

TOY SYSTEMS AND QUANTUM MASTER EQUATIONS

(PROVISIONAL TITLE)

DRAFT



A THESIS

PRESENTED TO

THE DIVISION OF MATHEMATICS AND NATURAL SCIENCES

REED COLLEGE



IN PARTIAL FULFILLMENT

OF THE REQUIREMENTS FOR THE DEGREE

BACHELOR OF ARTS



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NOVEMBER 20, 2020

APPROVED FOR THE DIVISION
(PHYSICS)

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Acknowledgements

I want to thank a few people.

Abstract

The preface pretty much says it all.

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Introduction

Introductory content.

Chapter 1

Closed systems

HOW DO THE SPINS interact with their environment? What do they even mean?
Argue quantization of electromagnetic field.

Dirac: [1, p. 246]

A Cartesian co-ordinate or momentum will in general have all characteristic values from $-\infty$ to ∞ , while an action variable has only a discrete set of characteristic values.

To motivate density operators and POVMs, try starting from [2]?

Chapter 2

Density operator theory

IF QUANTUM MECHANICS is so weird, then why aren't we? The answer lies in the phenomenon of **decoherence**, which was first considered in depth in the 1970's by Zeh [3]. Despite being a late comer to the history of quantum mechanics, the theory of decoherence is crucial to understanding how classical results are obtained from many interacting quantum systems. While there are other routes to decoherence, the most common is through interaction with a memoryless (Markovian) environment [4]. This leads to the theory of quantum Markovian master equations, which describe transformations of a system in the presence of such an environment. The most general form of these transformations was first extended to quantum mechanics by Gorini, Kosakowski, Lindblad, and Sudarshan to give the **GKLS** or **Lindblad equation** [5, 6].

This chapter will explain the relevant theoretical background in sections 2.1 and 2.2, before presenting the general theory which leads to the Lindblad equation in section 2.3, following the text of Breuer and Petruccione [7] and to a lesser extent [8] (which has some flaws). This leads us to consider the weak-coupling limit in section 2.4 and an application to atomic physics in section 2.6. Issues with the method are discussed briefly in section 2.7.

2.1 Different perspectives on density operators

For a statistical perspective on quantum mechanics, we will make two postulates. The mathematical background is the **Liouville space** $\mathcal{L}(\mathcal{H})$ for the Hilbert space \mathcal{H} .

Definition 1 (Liouville space). The space $\mathcal{L}(\mathcal{H})$ is the complex Hilbert space of operators A on \mathcal{H} for which the norm induced by the inner product $\langle A|B \rangle \equiv \text{tr}(A^\dagger B)$ is finite.

Postulate 1. A quantum system may be understood as a statistical ensemble ρ with observables O which are both described by elements of $\mathcal{L}(\mathcal{H})$, where the ensemble average of O is $\langle O \rangle_\rho \equiv \langle O|\rho \rangle$ and O is Hermitian.

The usual properties of the **density operator** ρ follow from considering various averages. The only way for $\langle \alpha I \rangle_\rho = \alpha$ for all physical constants $\alpha \in \mathbb{C}$ is if $\text{tr } \rho = 1$. For $\langle O \rangle_\rho$ to be real, ρ must be *self-adjoint*, and if O is also positive, then ρ must be *positive* for $\langle O \rangle_\rho$ to be positive [9].

Postulate 2. The density operator for an isolated system with Hamiltonian H evolves unitarily in time according to the **Liouville-von Neumann equation**

$$\dot{\rho} = [H, \rho]/i\hbar. \quad (2.1)$$

While we usually consider the density operator to change in time, the time dependence may be shifted onto the observables. Consider a quantum system with unitary time-evolution operator $U(t)$, so that we may express the density operator for the system as $\rho(t) = U(t)\rho U^\dagger(t)$, where $\rho = \rho(0)$. If we compute the ensemble average of an observable $O(t)$ and cycle the trace, we find

$$\langle O(t) \rangle_{\rho(t)} = \text{tr}(O(t)U(t)\rho U^\dagger(t)) \quad (2.2)$$

$$= \text{tr}(U^\dagger(t)O(t)U(t)\rho) \equiv \langle O_H(t) \rangle_\rho \quad (2.3)$$

where O_H is the observable in the **Heisenberg picture**, as opposed to the **Schrödinger picture**, where the operators are time-independent. If we can split the Hamiltonian into the form $H = H_0 + H_I(t)$, then $U(t)$ splits into the product of $U_0(t) = e^{H_0 t/i\hbar}$ and $U_I(t) = U_0^\dagger(t)U(t)$. Cycling over only $U_I(t)$ in eq. (2.2)[°] gives the **interaction picture** operators

$$O_I(t) = U_0^\dagger(t)O(t)U_0(t) \quad (2.4a)$$

$$\rho_I(t) = U_I(t)\rho U_I^\dagger(t). \quad (2.4b)$$

Without $H_I(t)$, eq. (2.4)[°] reduces to the Schrödinger picture, and without H_0 , eq. (2.4)[°] reduces to the Heisenberg picture. The time-dependence of the interaction picture density operator from differentiating eq. (2.4b)[°] is (suppressing time dependences)

$$\begin{aligned} i\hbar \dot{\rho}_I(t) &= i\hbar \frac{d}{dt} (U_0^\dagger \rho(t) U_0) \\ &= -U_0^\dagger H_0^\dagger \rho(t) U_0 + U_0^\dagger \rho(t) H_0 U_0 \\ &\quad + U_0^\dagger [H_0, \rho(t)] U_0 + U_0^\dagger [H_I, \rho(t)] U_0 \\ &= U_0^\dagger [U_0 H_I' U_0^\dagger, \rho(t)] U_0 \\ &= [H_I', \rho_I(t)], \end{aligned} \quad (2.5)$$

where H_I' denotes the interaction Hamiltonian $H_I(t)$ in the interaction picture. This is just eq. (2.1)[°] with the interaction Hamiltonian.

With this understanding of the behavior of isolated systems, it may be surprising that postulates 1 and 2[°] are actually insufficient to describe common systems. For example,

the allowed energies for the harmonic oscillator are unbounded, so the Hamiltonian is not an element of the Liouville space. We will see later how this issue is related to the dynamics of a composite quantum system in section 2.7,^{*} but will now move on to considering the more general dynamics of interacting quantum systems.

2.2 Composite quantum systems

Clean up inner product notation.

Consider two quantum systems described by Hilbert spaces \mathcal{H}_A and \mathcal{H}_B . We should be able to view both systems as parts of a composite quantum system described by some Hilbert space \mathcal{H} . For the moment, we will only consider the Hilbert spaces as vector spaces. Mathematically, we have a map $\phi : \mathcal{H}_A \times \mathcal{H}_B \rightarrow \mathcal{H}$. The simplest choice would be $\mathcal{H} = \mathcal{H}_A \times \mathcal{H}_B$, but this does not make physical sense. For the assignment of composite states to be consistent, if a linear combination is taken in \mathcal{H}_A then joined with \mathcal{H}_B , the result must be the same as first joining and then taking the linear combination. If $|a_1\rangle, |a_2\rangle \in \mathcal{H}_A$, $|b\rangle \in \mathcal{H}_B$, and $\alpha, \beta \in \mathbb{C}$, then

$$\phi(\alpha |a_1\rangle + \beta |a_2\rangle, |b\rangle) = \alpha \phi(|a_1\rangle, |b\rangle) + \beta \phi(|a_2\rangle, |b\rangle), \quad (2.6)$$

so that ϕ is bilinear.

Taking $\mathcal{H} = \mathcal{H}_A \times \mathcal{H}_B$ by doing operations elementwise is known as the **direct sum** $\mathcal{H}_A \oplus \mathcal{H}_B$. Applying $\phi' : \mathcal{H}_A \times \mathcal{H}_B \rightarrow \mathcal{H}_A \oplus \mathcal{H}_B$ gives

$$\alpha \phi'(|a_1\rangle, |b\rangle) + \beta \phi'(|a_2\rangle, |b\rangle) = \alpha(|a_1\rangle, |b\rangle) + \beta(|a_2\rangle, |b\rangle) \quad (2.7)$$

$$= (\alpha |a_1\rangle + \beta |a_2\rangle, 2 |b\rangle) \quad (2.8)$$

$$\neq (\alpha |a_1\rangle + \beta |a_2\rangle, |b\rangle) \quad (2.9)$$

$$= \phi'(\alpha |a_1\rangle + \beta |a_2\rangle, |b\rangle), \quad (2.10)$$

since $|b\rangle$ is normalized in \mathcal{H}_B . Thus the direct sum is not a physically consistent construction of a composite system.

Instead, we may define the composite system and corresponding map so that they satisfy eq. (2.6).^{*} We consider the combination of two states first as a symbol, giving the set of symbols

$$B = \{\tilde{\phi}(|a\rangle, |b\rangle) : |a\rangle \in \mathcal{H}_A, |b\rangle \in \mathcal{H}_B\}. \quad (2.11)$$

The formal complex linear combinations of elements of B form a vector space, known as the **free vector space** $F(\mathcal{H}_A \times \mathcal{H}_B)$. The composite system is then the quotient vector space $\mathcal{H} = F(\mathcal{H}_A \times \mathcal{H}_B) / \sim$, where \sim is an equivalence relation that identifies linear combinations like in eq. (2.6).^{*} These equivalence classes are known as **tensors**. We write the class $\phi(|a\rangle, |b\rangle) = [\tilde{\phi}(|a\rangle, |b\rangle)]$ as $|a\rangle \otimes |b\rangle$, which is often abbreviated to $|a\rangle |b\rangle$ or $|a, b\rangle$.

To make \mathcal{H} a Hilbert space, we may complete it with a suitable inner product. Consider the special case when the states are normalized and $\langle a_1 | a_2 \rangle = 0$. We have another consistency criterion: the composite state should also be normalized. We find

$$1 = \langle (\alpha |a_1\rangle + \beta |a_1\rangle) \otimes |b\rangle | (\alpha |a_1\rangle + \beta |a_1\rangle) \otimes |b\rangle \rangle \quad (2.12)$$

$$= |\alpha|^2 \langle |a_1\rangle \otimes |b\rangle | |a_1\rangle \otimes |b\rangle \rangle + |\beta|^2 \langle |a_2\rangle \otimes |b\rangle | |a_2\rangle \otimes |b\rangle \rangle \quad (2.13)$$

$$+ \alpha\beta^* \langle |a_1\rangle \otimes |b\rangle | |a_2\rangle \otimes |b\rangle \rangle + \alpha^*\beta \langle |a_2\rangle \otimes |b\rangle | |a_1\rangle \otimes |b\rangle \rangle \quad (2.14)$$

$$= |\alpha|^2 + |\beta|^2 + \alpha\beta^* \langle |a_1\rangle \otimes |b\rangle | |a_2\rangle \otimes |b\rangle \rangle + \alpha^*\beta \langle |a_2\rangle \otimes |b\rangle | |a_1\rangle \otimes |b\rangle \rangle. \quad (2.15)$$

This requires that

$$\alpha\beta^* \langle |a_1\rangle \otimes |b\rangle | |a_2\rangle \otimes |b\rangle \rangle = -\alpha^*\beta \langle |a_1\rangle \otimes |b\rangle | |a_2\rangle \otimes |b\rangle \rangle^*, \quad (2.16)$$

so if $\alpha, \beta \neq 0$, the inner product $\langle |a_1\rangle \otimes |b\rangle | |a_2\rangle \otimes |b\rangle \rangle$ must be purely imaginary. But since the superposition state is to 1, this establishes that $|a_1\rangle \otimes |b\rangle$ and $|a_2\rangle \otimes |b\rangle$ must be orthonormal. In general, consistency requires that

$$\langle |a_i\rangle \otimes |b_m\rangle | |a_j\rangle \otimes |b_n\rangle \rangle = \delta_{ij}\delta_{mn}. \quad (2.17)$$

Hence consistency has determined the inner product. For arbitrary vectors $|a\rangle = \sum_i c_i |a_i\rangle$, $|\tilde{a}\rangle = \sum_j c'_j |a_j\rangle$, $|b\rangle = \sum_m d_m |b_m\rangle$, and $|\tilde{b}\rangle = \sum_n d'_n |b_n\rangle$,

$$\langle |a\rangle \otimes |b\rangle | |\tilde{a}\rangle \otimes |\tilde{b}\rangle \rangle = \sum_{ijmn} c_i \tilde{c}_j^* d_m \tilde{d}_n^* \langle |a_i\rangle \otimes |b_m\rangle | |a_j\rangle \otimes |b_n\rangle \rangle \quad (2.18)$$

$$= \sum_{ijmn} c_i \tilde{c}_j^* d_m \tilde{d}_n^* \delta_{ij}\delta_{mn} \quad (2.19)$$

$$= \left(\sum_{ij} c_i \tilde{c}_j^* \langle a_i | a_j \rangle \right) \left(\sum_{mn} d_m \tilde{d}_n^* \langle b_m | b_n \rangle \right) \quad (2.20)$$

$$= \langle a | \tilde{a} \rangle \langle b | \tilde{b} \rangle. \quad (2.21)$$

Equation (2.21)^o is then a valid definition for the inner product, with consistency upheld by extending to linear combinations of tensors.

