B.17})$$

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

$$\sigma_i^+ \sigma_i^- = c_i^\dagger c_i \quad (\text{B.18})$$

$$\sigma_i^z = 2c_i^\dagger c_i - 1 \quad (\text{B.19})$$

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

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

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

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

$$= (c_i^\dagger + c_i) (1 - 2c_i^\dagger c_i) (c_{i+1}^\dagger + c_{i+1}) \quad (\text{B.23})$$

$$= (c_i^\dagger - c_i) (c_{i+1}^\dagger + c_{i+1}), \quad (\text{B.24})$$

and for $i = N - 1$,

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

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

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

We now Fourier transform with

$$c_i = \frac{1}{\sqrt{N}} \sum_k e^{iki} C_k \quad (\text{B.27a})$$

$$C_k = \frac{1}{\sqrt{N}} \sum_i e^{-iki} c_i \quad (\text{B.27b})$$

and

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-iki} C_k^\dagger \quad (\text{B.27c})$$

$$C_k^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{iki} c_i^\dagger. \quad (\text{B.27d})$$

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

$$c_0 = \frac{1}{\sqrt{N}} \sum_k C_k \quad (\text{B.28})$$

$$c_N = \frac{1}{\sqrt{N}} \sum_k e^{ikN} C_k. \quad (\text{B.29})$$

We then must require that

$$kN \equiv 0 \pmod{2\pi} \quad (\text{B.30})$$

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

For N odd, what is C_π ?

$$C_\pi = \frac{1}{\sqrt{N}} \sum_i e^{-i\pi i} c_i. \quad (\text{B.32})$$

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

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

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

$$C_k^\dagger = \sum_i U_{ik} c_i^\dagger. \quad (\text{B.33})$$

Then

$$\{C_k, C_{k'}^\dagger\} = \sum_{ij} U_{ik}^* U_{jk'} \{c_i, c_j^\dagger\} \quad (\text{B.34})$$

$$= \sum_i U_{ik}^* U_{ik'} \quad (\text{B.35})$$

$$= (U^\dagger U)_{kk'} \quad (\text{B.36})$$

$$= \delta_{kk'}, \quad (\text{B.37})$$

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

For the Fourier transform,

$$F_{ik} = \frac{1}{\sqrt{N}} e^{iki}. \quad (\text{B.38})$$

We may then confirm that

$$(F^\dagger F)_{kk'} = \sum_i \frac{1}{N} e^{i(k' - k)i} \quad (\text{B.39})$$

$$= \delta_{kk'}. \quad (\text{B.40})$$

Thus the Fourier transform is unitary. \square

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

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

and also

$$C_{-k} = C_k^* \quad (\text{B.42})$$

$$= \frac{1}{\sqrt{N}} \sum_i e^{-i(-k)i} c_i \quad (\text{B.43})$$

$$= \frac{1}{N} \sum_{ik'} e^{i(k'+k)i} C_{k'}, \quad (\text{B.44})$$

we have that

$$\sum_i c_i^\dagger c_i = \frac{1}{N} \sum_{ikk'} e^{i(k'-k)i} C_k^\dagger C_{k'} \quad (\text{B.45})$$

$$= \sum_k C_k^\dagger C_k, \quad (\text{B.46})$$

$$\sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) = \frac{1}{N} \sum_{ikk'} e^{i(k'-k)i} (e^{ik'} + e^{-ik}) C_k^\dagger C_{k'}, \quad (\text{B.47})$$

$$= \sum_k 2 \cos k C_k^\dagger C_k, \quad (\text{B.48})$$

$$\sum_i (c_{i+1} c_i + c_i^\dagger c_{i+1}^\dagger) = \frac{1}{N} \sum_{ikk'} (e^{i(k'+k)i} e^{ik} C_k C_{k'} + e^{-i(k'+k)i} e^{-ik'} C_k^\dagger C_{k'}^\dagger) \quad (\text{B.49})$$

$$= \sum_k (e^{-ik} C_{-k} C_k + e^{ik} C_k^\dagger C_{-k}^\dagger). \quad (\text{B.50})$$