Given an operator A on \mathcal{H}_A , what is the corresponding operator \tilde{A} on \mathcal{H} ? For $\langle a, b | \tilde{A} | a, b \rangle = \langle a | A | a \rangle$, we must have

$$\tilde{A} = A \otimes I, \quad (2.22)$$

where action of the operator $A \otimes B$ on \mathcal{H} is defined by

$$(A \otimes B)(|a\rangle \otimes |b\rangle) = A|a\rangle \otimes B|b\rangle. \quad (2.23)$$

The **adjoint** T^\dagger of $T : \mathcal{H}_A \rightarrow \mathcal{H}_B$ satisfies that

$$\langle T|a\rangle | |b\rangle \rangle = \langle |a\rangle | T^\dagger |b\rangle \rangle \quad \text{for } |a\rangle \in \mathcal{H}_A, |b\rangle \in \mathcal{H}_B. \quad (2.24)$$

Thus for $A \otimes B : \mathcal{H} \rightarrow \mathcal{H}$,

$$\langle (A \otimes B)(|a\rangle \otimes |b\rangle) | c\rangle \otimes |d\rangle \rangle = \langle A|a\rangle \otimes B|b\rangle | c\rangle \otimes |d\rangle \rangle \quad (2.25)$$

$$= \langle A|a\rangle | c\rangle \rangle \langle B|b\rangle | d\rangle \rangle \quad (2.26)$$

$$= \langle |a\rangle | A^\dagger | c\rangle \rangle \langle |b\rangle | B^\dagger | d\rangle \rangle \quad (2.27)$$

$$= \langle |a\rangle \otimes |b\rangle | A^\dagger | c\rangle \otimes B^\dagger | d\rangle \rangle \quad (2.28)$$

$$= \langle |a\rangle \otimes |b\rangle | (A^\dagger \otimes B^\dagger)(|c\rangle \otimes |d\rangle) \rangle. \quad (2.29)$$

Hence

$$(A \otimes B)^\dagger = A^\dagger \otimes B^\dagger. \quad (2.30)$$

Given $|a, b\rangle \in \mathcal{H}$, we will often use an operator on part of \mathcal{H} as if it were an operator on \mathcal{H} . For example, $A|a, b\rangle$ is taken to mean $(A \otimes I)|a, b\rangle$. This can be dangerous: we also write expressions like $(A + B)|a, b\rangle$, which we intend to mean $A|a\rangle \otimes B|b\rangle$, but this conflicts with using AB to do the same thing. Additionally, using the product notation makes $BA = (I \otimes B)(A \otimes I) = AB$ so that the “commutator” $[A, B] = 0$.

How might a density operator ρ for the composite system admit a **reduced density operator** ρ_A for system A ? Consider an observable O of system A , for which the corresponding composite observable is $O \otimes I$. Regardless of the representation (composite or subsystem), the ensemble average of O should be the same:

$$\langle O_A \otimes I \rangle_\rho = \langle O_A \rangle_{\rho_A}. \quad (2.31)$$

To see what ρ_A is, take an orthonormal complete basis $\{A_j\}$ of Hermitian operators for $\mathcal{L}(\mathcal{H}_A)$ and $\{B_k\}$ for $\mathcal{L}(\mathcal{H}_B)$, so the density operator may be expressed as

$$\rho = \sum_{jk} A_j \otimes B_k \langle A_j \otimes B_k | \rho \rangle. \quad (2.32)$$

We may then compute that

$$\rho_A = \sum_i A_i \langle A_i | \rho_A \rangle \quad (2.33)$$

$$= \sum_i A_i \langle A_i \otimes I | \rho \rangle \quad \text{eq. (2.31)}^\circ \quad (2.34)$$

$$= \sum_i A_i \langle A_i \otimes I | \sum_{jk} A_j \otimes B_k \langle A_j \otimes B_k | \rho \rangle \rangle \quad \text{eq. (2.32)}^\circ \quad (2.35)$$

$$= \sum_{ijk} A_i \langle A_i \otimes I | A_j \otimes B_k \rangle \langle A_j \otimes B_k | \rho \rangle \quad (2.36)$$

$$= \sum_{ijk} A_i \langle A_i | A_j \rangle \langle B_k | I \rangle \langle A_j \otimes B_k | \rho \rangle \quad (2.37)$$

$$= \sum_{ijk} A_i \delta_{ij} \text{tr } B_k \langle A_j \otimes B_k | \rho \rangle \quad (2.38)$$

$$= \sum_{jk} A_j \operatorname{tr} B_k \langle A_j \otimes B_k | \rho \rangle. \quad (2.39)$$

Definition 2. At this point, it makes sense to define the **partial trace** by

$$\operatorname{tr}_B (A \otimes B) = A \operatorname{tr} B \quad (2.40)$$

and extending linearly.

With this definition, we continue from eq. (2.39)^o to find that

$$\rho_A = \sum_{jk} \operatorname{tr}_B (A_j \otimes B_k) \langle A_j \otimes B_k | \rho \rangle \quad (2.41)$$

$$= \operatorname{tr}_B \left(\sum_{jk} A_j \otimes B_k \langle A_j \otimes B_k | \rho \rangle \right) \quad (2.42)$$

$$= \operatorname{tr}_B \rho. \quad (2.43)$$

Thus the reduced density matrix for system A is obtained from the full density matrix by taking the partial trace over system B .

However, the reduction of the density operator by “tracing out” B comes at the cost of losing information about the correlation between A and B . Quantitatively, the **relative entropy** between the correlated and uncorrelated density operators is

$$S(\rho \| \rho_A \otimes \rho_B) \quad (2.44)$$

$$\equiv \operatorname{tr} \rho (\ln \rho - \ln(\rho_A \otimes \rho_B)) \quad (2.45)$$

$$= \operatorname{tr}(\rho \ln \rho) - \operatorname{tr}_A \operatorname{tr}_B (\rho \ln(\rho_A \otimes I)) - \operatorname{tr}_B \operatorname{tr}_A (\rho \ln(I \otimes \rho_B)) \quad (2.46)$$

$$= S(\rho_A) + S(\rho_B) - S(\rho). \quad (2.47)$$

Together with the Klein inequality which states that relative entropies are non-negative (theorem 2.9.1^o), we have that

$$S(\rho) \leq S(\rho_A) + S(\rho_B), \quad (2.48)$$

with equality when $\rho = \rho_A \otimes \rho_B$. Other expected properties hold, such as that the relative entropy is invariant under unitary transformations (theorem 2.9.2^o), or that the relative entropy between subsystems is less than that between combined systems (theorem 2.9.3^o).

We would like to know the **reduced dynamics** of the quantum system S when in contact with an **environment** system B . We suppose that the composite system has a Hamiltonian of the form

$$H_{SB}(t) = H_S \otimes I + I \otimes H_B + H_I(t) \quad (2.49)$$

and that the environment is in equilibrium, so the composite density operator is $\rho(t) = \rho_S(t) \otimes \rho_B$. In terms of the unitary time-evolution operator $U(t)$ for the system, eq. (2.1)^o

becomes $\rho(t) = U(t)\rho(0)U^\dagger(t)$. Taking the partial trace over the environment gives the time-evolved system density operator

$$\rho_S(t) = \text{tr}_B \left(U(t)(\rho_S(0) \otimes \rho_B)U^\dagger(t) \right). \quad (2.50)$$

Whatever eq. (2.50)[◦] evaluates to, it will be an example of a **dynamical map** $\mathcal{V}(t)$ that time-evolves the system according to $\rho_S(t) = \mathcal{V}(t)\rho_S(0)$. While $\mathcal{V}(t)$ seems abstract, we know it should output a density operator. Then for $\mathcal{V}(t)$ to be a valid map on system density operators, it should *preserve the trace* of the input density operator. In fact, as a valid map $\mathcal{V}(t) \otimes I$ on the composite system, the composite density operator should remain positive. This property of $\mathcal{V}(t)$ is called **complete positivity**. Thus the valid maps on system density operators are **completely positive and trace-preserving (CPTP)**.

2.3 The Lindblad equation

With the idea of random interactions with an environment in mind, we will assume that the maps $\{\mathcal{V}(t) : t \geq 0\}$ are also *memoryless* or **Markovian**, so that they form a **quantum dynamical semigroup** satisfying

$$\mathcal{V}(t_1)\mathcal{V}(t_2) = \mathcal{V}(t_1 + t_2) \quad \text{for } t_1, t_2 \geq 0. \quad (2.51)$$

The action of the dynamical semigroup on the system describes an irreversible process. As such, the relative entropy between an arbitrary system ensemble $\rho(t)$ and an equilibrium ensemble ρ_0 cannot decrease (by eq. (2.50)[◦] and theorems 2.9.2 and 2.9.3[◦]):

$$S(\mathcal{V}(t)\rho \parallel \mathcal{V}(t)\rho_0) = S\left(\text{tr}_B \left[U(t)(\rho \otimes \rho_B)U^\dagger(t) \right] \parallel \rho_0\right) \quad (2.52)$$

$$\leq S\left(U(t)(\rho \otimes \rho_B)U^\dagger(t) \parallel \rho_0 \otimes \rho_B\right) \quad (2.53)$$

$$= S(\rho \otimes \rho_B \parallel \rho_0 \otimes \rho_B) \quad (2.54)$$

$$= S(\rho \parallel \rho_0). \quad (2.55)$$

We would like to determine the **infinitesimal generator** \mathcal{L} for the quantum dynamical semigroup which allows the dynamical maps to be expressed as $\mathcal{V}(t) = e^{\mathcal{L}t}$, analogously to how a time-independent Hamiltonian is a generator for the unitary time-evolution operator $e^{Ht/i\hbar}$. Following this analogy, the Schrödinger equation is replaced by the **Markovian quantum master equation** $\dot{\rho}_S = \mathcal{L}\rho_S$, which generalizes eq. (2.1)[◦] to typically non-unitary CTP maps of density operators, provided that they are Markovian.

We will find that the most general form of \mathcal{L} is given by the **Lindblad equation** eq. (2.67)[◦]. To obtain this result, first consider diagonalizing ρ_B as $\rho_B = \sum_j \lambda_j |\phi_j\rangle\langle\phi_j|$ with orthonormal vectors $\phi_j \in \mathcal{H}_B$, where $\sum_j \lambda_j = 1$. Then eq. (2.50)[◦] becomes (writing ρ_S as ρ)

$$\rho(t) = \sum_{ij} \langle\phi_i|U(t)(\rho(0) \otimes \lambda_j |\phi_j\rangle\langle\phi_j|)U^\dagger(t)|\phi_i\rangle \quad (2.56)$$

$$= \sum_{ij} \lambda_j \langle \phi_i | U(t) | \phi_j \rangle \rho(0) \langle \phi_j | U^\dagger(t) | \phi_i \rangle \quad (2.57)$$

$$= \sum_{ij} M_{ij}(t) \rho(0) M_{ij}^\dagger(t), \quad (2.58)$$

where $M_{ij}(t) \equiv \sqrt{\lambda_j} \langle \phi_i | U(t) | \phi_j \rangle$. This decomposition in terms of the M_{ij} is an instance of the Choi-Kraus representation theorem (theorem 2.9.4^o). We can express the M_{ij} in terms of an orthonormal complete basis $\{F_n\}$ for $\mathcal{L}(\mathcal{H}_S)$ as $M_{ij} = \sum_k F_k \langle F_k | M_{ij} \rangle$. Then eq. (2.58)^o becomes

$$\rho(t) = \sum_{mn} c_{mn}(t) F_m \rho(0) F_n^\dagger, \quad (2.59)$$

where

$$c_{mn}(t) \equiv \sum_{ij} \langle F_m | M_{ij}(t) \rangle \langle M_{ij}(t) | F_n \rangle. \quad (2.60)$$

For convenience, we may choose $F_d = I/\sqrt{d}$, where $d = \dim(\mathcal{H}_S)$. With an eye towards simplifying eq. (2.64)^o, we eliminate the explicit time dependence of eq. (2.60)^o by defining

$$a_{mn} \equiv \lim_{t \rightarrow 0^+} \frac{c_{mn}(t) - d \delta_{d^2} d^2}{t} \quad (2.61)$$

and introduce the sum of Kraus operators

$$F = \frac{1}{\sqrt{d}} \sum_{n=1}^{d^2-1} a_{nd^2} F_n \quad (2.62)$$

$$= \frac{F + F^\dagger}{2} + i \frac{F - F^\dagger}{2i} \equiv G + H/i\hbar, \quad (2.63)$$

where we have decomposed the sum F into Hermitian and anti-Hermitian parts and included \hbar so that H will have dimensions of energy. Now we may write the master equation $\mathcal{L}\rho = \dot{\rho}$ as

$$\begin{aligned} \dot{\rho} &= \lim_{\Delta t \rightarrow 0^+} \frac{\mathcal{V}(\Delta t)\rho - \rho}{\Delta t} \\ &= \lim_{\Delta t \rightarrow 0^+} \left(\frac{c_{d^2 d^2} - d}{d \Delta t} \rho + \sum_{m,n=1}^{d^2-1} \frac{c_{mn}(\Delta t)}{\Delta t} F_m \rho F_n^\dagger \right. \\ &\quad \left. + \frac{1}{\sqrt{d}} \sum_{n=1}^{d^2-1} \left(\frac{c_{nd^2}(\Delta t)}{\Delta t} F_n \rho + \frac{c_{d^2 n}(\Delta t)}{\Delta t} \rho F_n^\dagger \right) \right) \\ &= \frac{a_{d^2 d^2}}{d} \rho + F \rho + \rho F^\dagger + \sum_{m,n=1}^{d^2-1} a_{mn} F_m \rho F_n^\dagger \end{aligned} \quad (2.64)$$

$$\begin{aligned}
&= \frac{a_{d^2 d^2}}{d} \rho + \{G, \rho\} + \frac{[H, \rho]}{i\hbar} + \sum_{m,n=1}^{d^2-1} a_{mn} F_m \rho F_n^\dagger \\
&= \{G', \rho\} + \frac{[H, \rho]}{i\hbar} + \sum_{m,n=1}^{d^2-1} a_{mn} F_m \rho F_n^\dagger,
\end{aligned} \tag{2.65}$$

where $G' = G + a_{d^2 d^2} I/d$. Since $\mathcal{V}(t)$ is trace-preserving, $\text{tr } \dot{\rho} = 0$. Applying this condition to eq. (2.65)^o and cycling the trace gives

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

so $G' = -\sum_{m,n=1}^{d^2-1} a_{mn} F_n^\dagger F_m / 2$. This allows us to write eq. (2.65)^o as

$$\dot{\rho} = \frac{[H, \rho]}{i\hbar} + \sum_{m,n=1}^{d^2-1} a_{mn} \left(F_m \rho F_n^\dagger - \frac{1}{2} \{F_n^\dagger F_m, \rho\} \right), \tag{2.66}$$

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. (2.60)^o to be Hermitian, and eq. (2.61)^o 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 operators** L_n to find

$$\dot{\rho} = \frac{[H, \rho]}{i\hbar} + \sum_{k=1}^{d^2-1} \gamma_k \left(L_k \rho L_k^\dagger - \frac{1}{2} \{L_k^\dagger L_k, \rho\} \right) \equiv \mathcal{L} \rho, \tag{2.67}$$

which is the *diagonal form* of the Lindblad equation. The eigenvalues γ_k have dimensions of inverse time and the Lindblad operators may be taken to be traceless. The second term is often called the **dissipator** \mathcal{D} (see section 2.4^o), so the Lindbladian may be separated into unitary and non-unitary parts.

2.4 The weak-coupling limit

Now that we have found the general form for a stochastic CTCP generator, we must now determine the conditions for interaction Hamiltonian in eq. (2.49)^o to give rise to Markovian dynamics. While there are several different regimes where this is true, we will consider the **weak-coupling** limit which we justify by supposing that the environment is similar to a **harmonic bath** of many harmonic oscillators.

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

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

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

$$[H_S, A_{\alpha\omega}] = -\omega A_{\alpha\omega}. \quad (2.68)$$

Using eq. (2.68)[◦] to commute past the exponential in eq. (2.4a)[◦] gives $A'_{\alpha\omega} = e^{-i\omega t} A_{\alpha\omega}$ in the interaction picture. Thus the interaction Hamiltonian in the interaction picture is

$$H'_I = \sum_{\alpha\omega} e^{-i\omega t} A_{\alpha\omega} \otimes B'_\alpha, \quad (2.69)$$

where $B'_\alpha(t) = e^{-H_B t/i\hbar} B_\alpha e^{H_B t/i\hbar}$ per eq. (2.4a)[◦].

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

$$\langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle_{\rho_B} \quad (2.70)$$

and their one-sided Fourier transform

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty ds e^{i\omega s} \langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle_{\rho_B} \quad (2.71)$$

$$\equiv iS_{\alpha\beta}(\omega) + \gamma_{\alpha\beta}(\omega)/2, \quad (2.72)$$

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

$$\gamma_{\alpha\beta}(\omega) \equiv \int_{-\infty}^\infty ds e^{i\omega s} \langle B_\alpha^\dagger(t) B_\beta(t-s) \rangle_{\rho_B} \quad (2.73)$$

is positive.

With this setup, we may now move to the main derivation. It is helpful to consider the interaction picture time evolution eq. (2.5)[◦] in the integral form

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

Applying eq. (2.5)[◦] again and tracing out the environment gives the closed equation

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

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

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

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

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

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

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

$$\dot{\rho}_S = - \int_0^\infty ds \operatorname{tr}_B [H_I(t), [H_I(t-s), \rho_S(t) \otimes \rho_B]]. \quad (2.74)$$

This is justified when the reservoir correlation functions in eq. (2.71)[°] vanish quickly over a time τ_B that is smaller than the relaxation time τ_R (see section 2.7[°]). Substituting eq. (2.69)[°] into eq. (2.74)[°] and using eq. (2.71)[°] gives

$$\dot{\rho}_S = 2 \operatorname{He} \sum_{\alpha\beta\omega\omega'} e^{i(\omega' - \omega)t} \Gamma_{\alpha\beta}(\omega) (A_{\beta\omega} \rho_S A_{\alpha\omega'}^\dagger - A_{\alpha\omega'}^\dagger A_{\beta\omega} \rho_S), \quad (2.75)$$

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

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

for system evolution are large compared to the relaxation time τ_R , then the contribution from the fast-oscillating terms of eq. (2.75)[°] 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

$$\dot{\rho}_S = 2 \operatorname{He} \sum_{\alpha\beta\omega} \Gamma_{\alpha\beta}(\omega) (A_{\beta\omega} \rho_S A_{\alpha\omega}^\dagger - A_{\alpha\omega}^\dagger A_{\beta\omega} \rho_S). \quad (2.76)$$

Now applying the decomposition eq. (2.72)[°] gives the interaction picture Lindblad equation

$$\dot{\rho}_S = i[H_{LS}, \rho_S] + \mathcal{D}\rho_S, \quad (2.77)$$

where the **Lamb shift Hamiltonian** is

$$H_{LS} = \sum_{\alpha\beta\omega} S_{\alpha\beta}(\omega) A_{\alpha\omega}^\dagger A_{\beta\omega}, \quad (2.78)$$

and the *dissipator* is

$$\mathcal{D}\rho_S = \sum_{\alpha\beta\omega} \gamma_{\alpha\beta} \left(A_{\beta\omega} \rho_S A_{\alpha\omega}^\dagger - \frac{1}{2} \{ A_{\alpha\omega}^\dagger A_{\beta\omega}, \rho_S \} \right). \quad (2.79)$$

The Lamb shift (or environment renormalization) Hamiltonian commutes with the system Hamiltonian since eq. (2.68)[°] implies that $[H_S, A_{\alpha\omega}^\dagger A_{\beta\omega}] = 0$. Adding the system's Hamiltonian H_S to H_{LS} and diagonalizing gives the Schrödinger picture Lindblad equation eq. (2.67)[°].

2.5 Relaxation to thermal equilibrium

The system will generally relax from its initial configuration to a stationary solution of eq. (2.67)[°] (see section 2.7[°]). We expect that the thermal state

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

would be the equilibrium state. This is true when the reservoir correlation functions obey the KMS condition [I0, II]

$$\left\langle B_\alpha^\dagger(t) B_\beta(0) \right\rangle_{\rho_B} = \left\langle B_\beta(0) B_\alpha^\dagger(t + i\beta) \right\rangle_{\rho_B}, \quad (2.80)$$

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

2.6 A two-level atom

To demonstrate the use of the Lindblad equation, we will study a model for the decay of a two-level atom. Our aim is to glimpse why electrons in atoms undergo optical decay, even though excited states are stable atomic states. Suppose that the atom has Hamiltonian $H_S = \hbar\omega\sigma_3/2$, where $\sigma_3 = |1\rangle\langle 1| - |0\rangle\langle 0|$. The operators $\sigma_- = |0\rangle\langle 1|$ and $\sigma_+ = |1\rangle\langle 0|$ are Lindblad operators, since they are eigenoperators of the superoperator $[H_S, -]$, like in eq. (2.68)[°]. These correspond to lowering and raising the energy by $\hbar\omega$, and will be our analogues of the emission and absorption processes. The derivation of section 2.3[°] is similar for a bath of photons in equilibrium, and our assumptions are justified because typical atomic relaxation times of about 20 ns are much slower than the periods of electromagnetic waves [I2]. Ignoring the Lamb shift (which only offsets) and considering only the effects at ω , eq. (2.77)[°] becomes

$$\begin{aligned} \dot{\rho} = & \gamma_0(N+1) \left(\sigma_- \rho \sigma_+ - \frac{1}{2} \{ \sigma_+ \sigma_-, \rho \} \right) \\ & + \gamma_0 N \left(\sigma_+ \rho \sigma_- - \frac{1}{2} \{ \sigma_- \sigma_+, \rho \} \right) \equiv \mathcal{D}\rho, \end{aligned} \quad (2.81)$$

where $N = 1/(e^{\beta\hbar\omega} - 1)$. This is straightforward to solve given the properties of the Pauli matrices. From the initial density operator $\rho(0) = |1\rangle\langle 1|$, we find that the population of upper level is

$$\rho_{11}(t) = \frac{N}{2N+1} (1 - e^{-\gamma t}), \quad \text{where} \quad \gamma = \gamma_0(2N+1).$$

This is consistent with what we observe in atomic spectra: an exponential decay to an equilibrium level which gives Lorentzian peaks. At low temperatures ($N \rightarrow 0$) the system approaches the ground state in accordance with the third law of thermodynamics, and at high temperatures ($N \gg 1$), the level is half-occupied and the absorption is saturated [I3] (Cf. ¹).

¹It's cool how this provides a fundamental explanation of the *Doppler-free saturated absorption spectroscopy of Rubidium vapor* JLAB experiment that I did.

2.7 Limitations

Though the Lindblad equation is widely applicable, there are some situations in which key assumptions in its derivation break down. For one, we have glossed over the issue of *ergodicity* in considering a harmonic bath. Since we needed to assume a discrete spectrum, the correlation functions eq. (2.70)[°] will be quasi-periodic and will not decay as we required. It is only in the limit of a reservoir with infinitely many degrees of freedom that we expect non-periodic behavior like decay to emerge, but then there may be issues with unbounded operators. This can lead to the interesting behavior of spontaneous symmetry breaking and phase transitions.

There are also many systems with dynamics that occur on time scales comparable to the relaxation time. For example, a paper published less than a month ago (!) demonstrates how fast pulsed laser experiments can probe the relaxation of temporarily polarized gas molecules due to collisions [14, 15].

2.8 Conclusion

We have seen how the general consideration of Markovian CTCP maps on density operators leads to the Lindblad equation, and considered the weak-coupling limit as an example of a physical regime where the assumption of stochastic dynamics is valid. However, we have only scratched the surface of what can be done with the Lindblad equation, especially with respect to solving it. Since the two-level atom is a small system, it is simple to diagonalize, but larger systems provide more difficulty as the dimension of the Hilbert space grows. Numerical solutions are complicated by the additional requirement of trace preservation, but they can still be done in many situations [8, 14]. The theory of open quantum systems gives some fundamental justifications for the assumptions of equilibrium statistical mechanics, as was briefly noted in section 2.5,[°] and has made the picture of decoherence a bit more clear.

2.9 Mathematical details

Definition 3 (Tensor product). Consider vector spaces $V(k)$, $W(k)$, and Z . For any bilinear map $h : V \times W \rightarrow Z$, the **tensor product** $V \otimes W$ and associated bilinear map $\phi : V \times W \rightarrow V \otimes W$ map have the property that there is a unique linear map $g : V \otimes W \rightarrow Z$ such that $h = g \circ \phi$. For tensor products of Hilbert spaces, the inner product is defined on each element of a product and then the space is completed. There is then a natural correspondence between the element $v \otimes f$ of the tensor product $V \otimes V^*$ and the linear map $T : V \rightarrow V$ defined by $Tx = f(x)v$.