Thus eq. (B.26) is now

$$H = - \sum_k 2 \cos k C_k^\dagger C_k + \sum_k (e^{-ik} C_{-k} C_k + e^{ik} C_k^\dagger C_{-k}^\dagger) - \sum_k 2g C_k^\dagger C_k + gN1 \quad (\text{B.51})$$

$$= - \sum_k (g + \cos k) (C_k^\dagger C_k + C_{-k}^\dagger C_{-k}) + \sum_k i \sin k (C_{-k} C_k - C_k^\dagger C_{-k}^\dagger) + gN1 \quad (\text{B.52})$$

$$= - \sum_k (g + \cos k) (C_k^\dagger C_k - C_{-k} C_{-k}^\dagger) + \sum_k i \sin k (C_{-k} C_k - C_k^\dagger C_{-k}^\dagger) \quad (\text{B.53})$$

$$= \sum_k \mathbf{v}_k^\dagger \mathbf{H}_k \mathbf{v}_k, \quad (\text{B.54})$$

where

$$\mathbf{H}_k = \begin{bmatrix} -(g + \cos k) & -i \sin k \\ i \sin k & g + \cos k \end{bmatrix}, \quad (\text{B.55})$$

$$\mathbf{v}_k = \begin{bmatrix} C_k \\ C_{-k}^\dagger \end{bmatrix}, \quad (\text{B.56})$$

and we have used that

$$\sum_k \cos k = 0. \quad (\text{B.57})$$

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

$$E_k^\pm = \pm \sqrt{-\det \mathbf{H}_k} \quad (\text{B.63})$$

$$= \pm \sqrt{g^2 + 2g \cos k + \cos^2 k + \sin^2 k} \quad (\text{B.64})$$

$$= \pm \sqrt{g^2 + 2g \cos k + 1}. \quad (\text{B.65})$$

The eigenvectors are then

$$\mathbf{q}_k^\pm = \begin{bmatrix} -i \sin k \\ E_k^\pm + g + \cos k \end{bmatrix}, \quad (\text{B.66})$$

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

$$\mathbf{q}_k^- = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \mathbf{q}_k^+ = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \quad (\text{B.67})$$

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

$$C_k = u f_k + v g_k^\dagger \quad (\text{B.58a})$$

and

$$C_{-k} = -v f_k^\dagger + u g_k. \quad (\text{B.58b})$$

For these transformations to preserve the CARs,

$$\{C_k^\dagger, C_k\} = |u|^2 \{f_k^\dagger, f_k\} + |v|^2 \{g_k, g_k^\dagger\} + u^* v \{f_k^\dagger, g_k^\dagger\} + v^* u \{g_k, f_k\} \quad (\text{B.59})$$

$$= (|u|^2 + |v|^2) 1, \quad (\text{B.60})$$

so we must have

$$|u|^2 + |v|^2 = 1. \quad (\text{B.61})$$

We may choose

$$u = e^{i\phi_1} \cos \theta \quad (\text{B.62a})$$

$$v = e^{i\phi_2} \sin \theta \quad (\text{B.62b})$$

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

$$\|\mathbf{q}_k^\pm\|^2 = (E_k^\pm + g + \cos k)^2 + \sin^2 k \quad (\text{B.68})$$

$$= (E_k^\pm)^2 + g^2 + \cos^2 k + 2g \cos k + 2E_k^\pm(g + \cos k) + 1 - \cos^2 k \quad (\text{B.69})$$

$$= 2E_k^\pm(E_k^\pm + g + \cos k). \quad (\text{B.70})$$

Now

$$\frac{(\mathbf{q}_k^\pm)_1}{\|\mathbf{q}_k^\pm\|} = \frac{-i \sin k}{\sqrt{2E_k^\pm(E_k^\pm + g + \cos k)}} \quad (\text{B.71})$$

$$= \frac{-i \sin k}{\sqrt{2|E_k^\pm|(|E_k^\pm| \pm (g + \cos k))}} \quad (\text{B.72})$$

and

$$\frac{(\mathbf{q}_k^\pm)_2}{\|\mathbf{q}_k^\pm\|} = \pm \sqrt{\frac{E_k^\pm + (g + \cos k)}{2E_k^\pm}} \quad (\text{B.73})$$

$$= \pm \sqrt{\frac{|E_k^\pm| \pm (g + \cos k)}{2|E_k^\pm|}} \quad (\text{B.74})$$

$$\mathbf{U}_k^\dagger = \begin{bmatrix} (\hat{\mathbf{q}}_k^-)^\dagger \\ (\hat{\mathbf{q}}_k^+)^\dagger \end{bmatrix}. \quad (\text{B.75})$$