This induces an extension of Dirac notation where all pairs $f \otimes x$ of dual and usual vectors from the same space are evaluated as $\langle f|x \rangle = f(x)$ and extended linearly. For example, given a linear operator $U : V \otimes W \rightarrow V \otimes W$ and a basis $|\phi_i\rangle$ for W , the partial

trace over W may be expressed as $\text{tr}_W U = \langle \phi_i | U | \phi_i \rangle$. This forms the justification of the step from eq. (2.56)[◦] to eq. (2.57)[◦] and of the manipulations in theorem 2.9.4.[◦]

Theorem 2.9.1 (Klein inequality). *For density operators ρ and ρ' , $S(\rho \| \rho') \geq 0$, with equality if and only if $\rho = \rho'$.*

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

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

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

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

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

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

which evaluates to

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

Theorem 2.9.2. *For a unitary operator U and density operators ρ and ρ' ,*

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

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

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

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

Theorem 2.9.3. *For density operators ρ and ρ' ,*

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

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

Theorem 2.9.4 (Choi-Kraus representation [8]). *A superoperator \mathcal{S} on a density operator ρ is completely positive and trace-preserving if and only if it may be represented as*

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

2.10 The Born-Markov approximation for the Ising chain in a bath

We consider the Hamiltonian (in natural units)

$$H = \left(-J \sum_i \sigma_{zi} \sigma_{z(i+1)} - h \sum_i \sigma_{xi} \right) + \sum_{ik} \omega_{ik} a_{ik}^\dagger a_{ik} + \sum_{ik} C_k (a_{ik}^\dagger + a_{ik}) \sigma_{zi} \quad (2.82)$$

$$\equiv H_S \otimes I + I \otimes H_B + H_I. \quad (2.83)$$

The Schrodinger picture operators of the interaction Hamiltonian

$$H_I = \sum_i A_i \otimes B_i \quad (2.84)$$

are

$$A_i = \sigma_{zi} \quad (2.85)$$

$$B_i = \sum_k C_k (a_{ik}^\dagger + a_{ik}) \equiv \sum_k B_{ik}. \quad (2.86)$$

In the interaction picture,

$$A_i(t) = \sigma_{zi} \quad (2.87)$$

and

$$B_{ik}(t) = C_k (e^{i\omega_{ik}t} a_{ik}^\dagger + e^{-i\omega_{ik}t} a_{ik}). \quad (2.88)$$

Proof. Consider an observable A which satisfies

$$[H, A] = \omega A \quad (2.89)$$

for a Hamiltonian H . Such an **eigenoperator** of H has

$$H^n A = H^{n-1} A H + H^{n-1} [H, A] \quad (2.90)$$

$$= H^{n-1} A (H + \omega I) \quad (2.91)$$

$$= A (H + \omega I)^n. \quad (2.92)$$

Then

$$e^H A = \sum_{n \geq 0} \frac{H^n A}{n!} \quad (2.93)$$

$$= A \sum_{n \geq 0} \frac{(H + \omega I)^n}{n!} \quad (2.94)$$

$$= A e^{H + \omega I} \quad (2.95)$$

$$= A e^\omega e^H, \quad \text{BCH} \quad (2.96)$$

so the interaction picture operator is

$$A(t) = e^{iHt} A e^{-iHt} \quad (2.97)$$

$$= e^{i\omega t} A e^{iHt} e^{-iHt} \quad (2.98)$$

$$= e^{i\omega t} A. \quad (2.99)$$

In our case, $H = H_B$ and we have the eigenoperators

$$[H_B, a_{jl}] = \sum_{ik} [a_{ik}^\dagger a_{ik}, a_{jl}] \quad \text{definition of } H_B \quad (2.100)$$

$$= - \sum_{ik} \delta_{ij} \delta_{kl} a_{jl} \quad \text{commutation relations} \quad (2.101)$$

$$= -a_{jl}, \quad (2.102)$$

which follows from the commutation relations

$$[a^\dagger a, a] = a^\dagger a a - a a^\dagger a \quad (2.103)$$

$$= a^\dagger a a - a^\dagger a a - a[a, a^\dagger] \quad (2.104)$$

$$= -a \quad (2.105)$$

and

$$[a^\dagger a, a^\dagger] = a^\dagger a a^\dagger - a^\dagger a^\dagger a \quad (2.106)$$

$$= a^\dagger a a^\dagger - a^\dagger a a^\dagger - a^\dagger[a, a^\dagger] \quad (2.107)$$

$$= a^\dagger.$$

□

For the Born-Markov approximation to hold, we must verify that

1. $\text{tr}_B [H_I(t), \rho_0] = 0$, or also that $0 = \langle B_{ik}(t) \rangle_{\rho_B^{(I)}(t)} = \langle B_{ik} \rangle_{\rho_B^{(S)}(t)}$.
2. $\rho(t) \approx \rho_S(t) \otimes \rho_B$ (see [7, p. 131]).
3. The reservoir correlation functions $\langle B_{ik}^\dagger(t) B_{jl}(t-s) \rangle_{\rho_B^{(I)}(t)}$ decay quickly over a time τ_B much less than the relaxation time τ_R .

Condition 1 is satisfied if the bath is in a thermal state, which we will also assume at $t = 0$ for condition 2. The validity of 2 rests on 3: we do not require that the bath is truly stationary, but only that it is approximately so on the coarser timescale of system evolution.

In the thermal state

$$\rho_{\text{th}} = \frac{e^{-\beta H_B}}{\text{tr } e^{-\beta H_B}}, \quad (2.108)$$

the reservoir correlation functions are

$$\langle B_{ik}^\dagger(t) B_{jl}(t-s) \rangle = \langle B_{ik}^\dagger(s) B_{jl}(0) \rangle \quad (2.109)$$

$$= \delta_{ij} \delta_{kl} C_k C_l \left(e^{-i\omega_{ik}s} (n_B(\omega_{ik}) + 1) + e^{i\omega_{ik}s} n_B(\omega_{ik}) \right). \quad (2.110)$$

Proof. We have that [7, p. 144]

$$\langle a_{ik} a_{jl} \rangle = 0 \quad (2.111)$$

$$\langle a_{ik}^\dagger a_{jl}^\dagger \rangle = 0 \quad (2.112)$$

$$\langle a_{ik}^\dagger a_{jl} \rangle = \delta_{ij} \delta_{kl} n_B(\omega_{ik}) \quad (2.113)$$

$$\langle a_{ik} a_{jl}^\dagger \rangle = \delta_{ij} \delta_{kl} (n_B(\omega_{ik}) + 1), \quad (2.114)$$

where

$$n_B(\omega) = \frac{1}{e^{\beta\omega} - 1} \quad (2.115)$$

is the **Planck distribution**. We may then compute that

$$\langle B_{ik}^\dagger(t) B_{jl}(t-s) \rangle \quad (2.116)$$

$$= C_k C_l \langle (e^{-i\omega_{ik}t} a_{ik} + e^{i\omega_{ik}t} a_{ik}^\dagger) (e^{i\omega_{jl}(t-s)} a_{jl}^\dagger + e^{-i\omega_{jl}(t-s)} a_{jl}) \rangle \quad (2.117)$$

$$= C_k C_l \left(e^{-i\omega_{ik}t + i\omega_{jl}(t-s)} \langle a_{ik} a_{jl}^\dagger \rangle + e^{-i\omega_{ik}t - i\omega_{jl}(t-s)} \langle a_{ik} a_{jl} \rangle \right. \quad (2.118)$$

$$\left. + e^{i\omega_{ik}t + i\omega_{jl}(t-s)} \langle a_{ik}^\dagger a_{jl}^\dagger \rangle + e^{i\omega_{ik}t - i\omega_{jl}(t-s)} \langle a_{ik}^\dagger a_{jl} \rangle \right). \quad (2.119)$$

$$= \delta_{ij} \delta_{kl} C_k C_l (e^{-i\omega_{ik}s} (n_B(\omega_{ik}) + 1) + e^{i\omega_{ik}s} n_B(\omega_{ik})). \quad \square$$

Thus the **spectral correlation tensor** is

$$\Gamma_{ij}(\omega) \equiv \sum_{kl} \int_0^\infty ds e^{i\omega s} \langle B_{ik}^\dagger(t) B_{jl}(t-s) \rangle_{\rho_B} \quad (2.120)$$

$$= \delta_{ij} \sum_k \int_0^\infty ds C_k^2 (e^{i(\omega - \omega_{ik})s} (n_B(\omega_{ik}) + 1) + e^{i(\omega + \omega_{ik})s} n_B(\omega_{ik})) \quad (2.121)$$

$$= \delta_{ij} \sum_k C_k^2 \left(\pi \delta(\omega_{ik} - \omega) - i \mathcal{P} \frac{1}{\omega_{ik} - \omega} \right) (n_B(\omega_{ik}) + 1) \quad (2.122)$$

$$+ \left(\pi \delta(-\omega_{ik} - \omega) + i \mathcal{P} \frac{1}{\omega_{ik} + \omega} \right) n_B(\omega_{ik}) \quad (2.123)$$

$$\equiv \delta_{ij} \left(\frac{\gamma(\omega)}{2} + i S(\omega) \right), \quad (2.124)$$

where we have used that

$$\int_0^\infty ds e^{-i\omega s} = \pi \delta(\omega) - i \mathcal{P} \frac{1}{\omega}, \quad (2.125)$$

and \mathcal{P} denotes the Cauchy principal value. We now take the continuum limit of a large 1D cavity (with $\omega = ck$)²

$$\sum_k \mapsto \frac{L}{\pi} \int_0^\infty dk = \frac{L}{\pi c} \int_0^\infty d\omega \quad (2.126)$$

²We are assuming that there is only one mode per frequency per site in 1D, rather than that there may be many modes for a given frequency, as usual in 3D.

so that we have³

$$\gamma(\omega) = \frac{2L}{c} C(\omega)^2 (n_B(\omega) + 1) \quad (2.127)$$

and

$$S(\omega) = \mathcal{P} \int_0^\infty d\omega_k \frac{L}{c} C(\omega_k)^2 \left(\frac{n_B(\omega_{ik}) + 1}{\omega - \omega_{ik}} + \frac{n_B(\omega_{ik})}{\omega + \omega_{ik}} \right). \quad (2.128)$$

Since the only eigenvalue of H_S is $\omega = 0$, we must require that

$$\gamma(0) = \lim_{\omega \rightarrow 0} \frac{2L}{c} C(\omega)^2 (n_B(\omega) + 1) \quad (2.129)$$

is finite. There are two relevant cases.

If $C(\omega)$ initially grows faster than $\sqrt{\omega}$, then $\gamma(0) = 0$ and the jump operators vanish, leaving just the Lamb shift. We then evaluate

$$S(0) = \mathcal{P} \int_0^\infty d\omega_k \frac{L}{c} C(\omega_k)^2 \left(\frac{n_B(\omega_{ik}) + 1}{-\omega_{ik}} + \frac{n_B(\omega_{ik})}{\omega_{ik}} \right) \quad (2.130)$$

$$= -\frac{L}{c} \mathcal{P} \int_0^\infty d\omega_k \frac{C(\omega_k)^2}{\omega_k} \quad \text{let } \omega_{ik} := \omega_k \quad (2.131)$$

In this case, the exact form of $C(\omega_k)$ does not matter much. So long as it also goes to zero, $S(0)$ will take some constant negative value.

If instead, $C(\omega) \propto \sqrt{\omega}$, then $\gamma(0)$ is finite. A common choice makes the **spectral density**

$$J(\omega) \equiv \frac{2\alpha}{\pi} \int_0^\infty d\omega_k C(\omega_k)^2 \delta(\omega - \omega_k) \quad (2.132)$$

$$= \frac{2\alpha}{\pi} C(\omega)^2 \quad (2.133)$$

be

$$J(\omega) = \frac{2\alpha}{\pi} \frac{\omega}{1 + (\omega/\Omega)^2}. \quad (2.134)$$

This is known as the **Ohmic spectral density** with cutoff frequency Ω , which gives rise to frequency-independent damping with a rate proportional to α [7, p. 175]. Then

$$S(0) = -\frac{2\alpha}{\pi} \mathcal{P} \int_0^\infty \frac{d\omega_k}{1 + (\omega_k/\Omega)^2} \quad (2.135)$$

$$= -\frac{\Omega}{\alpha}. \quad (2.136)$$

Thus the Lamb shift Hamiltonian

$$H_{LS} = \sum_{ij} \delta_{ij} S(0) \sigma_{zi} \sigma_{zj} = -\frac{N\Omega}{\alpha} I$$

³Note that the Planck distribution satisfies $n_B(\omega) + 1 = -n_B(-\omega)$.

only shifts the energy of the chain. With an Ohmic bath, we find

$$\gamma(0) = \lim_{\omega \rightarrow 0} \frac{4\alpha L}{\pi c} \frac{\omega}{1 + (\omega/\Omega)^2} (n_B(\omega) + 1) \quad (2.I37)$$

$$= \frac{2L}{c} \frac{1}{\beta}, \quad (2.I38)$$

so the dissipator is

$$\mathcal{D}\rho_S = \frac{4L}{\pi c} \frac{\alpha}{\beta} \sum_i (\sigma_{zi} \rho_S \sigma_{zi} - \rho_S). \quad (2.I39)$$

Thus neglecting the Lamb shift and $4L/\pi c$, we have that the system density matrix in the interaction picture obeys

$$\dot{\rho}_S(t) = \frac{\alpha}{\beta} \sum_i (\sigma_{zi} \rho_S(t) \sigma_{zi} - \rho_S(t)) \quad (2.I40)$$

$$= \frac{\alpha}{\beta} \sum_i [\sigma_{zi}, \rho_S(t)] \sigma_{zi}. \quad (2.I41)$$

The reduced density matrix entries for each site are then determined by the equations

$$\dot{\rho}_{00} = 0 \quad (2.I42)$$

$$\dot{\rho}_{11} = 0 \quad (2.I43)$$

$$\dot{\rho}_{01} = -\frac{2\alpha}{\beta} \rho_{01} \quad (2.I44)$$

$$\dot{\rho}_{01} = -\frac{2\alpha}{\beta} \rho_{10}. \quad (2.I45)$$

Proof. If $A|a\rangle = a|a\rangle$, then

$$A \angle |a\rangle\langle b| = (a - b) |a\rangle\langle b|,$$

where the superoperator $A \angle$ is defined by $A \angle B \equiv [A, B]$. □

2.11 Solving eigenoperator problems in coordinates

Given a complete basis A_i for $\mathcal{L}(\mathcal{H}_A)$ and the Hamiltonian

$$H = \sum_i h_i A_i, \quad (2.I46)$$

we want to find eigenoperators

$$A = \sum_j a_j A_j, \quad (2.I47)$$

of $H\angle$. If

$$[A_i, A_j] = \sum_k s_{ijk} A_k \quad (2.148)$$

$$s_{ijk} = \langle [A_i, A_j] | A_k \rangle, \quad (2.149)$$

then the eigenvalue equation is

$$[H, A] = \omega A \quad (2.150)$$

$$\sum_{ijk} h_i a_j s_{ijk} A_k = \sum_j \omega a_j A_j \quad (2.151)$$

$$\sum_{jk} S_{jk} a_j A_k = \sum_j \omega a_j A_j, \quad (2.152)$$

where the matrix S has coefficients

$$S_{jk} = \sum_i h_i s_{ijk} = \langle A_j | H\angle | A_k \rangle. \quad (2.153)$$

Thus eigenoperators may be found by solving the ordinary eigenvalue problem

$$S^T \mathbf{a} = \omega \mathbf{a}. \quad (2.154)$$

2.12 Eigenoperators for the transverse Ising Hamiltonian

Pfeuty algebra time.

Chapter 3

The Ising model as an open quantum system

3.1 Solution of the transverse Ising model

We consider the Hamiltonian

$$H = -J \sum_{i \in \mathbb{Z}_N} S_i^x S_{i+1}^x - \Gamma \sum_{i \in \mathbb{Z}_N} S_i^z, \quad (3.1)$$

which we nondimensionalize as

$$\frac{4}{J}H = - \sum_{i \in \mathbb{Z}_N} \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i \in \mathbb{Z}_N} \sigma_i^z \quad (3.2)$$

Note that H does not have $4/J$ below. Fix this and change λ (Striff) to $-\alpha$.

for the periodic transverse Ising chain with N spins. We notice that the operators

$$\sigma_i^\pm = \frac{\sigma_i^x \pm i\sigma_i^y}{2} \quad (3.3)$$

satisfy

$$\sigma_i^z = 2\sigma_i^+ \sigma_i^- - I \quad (3.4)$$

and have commutators

$$[\sigma_i^+, \sigma_j^-] = \frac{1}{4} [\sigma_i^x + i\sigma_i^y, \sigma_j^x - i\sigma_j^y] \quad (3.5)$$

$$= \frac{1}{4} ([\sigma_i^x, \sigma_j^x] + [\sigma_i^y, \sigma_j^y] + i[\sigma_i^y, \sigma_j^x] - i[\sigma_i^x, \sigma_j^y]) \quad (3.6)$$

$$= \delta_{ij} \sigma_i^z. \quad (3.7)$$

Thus their anticommutators are

$$\{\sigma_i^+, \sigma_j^-\} = 2\sigma_i^+ \sigma_j^- - [\sigma_i^+, \sigma_j^-] \quad (3.8)$$

$$= 2\sigma_i^+ \sigma_j^- - \delta_{ij} \sigma_i^z \quad (3.9)$$

$$= \delta_{ij} I + 2\sigma_i^+ \sigma_j^- (1 - \delta_{ij}). \quad (3.10)$$

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

$$|\mathbf{n}\rangle = \prod_{i \in \mathbb{Z}_N} (c_i^\dagger)^{n_i} |0\rangle, \quad (3.11)$$

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

$$c_i |\mathbf{n}\rangle = -n_i (-1)^{n_{<i}} |\mathbf{n}_{i \leftarrow 0}\rangle \quad (3.12)$$

$$c_i^\dagger |\mathbf{n}\rangle = -(1 - n_i) (-1)^{n_{<i}} |\mathbf{n}_{i \leftarrow 1}\rangle, \quad (3.13)$$

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

$$c_i^\dagger c_i |\mathbf{n}\rangle = (1 - 0) (-1)^{n_{<i}} n_i (-1)^{n_{<i}} |\mathbf{n}_{i \leftarrow 1}\rangle \quad (3.14)$$

$$= n_i |\mathbf{n}\rangle. \quad (3.15)$$

This leads us to consider

$$c_i = - \left(\prod_{j < i} -\sigma_j^z \right) \sigma_j^- \quad (3.16)$$

acting on the states

$$|\mathbf{n}\rangle = \prod_{i \in \mathbb{Z}_N} (\sigma_i^+)^{n_i} |0\rangle, \quad (3.17)$$

Fix my sign errors.

where $|0\rangle = |\uparrow\rangle^{\otimes N}$ is the state with all z -spins up, or all zero qubits. This gives the same result as eq. (3.12), 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

$$\sigma_i^+ \sigma_i^- = c_i^\dagger c_i \quad (3.18)$$

$$\sigma_i^z = 2c_i^\dagger c_i - I \quad (3.19)$$

$$\sigma_i^x = -\left(\prod_{j<i} (I - 2c_j^\dagger c_j)\right)(c_i^\dagger + c_i) \quad (3.20)$$

$$\sigma_i^y = i\left(\prod_{j<i} (I - 2c_j^\dagger c_j)\right)(c_i^\dagger - c_i). \quad (3.21)$$

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

$$\sigma_i^x \sigma_{i+1}^x = \left(\prod_{j<i} (2c_j^\dagger c_j - I)\right)(c_i^\dagger + c_i) \left(\prod_{j<i+1} (2c_j^\dagger c_j - I)\right)(c_{i+1}^\dagger + c_{i+1}) \quad (3.22)$$

$$= (c_i^\dagger + c_i)(I - 2c_i^\dagger c_i)(c_{i+1}^\dagger + c_{i+1}) \quad (3.23)$$

$$= (c_i^\dagger - c_i)(c_{i+1}^\dagger + c_{i+1}), \quad (3.24)$$

and for $i = N - 1$,

$$\sigma_{N-1}^x \sigma_0^x = \left(\prod_{j<N-1} (2c_j^\dagger c_j - I)\right)(c_{N-1}^\dagger + c_{N-1})(c_0^\dagger + c_0). \quad (3.25)$$

We may now perform the Jordan-Wigner transformation of eq. (3.2)^{*} to obtain

Check boundary term to Pfeuty (2.4). Why can it be neglected for large N ?

$$H = \sum_i (c_i - c_i^\dagger)(c_{i+1}^\dagger + c_{i+1}) + \lambda \sum_i 2c_i^\dagger c_i - \lambda N I \quad (3.26)$$

$$- \left(I - \prod_{j<N-1} (2c_j^\dagger c_j - I)\right)(c_{N-1} - c_{N-1}^\dagger)(c_0^\dagger + c_0) \quad (3.27)$$

We now Fourier transform with

$$c_i = \frac{1}{\sqrt{N}} \sum_k e^{iki} C_k \quad (3.28a)$$

$$C_k = \frac{1}{\sqrt{N}} \sum_i e^{-iki} c_i \quad (3.28b)$$

and

$$c_i^\dagger = \frac{1}{\sqrt{N}} \sum_k e^{-iki} C_k^\dagger \quad (3.28c)$$

$$C_k^\dagger = \frac{1}{\sqrt{N}} \sum_i e^{iki} c_i^\dagger. \quad (3.28d)$$

Proof.

$$c_0 = \frac{1}{\sqrt{N}} \sum_k C_k \quad (3.29)$$

$$c_N = \frac{1}{\sqrt{N}} \sum_k e^{ikN} C_k. \quad (3.30)$$

We then must require that

$$kN \equiv 0 \pmod{2\pi} \quad (3.31)$$

$$k = \frac{2\pi n}{N} - \frac{N - [N \text{ odd}]}{N} \pi, \quad n \in \mathbb{Z}_N. \quad (3.32)$$

For N odd, what is C_π ?

$$C_\pi = \frac{1}{\sqrt{N}} \sum_i e^{-i\pi i} c_i. \quad (3.33)$$

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

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

$$C_k^\dagger = \sum_i U_{ik} c_i^\dagger. \quad (3.34)$$

Then

$$\{C_k, C_{k'}^\dagger\} = \sum_{ij} U_{ik}^* U_{jk'} \{c_i, c_j^\dagger\} \quad (3.35)$$

$$= \sum_i U_{ik}^* U_{ik'} \quad (3.36)$$

$$= (U^\dagger U)_{kk'} \quad (3.37)$$

$$= \delta_{kk'}, \quad (3.38)$$

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

Proof. For the Fourier transform,

$$F_{ik} = \frac{1}{\sqrt{N}} e^{iki}. \quad (3.39)$$

We may then confirm that

$$(F^\dagger F)_{kk'} = \sum_i \frac{1}{N} e^{i(k'-k)i} \quad (3.40)$$

$$= \delta_{kk'}. \quad (3.41)$$

Thus the Fourier transform is unitary. \square

Now since

$$\frac{1}{N} \sum_{i \in \mathbb{Z}_N} e^{i(k'-k)i} = \delta_{kk'}, \quad (3.42)$$

and also

$$C_{-k} = C_k^* \quad (3.43)$$

$$= \frac{1}{\sqrt{N}} \sum_i e^{-i(-k)i} c_i \quad (3.44)$$

$$= \frac{1}{N} \sum_{ik'} e^{i(k'+k)i} C_{k'}, \quad (3.45)$$

we have that

$$\sum_i c_i^\dagger c_i = \frac{1}{N} \sum_{ikk'} e^{i(k'-k)i} C_k^\dagger C_{k'} \quad (3.46)$$

$$= \sum_k C_k^\dagger C_k, \quad (3.47)$$

$$\sum_i (c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i) = \frac{1}{N} \sum_{ikk'} e^{i(k'-k)i} (e^{ik'} + e^{-ik}) C_k^\dagger C_{k'} \quad (3.48)$$

$$= \sum_k 2 \cos k C_k^\dagger C_k, \quad (3.49)$$

$$\sum_i (c_{i+1} c_i + c_i^\dagger c_{i+1}^\dagger) = \frac{1}{N} \sum_{ikk'} (e^{i(k'+k)i} e^{ik} C_k C_{k'} + e^{-i(k'+k)i} e^{-ik'} C_k^\dagger C_{k'}^\dagger) \quad (3.50)$$

$$= \sum_k (e^{-ik} C_{-k} C_k + e^{ik} C_k^\dagger C_{-k}^\dagger). \quad (3.51)$$