Then with $E_k = |E_k^\pm|$,

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

so that

$$\{(\eta_k^\pm)^\dagger, \eta_k^\pm\} = \frac{\sin^2 k}{2E_k(E_k \pm (g + \cos k))} 1 + \frac{E_k \pm (g + \cos k)}{2E_k} 1 \quad (\text{B.77})$$

$$= 1 \quad (\text{B.78})$$

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

$$(\text{B.80})$$

Note that eq. (B.76) is consistent with the edge cases in the limits $k \rightarrow -\pi$ and $k \rightarrow 0$. If also $g = 1$, then we impose that $\eta_{-\pi} = C_\pi^\dagger$, which is the same as if $g \neq 1$.

Equation (B.54) becomes

$$H = \sum_k E_k^+ (\eta_k^+)^\dagger \eta_k^+ + \sum_k E_k^- (\eta_k^-)^\dagger \eta_k^-. \quad (\text{B.81})$$

Since

$$(\eta_{-k}^-)^\dagger = \eta_k^+ =: \eta_k \quad (\text{B.82})$$

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

$$H = \sum_k E_k \eta_k^\dagger \eta_k - \sum_k E_k (1 - \eta_k^\dagger \eta_k) \quad (\text{B.83})$$

$$= \sum_k 2E_k \eta_k^\dagger \eta_k - 1 \sum_k E_k. \quad (\text{B.84})$$

APPENDIX C

COMPUTER DETAILS

C.1 JULIA VERSION INFORMATION

```
versioninfo()
```

```
Julia Version 1.6.0
```

```
Commit f9720dc2eb (2021-03-24 12:55 UTC)
```

```
Platform Info:
```

```
  OS: Linux (x86_64-pc-linux-gnu)
```

```
  CPU: Intel(R) Core(TM) i7-4710MQ CPU @ 2.50GHz
```

```
  WORD_SIZE: 64
```

```
  LIBM: libopenlibm
```

```
  LLVM: libLLVM-11.0.1 (ORCJIT, haswell)
```

```
Environment:
```

```
  JULIA_PROJECT = .
```

```
  JULIA_NUM_THREADS = 8
```

```
using Pkg
```

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

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

```
Pkg.status()
```

```

    Status `~/drive/thesis/notebooks/Project.toml`
[537997a7] AbstractPlotting v0.15.27
[7d9fca2a] Arpack v0.4.0
[6e4b80f9] BenchmarkTools v0.7.0
[ad839575] Blink v0.12.5
[13f3f980] CairoMakie v0.3.19
[5ae59095] Colors v0.12.7
[150eb455] CoordinateTransformations v0.6.1
[e9467ef8] GLMakie v0.1.30
[7073ff75] IJulia v1.23.2
[d1acc4aa] IntervalArithmetic v0.17.8
[c8e1da08] IterTools v1.3.0
[5ab0869b] KernelDensity v0.6.2
[b964fa9f] LaTeXStrings v1.2.1
[2fda8390] LsqFit v0.12.0
[ee78f7c6] Makie v0.12.0
[eff96d63] Measurements v2.5.0
[3b7a836e] PGFPlots v3.3.6
[ccf2f8ad] PlotThemes v2.0.1
[58dd65bb] Plotly v0.3.0
[91a5bcd] Plots v1.11.2
[92933f4c] ProgressMeter v1.5.0
[438e738f] PyCall v1.92.3
[6e0679c1] QuantumOptics v0.8.2
[4f57444f] QuantumOpticsBase v0.2.7
[189a3867] Reexport v0.2.0
[f3b207a7] StatsPlots v0.14.19
[24249f21] SymPy v1.0.42
[ac1d9e8a] ThreadsX v0.1.7
[1986cc42] Unitful v1.7.0
[276b4fcb] WGLMakie v0.3.4
[0f1e0344] WebIO v0.8.15
[37e2e46d] LinearAlgebra

```

```

using LinearAlgebra
BLAS.vendor()

```

```
:openblas64
```

C.2 NOTEBOOK PREAMBLE

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

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

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

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

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

⊗k(a, b) = kron(b, a);
```

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


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