Thus eq. (3.27)^o is now

$$H = - \sum_k 2 \cos k C_k^\dagger C_k + \sum_k (e^{-ik} C_{-k} C_k + e^{ik} C_k^\dagger C_{-k}^\dagger) + \sum_k 2\lambda C_k^\dagger C_k - \lambda N I \quad (3.52)$$

$$= \sum_k (\lambda - \cos k) (C_k^\dagger C_k + C_{-k}^\dagger C_{-k}) + \sum_k i \sin k (C_{-k} C_k - C_k^\dagger C_{-k}^\dagger) - \lambda N I \quad (3.53)$$

$$= \sum_k (\lambda - \cos k) (C_k^\dagger C_k - C_{-k} C_{-k}^\dagger) + \sum_k i \sin k (C_{-k} C_k - C_k^\dagger C_{-k}^\dagger) \quad (3.54)$$

$$= \sum_k \mathbf{v}_k^\dagger \mathbf{H}_k \mathbf{v}_k, \quad (3.55)$$

where

$$\mathbf{H}_k = \begin{bmatrix} \lambda - \cos k & -i \sin k \\ i \sin k & \cos k - \lambda \end{bmatrix}, \quad (3.56)$$

$$\mathbf{v}_k = \begin{bmatrix} C_k \\ C_{-k}^\dagger \end{bmatrix}, \quad (3.57)$$

and we have used that

$$\sum_k \cos k = 0. \quad (3.58)$$

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

$$E_k^\pm = \pm \sqrt{-\det H_k} \quad (3.59)$$

$$= \pm \sqrt{\lambda^2 - 2\lambda \cos k + \cos^2 k + \sin^2 k} \quad (3.60)$$

$$= \pm \sqrt{\lambda^2 - 2\lambda \cos k + 1}. \quad (3.61)$$

The eigenvectors are then

$$\mathbf{q}_k^\pm = \begin{bmatrix} -i \sin k \\ E_k^\pm - (\lambda - \cos k) \end{bmatrix}, \quad (3.62)$$

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

$$\mathbf{q}_k^- = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \quad \text{and} \quad \mathbf{q}_k^+ = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \quad (3.63)$$

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

$$\|\mathbf{q}_k^\pm\|^2 = (E_k^\pm - (\lambda - \cos k))^2 + \sin^2 k \quad (3.64)$$

$$= (E_k^\pm)^2 + \lambda^2 + \cos^2 k - 2\lambda \cos k - 2E_k^\pm(\lambda - \cos k) + 1 - \cos^2 k \quad (3.65)$$

$$= 2E_k^\pm(E_k^\pm - (\lambda - \cos k)). \quad (3.66)$$

Now

$$\frac{(\mathbf{q}_k^\pm)_1}{\|\mathbf{q}_k^\pm\|} = \frac{-i \sin k}{\sqrt{2E_k^\pm(E_k^\pm - (\lambda - \cos k))}} \quad (3.67)$$

$$= \frac{-i \sin k}{\sqrt{2|E_k^\pm|(|E_k^\pm| \mp (\lambda - \cos k))}} \quad (3.68)$$

and

$$\frac{(\mathbf{q}_k^\pm)_2}{\|\mathbf{q}_k^\pm\|} = \pm \sqrt{\frac{E_k^\pm - (\lambda - \cos k)}{2E_k^\pm}} \quad (3.69)$$

$$= \pm \sqrt{\frac{|E_k^\pm| \mp (\lambda - \cos k)}{2|E_k^\pm|}} \quad (3.70)$$

$$U_k^\dagger = \begin{bmatrix} (\hat{q}_k^-)^\dagger \\ (\hat{q}_k^+)^\dagger \end{bmatrix}. \quad (3.71)$$

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

$$\eta_k^\pm = \frac{i \sin k}{\sqrt{2E_k(E_k \pm (\cos k - \lambda))}} C_k \pm \sqrt{\frac{E_k \pm (\cos k - \lambda)}{2E_k}} C_{-k}^\dagger \quad (3.72)$$

so that

$$\{(\eta_k^\pm)^\dagger, \eta_k^\pm\} = \frac{\sin^2 k}{2E_k(E_k \pm (\cos k - \lambda))} I + \frac{E_k \pm (\cos k - \lambda)}{2E_k} I \quad (3.73)$$

$$= I \quad (3.74)$$

$$\begin{aligned} \{(\eta_k^\pm)^\dagger, \eta_k^\mp\} &= \frac{\sin^2 k}{2E_k \sqrt{E_k \pm (\cos k - \lambda)} \sqrt{E_k \mp (\cos k - \lambda)}} I \\ &\quad - \frac{\sqrt{E_k \pm (\cos k - \lambda)} \sqrt{E_k \mp (\cos k - \lambda)}}{2E_k} I \end{aligned} \quad (3.75)$$

$$= 0. \quad (3.76)$$

Note that eq. (3.72)^o is consistent with the edge cases in the limits $k \rightarrow -\pi$ and $k \rightarrow 0$. If also $\lambda = -1$, then we impose that $\eta_{-\pi} = C_\pi^\dagger$, which is the same as if $\lambda \neq -1$.

Equation (3.55)^o becomes

$$H = \sum_k E_k^+ (\eta_k^+)^\dagger \eta_k^+ + \sum_k E_k^- (\eta_k^-)^\dagger \eta_k^-. \quad (3.77)$$

Since

$$(\eta_{-k}^-)^\dagger = \eta_k^+ =: \eta_k \quad (3.78)$$

and $E_{-k}^\pm = E_k^\pm$, we may reduce eq. (3.77)^o to

$$H = \sum_k E_k \eta_k^\dagger \eta_k - \sum_k E_k (I - \eta_k^\dagger \eta_k) \quad (3.79)$$

$$= \sum_k 2E_k \eta_k^\dagger \eta_k - I \sum_k E_k. \quad (3.80)$$

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

$$C_k = u f_k + v g_k^\dagger \quad (3.81a)$$

and

$$C_{-k} = -v f_k^\dagger + u g_k. \quad (3.81b)$$

For these transformations to preserve the CARs,

$$\{C_k^\dagger, C_k\} = |u|^2 \{f_k^\dagger, f_k\} + |v|^2 \{g_k, g_k^\dagger\} + u^* v \{f_k^\dagger, g_k^\dagger\} + v^* u \{g_k, f_k\} \quad (3.82)$$

$$= (|u|^2 + |v|^2)I, \quad (3.83)$$

so we must have

$$|u|^2 + |v|^2 = 1. \quad (3.84)$$

We may choose

$$u = e^{i\phi_1} \cos \theta \quad (3.85)$$

$$v = e^{i\phi_2} \sin \theta \quad (3.86)$$

for real angles ϕ_1 , ϕ_2 , and θ .

It remains to perform the inverse transformations to obtain the σ_i^x in terms of the η_k^\pm . Shift of perspective: Instead of decomposing the Hilbert space as the tensor product of spin operators, we decompose it as the tensor product of fermionic operators, where the fermionic operators are restricted to their subspaces in order to form an orthonormal basis for the Liouville space. We may then recover σ_i^x by the corresponding isomorphism of Liouville spaces. We choose

$$c, \quad c^\dagger, \quad c^\dagger c, \quad \text{and} \quad c c^\dagger \quad (3.87)$$

as our basis, since they are both orthonormal and eigenoperators of $c^\dagger c$ with respective eigenvalues

$$-1, \quad 1, \quad 2, \quad \text{and} \quad 0.$$

Theorem 3.1.1. *The fermionic operators $\bigcup_i \{c_i, c_i^\dagger, c_i^\dagger c_i, c_i c_i^\dagger\}$ form an orthonormal complete basis for the Liouville space $\mathcal{L}(\mathcal{H}_2^{\otimes N})$?*

Proof. We apply the CARs to show orthogonality.

$$\langle c_i | c_j \rangle = \text{tr}(c_i^\dagger c_j) \quad (3.88)$$

$$= \text{tr}(\delta_{ij}I - c_j c_i^\dagger) \quad (3.89)$$

$$= \delta_{ij} \text{tr} I - \text{tr}(c_j c_i^\dagger) \quad (3.90)$$

$$= 2^N \delta_{ij} - \text{tr}(c_i^\dagger c_j) \quad (3.91)$$

$$= 2^{N-1} \delta_{ij}, \quad (3.92)$$

$$\langle c_i^\dagger | c_j^\dagger \rangle = \text{tr}(c_i c_j^\dagger) \quad (3.93)$$

$$= 2^{N-1} \delta_{ij}, \quad (3.94)$$

$$\langle c_i^\dagger | c_j \rangle = \text{tr}(c_i c_j) \quad (3.95)$$

$$= -\text{tr}(c_j c_i) \quad (3.96)$$

$$= 0, \quad (3.97)$$

$$\langle c_i | c_j^\dagger \rangle = \text{tr}(c_i^\dagger c_j^\dagger) \quad (3.98)$$

$$= -\text{tr}(c_j^\dagger c_i^\dagger) \quad (3.99)$$

$$= 0, \quad (3.100)$$

$$\langle c_i^\dagger c_i | c_j \rangle = \text{tr}(c_i^\dagger c_i c_j) \quad (3.101)$$

$$= -\text{tr}(c_i^\dagger c_j c_i) \quad (3.102)$$

$$= -\text{tr}(c_i c_i^\dagger c_j) \quad (3.103)$$

$$\langle c_i^\dagger c_i | c_j^\dagger c_j \rangle = \text{tr}(c_i^\dagger c_i c_j^\dagger c_j) \quad (3.104)$$

$$= \delta_{ij} \text{tr}(c_i^\dagger c_j) - \text{tr}(c_i^\dagger c_j^\dagger c_i c_j) \quad (3.105)$$

$$= \delta_{ij} \text{tr}(c_i^\dagger c_j) + \text{tr}(c_i^\dagger c_j^\dagger c_j c_i) \quad (3.106)$$

$$= \delta_{ij} \text{tr}(c_i^\dagger c_j) + \text{tr}(c_i c_i^\dagger c_j^\dagger c_j) \quad (3.107)$$

$$= \delta_{ij} \text{tr}(c_i^\dagger c_j) + \text{tr}(c_j^\dagger c_j) - \text{tr}(c_i^\dagger c_i c_j^\dagger c_j) \quad (3.108)$$

$$= \frac{\delta_{ij}}{2} 2^{N-1} + \frac{1}{2} 2^{N-1} \quad (3.109)$$

$$= (\delta_{ij} + 1) 2^{N-2}, \quad (3.110)$$

$$\langle c_i^\dagger c_i | c_j c_j^\dagger \rangle = \text{tr}(c_i^\dagger c_i c_j c_j^\dagger) \quad (3.111)$$

$$= \text{tr}(c_i^\dagger c_i) - \text{tr}(c_i^\dagger c_i c_j^\dagger c_j) \quad (3.112)$$

$$= 2^{N-1} - (\delta_{ij} + 1) 2^{N-2} \quad (3.113)$$

$$= (1 - \delta_{ij}) 2^{N-2}. \quad (3.114)$$

Thus only c_i and c_i^\dagger are orthogonal, but still require normalization. The full set is not orthogonal. \square

We may then write

$$\sigma_x = \sum_{ia} x_{ia} c_{ia}, \quad (3.115)$$

where

$$x_{ia} = \langle \sigma_x | c_{ia} \rangle \quad (3.116)$$

and c_{ia} is restricted to subspace i . That is,

$$c_{1a} = c_a \otimes 0^{\otimes(N-1)}, \quad (3.117)$$

not

$$c_{1a} = c_a \otimes I^{\otimes(N-1)} \quad (3.118)$$

as usual.

Combining eqs. (3.28) and (3.72)^o gives

$$\eta_k = \frac{-i \sin k}{\sqrt{2E_k(E_k + (\cos k - \lambda))}} \frac{1}{\sqrt{N}} \sum_i e^{-iki} c_i \quad (3.119)$$

$$+ \sqrt{\frac{E_k + (\cos k - \lambda)}{2E_k}} \frac{1}{\sqrt{N}} \sum_i e^{-iki} c_i^\dagger. \quad (3.120)$$

$$\eta_k^\dagger \eta_k = \frac{\sin^2 k}{2E_k(E_k + (\cos k - \lambda))} \frac{1}{N} \sum_{ij} e^{ik(i-j)} c_i^\dagger c_j \quad (3.121)$$

$$+ \frac{E_k + (\cos k - \lambda)}{2E_k} \frac{1}{N} \sum_{ij} e^{ik(i-j)} c_i c_j^\dagger \quad (3.122)$$

$$+ \frac{i \sin k}{2E_k} \frac{1}{N} \sum_{ij} e^{ik(i-j)} (c_i^\dagger c_j^\dagger - c_i c_j) \quad (3.123)$$

Should the η_k match Pfeuty? If so, then hmm: these coefficients are complex while Pfeuty's are real. But I don't think they need to match. Having the same Hamiltonian and spectrum of energies says that the two representations of the Hamiltonian in the occupation basis for the different η_k are the same (up to permutation). However, since the spectrum is degenerate (Mathematica), these states may be rotated around within each degenerate eigenspace without changing the representation. It is thus possible that Pfeuty's and my η_k are both correct. While my way of obtaining the η_k through a Fourier transform is more straightforward, it gives more complicated coefficients for the c_i than the method of Lieb et. al., which is less direct (a harder eigenvalue problem than 2×2 matrices), but gives nice coefficients for the c_i [16, pp. 452–454].

We recall eq. (3.20)^o as

$$\sigma_i^x = - \left(\prod_{j < i} (c_j^\dagger c_j - c_j c_j^\dagger) \right) (c_i^\dagger + c_i), \quad (3.124)$$

and write

$$\eta_k = \sum_i a_{ik} c_i + b_{ik} c_i^\dagger \quad (3.125)$$

$$\eta_k^\dagger \eta_k = \sum_{ij} \left(a_{ik}^* c_i^\dagger + b_{ik}^* c_i \right) \left(a_{jk} c_j + b_{jk} c_j^\dagger \right) \quad (3.126)$$

$$= \sum_{ij} \left(a_{ik}^* a_{jk} c_i^\dagger c_j + b_{ik}^* b_{jk} c_i c_j^\dagger + a_{ik}^* b_{jk} c_i^\dagger c_j^\dagger + b_{ik}^* a_{jk} c_i c_j \right) \quad (3.127)$$

$$= \sum_i \left(|a_{ik}|^2 c_i^\dagger c_i + |b_{ik}|^2 c_i c_i^\dagger \right) \quad (3.128)$$

$$+ \sum_{i \neq j} \left(a_{ik}^* a_{jk} c_i^\dagger c_j + b_{ik}^* b_{jk} c_i c_j^\dagger + a_{ik}^* b_{jk} c_i^\dagger c_j^\dagger + b_{ik}^* a_{jk} c_i c_j \right). \quad (3.129)$$

Suppose that eq. (3.125)^o has been inverted to give coefficients α_{ik} and β_{ik} such that

$$c_i = \sum_k \alpha_{ik} \eta_k + \beta_{ik} \eta_k^\dagger. \quad (3.130)$$

We may then expand eq. (3.20)^o as

$$\sigma_i^x = - \left(\prod_{j < i} (2c_j^\dagger c_j - I) \right) (c_i^\dagger + c_i) \quad (3.131)$$

$$= - \left(\prod_{j < i} \left(2 \left(\sum_{kk'} \alpha_{ik}^* \alpha_{jk} \eta_k^\dagger \eta_{k'} + \alpha_{ik}^* \beta_{jk} \eta_k^\dagger \eta_{k'}^\dagger + \beta_{ik}^* \alpha_{jk} \eta_k \eta_{k'} + \beta_{ik}^* \beta_{jk} \eta_k \eta_{k'}^\dagger \right) - I \right) \right) \quad (3.132)$$

$$\left(\sum_k (\alpha_{ik} + \beta_{ik}^\dagger) \eta_k + (\alpha_{ik}^\dagger + \beta_{ik}) \eta_k^\dagger \right) \quad (3.133)$$

$$\sim - \left(\prod_j (x_j - I) \right) \quad (3.134)$$

$$\left(\sum_k (\alpha_{ik} + \beta_{ik}^\dagger) \eta_k + (\alpha_{ik}^\dagger + \beta_{ik}) \eta_k^\dagger \right) \quad (3.135)$$

$$\sim - \left(\sum_{I: J \rightarrow \mathbb{Z}_2} \prod_{j \in J} (-1)^{I(j)+1} x_j^{I(j)} \right) \quad (3.136)$$

$$\left(\sum_k (\alpha_{ik} + \beta_{ik}^\dagger) \eta_k + (\alpha_{ik}^\dagger + \beta_{ik}) \eta_k^\dagger \right) \quad (3.137)$$

We see that σ_i^x is a generic normal order expression in the η_k , so the eigenoperators we found at each site do not suffice, even if we got around them not being orthogonal.

Evaluation with projectors is intractable because a projector has one occupation state, but an η_k has many. Normal order expressions will have an intermediate number of non-identity factors.

Therefore, evaluate with 2^N dimensional matrices on a computer? Then ρ will only be known in coordinates and we may only consider numerical solutions for small N .

3.2 Computation of transverse-Ising superoperators

TODO: Redefine spin operators and the rest to depend on N and maybe λ , so that we can look at what happens as those parameters are varied.

3.2.1 Utility functions

```
trnorm(op) = tracenorm(dense(op))
acomm(x, y) = x*y + y*x
matriximage(A) = Gray.(1 .- abs.(A))
matriximage(A::Operator) = matriximage(dense(A).data)

function acomm_table(a, b, N, image)
    A = Matrix{Float64}(undef, N, N)
    for i in 1:N, j in i:N
        A[j, i] = trnorm(acomm(a(i), b(j))) / 2^N
    end
    L = LowerTriangular(A)
    image ? matriximage(L) : L
end

function acomm_tables(c, N=Int(log2(size(c(1))[1])); image=true)
    ct = dagger * c
    acommms = [
        acomm_table(ct, c, N, image),
        acomm_table(c, c, N, image),
        acomm_table(ct, ct, N, image),
    ]
    if image
        hcat(acommms...)
    else
        for ac in acommms
            display(ac)
        end
    end
end
```

```

    end
end

tpow(x, n) = ⊗(repeat([x], n)...);

```

3.2.2 Spins

First, we set up the spin-1/2 sites and Pauli operators.

```

sb = SpinBasis(1//2)
sx, sy, sz, sp, sm = sigmax(sb), sigmay(sb), sigmaz(sb), sigmap(sb), sigmam(sb)
up, down = spinup(sb), spindown(sb)
ψx = eigenstates(dense(sx))[2][1];

```

3.2.3 Ising model

To create a N -site spin loop, we need to construct the basis for the loop and operators for each site.

```

N = 8
sB = tpow(sb, N)
I = identityoperator(sB)
site(i, op) = embed(sB, (i-1)%N + 1, op) # Periodic boundary
acomm_tables(i → site(i, sm))

```



Figure 3.1

We now construct the transverse-field Ising Hamiltonian (Pfeuty)

$$\frac{4H}{J} = -\frac{1}{\lambda} \sum_i \sigma_z^i - \sum_{i=1}^N \sigma_i^x \sigma_{i+1}^x, \quad (3.138)$$

where $2\lambda = J/\Gamma$.

```

λ = 0.5 # Pfeuty with Γ=1, so
# Hs = -sum(site(i, sz)/2 + 2λ*site(i, sx)*site(i+1, sx)/4 for i in 1:N);
Hs = -sum((1/λ)*site(i, sz) + site(i, sx)*site(i+1, sx) for i in 1:N);

```

3.2.4 Fermion definitions

```

k(m, N=N) = 2π*(m-1)/N - π*(N - (N%2))/N; # for m in 1:N
function c(i) # for i in 1:N
    i = (i-1)%N + 1
    A = -(i == 1
        ? I
        : prod(-site(j, sz) for j in 1:(i-1)))
    A * site(i, sm)
end
ct(i) = dagger(c(i))
acomm_tables(c)

```

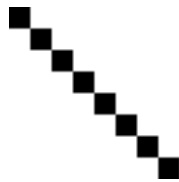


Figure 3.2

Verify that the inverse Jordan-Wigner transformation reproduces all the σ_i^x :

```

csx(i) = -(i == 1 ? I : prod(I - 2*ct(j)*c(j) for j in 1:(i-1))) * (ct(i) + c(i))
[csx(i) - site(i, sx) for i in 1:N]' .|> trnorm
1×8 Array{Float64,2}:
 0.0  0.0  0.0  0.0  0.0  0.0  0.0  0.0

```

The Jordan-Wigner transformed Hamiltonian:

```

L = sum(ct(i)*c(i) for i in 1:N)
Hend = (ct(N) - c(N))*(ct(1) + c(1))*((sparse ∘ exp ∘ dense)(im*π*L) + I)
Hc = I*(N/λ) + Hend - sum(
    (2/λ)*ct(i)*c(i) + (ct(i) - c(i))*(ct(i+1) + c(i+1))
    for i in 1:N)
trnorm(Hs - Hc) / 2^N
9.723409710616653e-16

```

It looks like the trace norm of the boundary term relative to that of the whole Hamiltonian diminishes with increasing N . But does this imply that it may be dropped?

```
trnorm(Hend) / trnorm(Hs)
0.19610389063966407
```

```
matriximage(Hend)
```

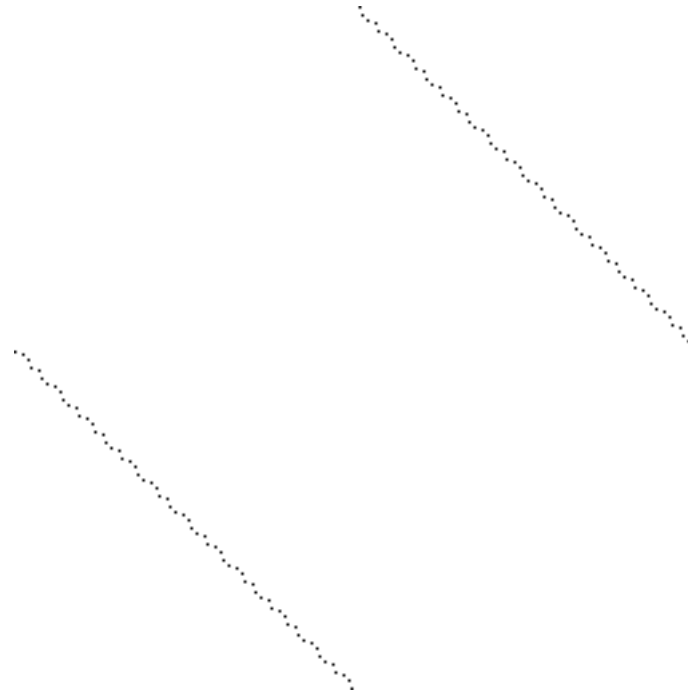


Figure 3.3

Striff

My λ differs from Pfeuty's (**TODO:** $\lambda \mapsto -\alpha$)

```
 $\lambda S = -1 / \lambda$ 
```

```
-2.0
```

First, we define the Fourier-transformed fermion operators and verify that the corresponding Hamiltonian is correct.

```
 $C(k) = \text{sum}(\exp(-im*k*i) * c(i) \text{ for } i \text{ in } 1:N) / \sqrt{N}$ 
```

```
 $Ct(k) = \text{dagger}(C(k))$ 
```

```
 $Hk(k) = [$ 
```

```
     $\lambda S - \cos(k) \quad -im*\sin(k)$ 
```

```
     $im*\sin(k) \quad \cos(k) - \lambda S$ 
```

```

]
vk(k) = [C(k); Ct(-k)]
vkt(k) = [Ct(k) C(-k)];

acomm_tables(C*k)

```



Figure 3.4

```

HC = sum((vkt(k(m))*Hk(k(m))*vk(k(m)))[1] for m in 1:N)
(trnorm((Hs - Hend) - HC), trnorm(Hs - HC)) ./ 2^N

(1.8522324463453775e-15, 1.0000000000000004)

```

Now, we define E_k and the operators $\eta_k = \eta_k^\dagger$.

```

E(m, N=N) = sqrt(lambda^2 - 2*lambda*cos(k(m, N)) + 1)
# aS(m) = ((N%2 == 0 && m == 1) || m == 1 + floor(N/2) ? 0 :
#         -im*sin(k(m)) / sqrt(2E(m)*(E(m) + cos(k(m)) - lambda)))
aS(m) = ((N%2 == 0 && m == 1) || m == 1 + floor(N/2) ? 0 :
         im*sin(k(m)) / sqrt(2E(m)*(E(m) + cos(k(m)) - lambda)))
bS(m) = ((N%2 == 0 && m == 1) || m == 1 + floor(N/2) ? 1 :
         sqrt((E(m) + cos(k(m)) - lambda) / (2E(m))))
etaS(m) = aS(m)*C(k(m)) + bS(m)*Ct(-k(m))
etaSt(m) = dagger(etaS(m))
acomm_tables(etaS)

```

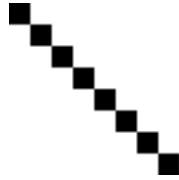


Figure 3.5

Check if the Striff η_k Hamiltonian is correct:

```

E0S = -sum(E(m) for m in 1:N);
HetaS = sum(2E(m)*etaSt(m)*etaS(m) for m in 1:N) + E0S*I
(trnorm((Hs - Hend) - HetaS), trnorm(Hs - HetaS)) ./ 2^N

```

(1.901556843519662e-15, 1.0)

Try to directly diagonalize H_k to find the η_k^\pm :

```
Heigs = [eigen(Hk(k(m))) for m in 1:N]
EC(m) = Heigs[m].values[2] # Positive energy
ηC(m) = (Heigs[m].vectors)'[2,1] * C(k(m)) + (Heigs[m].vectors)'[2,2] *
    ↪ Ct(-k(m))
ηCt(m) = dagger(ηC(m))
acomm_tables(ηC)
```

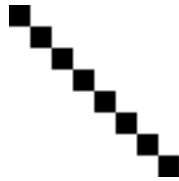


Figure 3.6

```
[ηC(m) - ηS(m) for m in 1:N]' .|> trnorm
1×8 Array{Float64,2}:
 7.83774e-15  0.0  1.2473e-30  0.0  0.0  0.0  1.2473e-30  0.0

HηC = sum(2EC(m) * (ηCt(m)*ηC(m) - I/2) for m in 1:N)
(trnorm((Hs - Hnd) - HηC), trnorm(Hs - HηC)) ./ 2^N
(5.232715105722094e-15, 1.0000000000000002)
```

Thus the diagonalization is correct. We may now construct the vacuum state from the sum of number operators.

```
NηS = sum(ηSt(m)*ηS(m) for m in 1:N)
vacS = eigenstates(NηS, 1, info=false)[2][1] # Indices select first eigenstate
((ηSt(1)*ηS(1) + ηSt(2)*ηS(2)) - 2*I) * (ηSt(1) * ηSt(2) * vacS) |> norm
4.451931037434651e-16
```

Pfeuty

Pfeuty: η 's do not satisfy the CARs? Typo, or **problem**?

```

 $\Lambda(m) = \sqrt{(\lambda^2 + 2\lambda \cos(k(m)) + 1)}$ 
 $\phi(k, i) = \sqrt{2/N} * (k > 0 ? \sin(k*i) : \cos(k*i))$ 
 $\psi(k, i) = -((1 + \lambda \cos(k)) * \phi(k, i) + \lambda \sin(k) * \phi(-k, i)) / \Lambda(k)$ 
 $a(m, i) = (\phi(k(m), i) + \psi(k(m), i)) / 2$ 
 $b(m, i) = (\phi(k(m), i) - \psi(k(m), i)) / 2$ 
 $\eta(m) = \text{sum}(a(m, i) * c(i) + b(m, i) * ct(i) \text{ for } i \text{ in } 1:N)$ 
 $\eta t(m) = \text{dagger}(\eta(m));$ 

acomm_tables( $\eta$ )

```



Figure 3.7

Check if the Pfeuty Hamiltonian is correct:

```

 $E0 = -\text{sum}(\Lambda(m) \text{ for } m \text{ in } 1:N) / 2;$ 
 $H\eta = \text{sum}(\Lambda(m) * \eta t(m) * \eta(m) \text{ for } m \text{ in } 1:N) + E0 * I;$ 
 $(Hs - \text{Hend}) - H\eta \triangleright \text{matriximage}$ 

```



Figure 3.8

```

 $(\text{trnorm}((Hs - \text{Hend}) - H\eta), \text{trnorm}(Hs - H\eta)) ./ 2^N$ 

```


(6.219280775999115, 6.254978848074612)

3.2.5 Starting from the many-body basis instead

It looks like create and destroy do not change the signs of occupation states, and thus do not anticommute.

TODO: Make correct creation and annihilation operators.

```
f = NLevelBasis(N) # "Levels" 1 to N are indices of k's
mbb = ManyBodyBasis(f, fermionstates(f, [0:N...]))
ηmb(m) = destroy(mbb, m)
ηtmb(m) = create(mbb, m)
Hf = diagonaloperator(f, @. Λ(k(1:N)) + E0)
Hmb = manybodyoperator(mbb, Hf);

A = reshape([a(m, i) for i in 1:N for m in 1:N], (N, N))
B = reshape([b(m, i) for i in 1:N for m in 1:N], (N, N))
η2c = inv([A B; conj(B) conj(A)]);

ηmbs = [[ηmb(m) for m in 1:N]; [ηtmb(m) for m in 1:N]]
cmbs = η2c * ηmbs
cmb(i) = cmbs[i];
cmbt(i) = cmbs[i+N];

[cmbt(i) - dagger(cmb(i)) for i in 1:N]' .|> dense .|> tracenorm

1×8 Array{Float64,2}:
 8.27619e-14  8.21719e-14  7.42067e-14  ...  7.63235e-14  6.3484e-14

acomm_tables(ηmb)
```



Figure 3.9

```
acomm_tables(cmb)
```

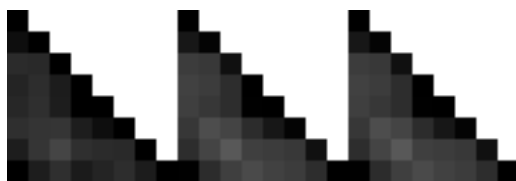


Figure 3.10

3.2.6 Energy spacings

The eigenvalues of the eigenoperators we seek are energy spacings. We should then figure out how they are distributed, and verify that the smallest energy spacing is large enough to be represented as a floating point number. Even with floating point errors, we may find rigorous bounds on the minimum energy difference using interval arithmetic.

```
using IntervalArithmetic
setformat(:midpoint);
```

Note that ΔE s generally double-counts due to parity symmetry.

```
function  $\Delta E$ s(NE)
    Eks = (m  $\rightarrow$  E(@interval(m), NE)).(1:NE)
    diffweights = Iterators.product(repeat([-1,0,1], NE)...)
    Ediffs = (abs(w  $\cdot$  Eks) for w in diffweights)
    Ediffs = Ediffs ./ abs(-(extrema(Ediffs)...))
    Ediffs  $\triangleright$  collect  $\triangleright$  vec  $\triangleright$  sort
end
;

NE = 4
 $\Delta E$ plot = plot(mid. ( $\Delta E$ s(NE)), 0:1/3^NE:1-eps(),
    label=latexstring("N = $NE"),
    xlim=(0, 1),
    ylim=(0, 1),
    key=:bottomright,
    xlabel=L"x \in \mathrm{supp}(\Delta E/\Delta E_{\text{max}})",
    ylabel=L"P(\Delta E/\Delta E_{\text{max}} \leqslant x)")
for NE in 5:10
    plot!( $\Delta E$ plot, mid. ( $\Delta E$ s(NE)), 0:1/3^NE:1-eps(), label=latexstring("N = $NE"))
end
 $\Delta E$ plot
```

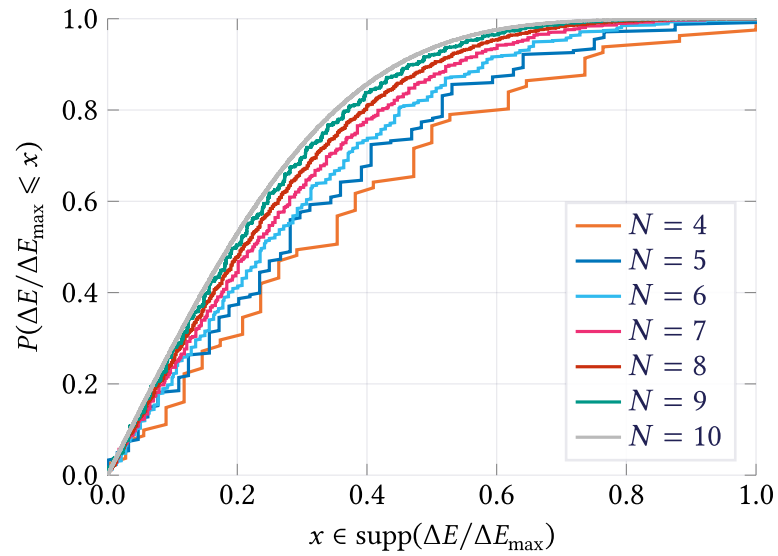


Figure 3.11

As expected, the density approaches a truncated normal distribution.

```
using KernelDensity
ΔE_kde = kde(mid.(ΔEs(12)))
plot(ΔE_kde.x, ΔE_kde.density)
```

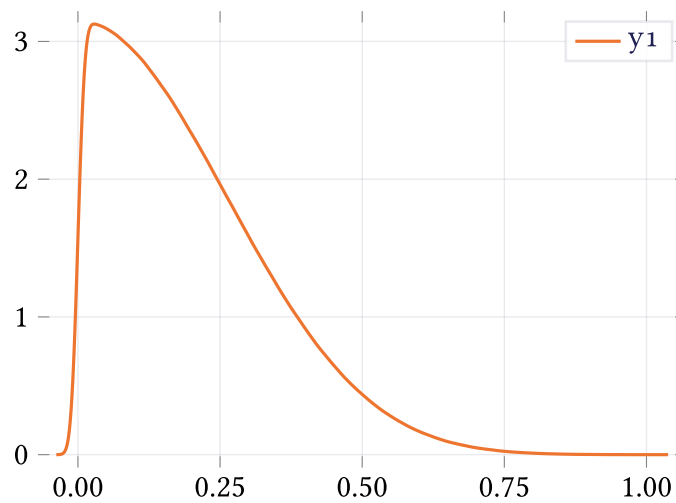


Figure 3.12

This rigorously shows that the smallest ΔE is either within the first interval (nonzero) or the second interval (very close to zero).

```
minΔEs = [NE ⇒ foldr((x, (m, z)) → 0 ∈ x ? (m, x ∪ z) : (min(x, m), z),
  ↪ ΔEs(NE), init=(@interval(Inf), @interval(0))) for NE in 2:15]
```

```

14-element Array{Pair{Int64,Tuple{Interval{Float64},Interval{Float64}}},1}:
 2 => (0.25 ± 5.55112e-17, 0 ± 0)
 3 => (0.0717968 ± 1.80412e-16, 1.03051e-16 ± 1.03052e-16)
 4 => (0.027864 ± 7.28584e-17, 5.24176e-17 ± 5.24177e-17)
 5 => (0.0149333 ± 8.84709e-17, 6.25437e-17 ± 6.25438e-17)
 6 => (0.00676561 ± 8.93383e-17, 1.04446e-16 ± 1.04446e-16)
 7 => (0.00492663 ± 9.1073e-17, 8.94574e-17 ± 8.94575e-17)
 8 => (8.75569e-05 ± 8.4866e-17, 6.52487e-17 ± 6.52487e-17)
 9 => (0.000111021 ± 1.21851e-16, 1.56578e-16 ± 1.56578e-16)
10 => (0.000484994 ± 8.89588e-17, 1.0961e-16 ± 1.09611e-16)
11 => (0.000260287 ± 1.94777e-16, 1.66072e-16 ± 1.66073e-16)
12 => (4.47363e-05 ± 1.13123e-16, 1.34836e-16 ± 1.34837e-16)
13 => (2.69225e-05 ± 1.96756e-16, 1.76658e-16 ± 1.76659e-16)
14 => (6.73035e-07 ± 1.60313e-16, 1.67768e-16 ± 1.67769e-16)
15 => (1.19663e-07 ± 1.53104e-16, 1.67022e-16 ± 1.67023e-16)

```

From the plot, we can derive an approximate lower bound for the smallest energy spacing. From the small N plots, it is clear that the energy differences are not uniformly separated. However, the CDF (from sorted indices) is uniformly spaced. Since we have computed 3^N energy differences, we may then expect the typical spacing between ΔE values at x to be $Q'(x)3^{-N}$, where $Q(x)$ is the limiting differentiable quantile function (inverse CDF). Suppose that for large N , $Q'(0) \rightarrow k$. From the plots, we estimate that $k > 1/3$. We may then make the following estimates:

```
[NE => (1/3) * 3.0^-NE for NE in 2:15]
```

```

14-element Array{Pair{Int64,Float64},1}:
 2 => 0.037037037037037035
 3 => 0.012345679012345678
 4 => 0.004115226337448559
 5 => 0.0013717421124828533
 6 => 0.00045724737082761767
 7 => 0.00015241579027587256
 8 => 5.080526342529086e-5
 9 => 1.6935087808430286e-5
10 => 5.645029269476761e-6
11 => 1.8816764231589206e-6
12 => 6.272254743863069e-7
13 => 2.0907515812876897e-7
14 => 6.969171937625632e-8
15 => 2.3230573125418773e-8

```

Note that these are all smaller than the actual minimum energy differences, as desired.

Now we may estimate the N where the spacing is small enough to cause problems to be around

```
-log(3, 3*eps()) > floor > Int
```

31

3.2.7 Construction of superoperators

TODO: Sort spectrum to group projectors together, etc.

3.2.8 Time evolution

We start the system off with all x -oriented spins.

```
#  $\psi_s = \text{tpow}(\text{down}, N);$   
 $\psi_s = \text{tpow}(\psi_x, N);$ 
```

Now we time-evolve the system and look at the expectation values of some reduced operators on the spin chain. We start with just the isolated chain.

```
fout(t,  $\rho$ ) = real([  
    expect(site(1, sz),  $\rho$ )  
    expect(embed(sB, [1, 2], [sz, sz]),  $\rho$ )  
    expect(site(1, sx),  $\rho$ )  
])  
ts, fouts = timeevolution.schroedinger([0:0.05:20;],  $\psi_s$ , Hs, fout=fout);  
  
plot(xlabel="Time", ylabel="Expectation Value")  
plot!(ts, hcat(fouts...)',  
    title = latexstring("$N$ spins,  $\lambda = \lambda$ "),  
    label = [  
        L"\left\langle \text{pauli}_1^z \right\rangle"  
        L"\left\langle \text{pauli}_1^z \text{pauli}_2^z \right\rangle"  
        L"\left\langle \text{pauli}_1^x \right\rangle"  
    ])
```

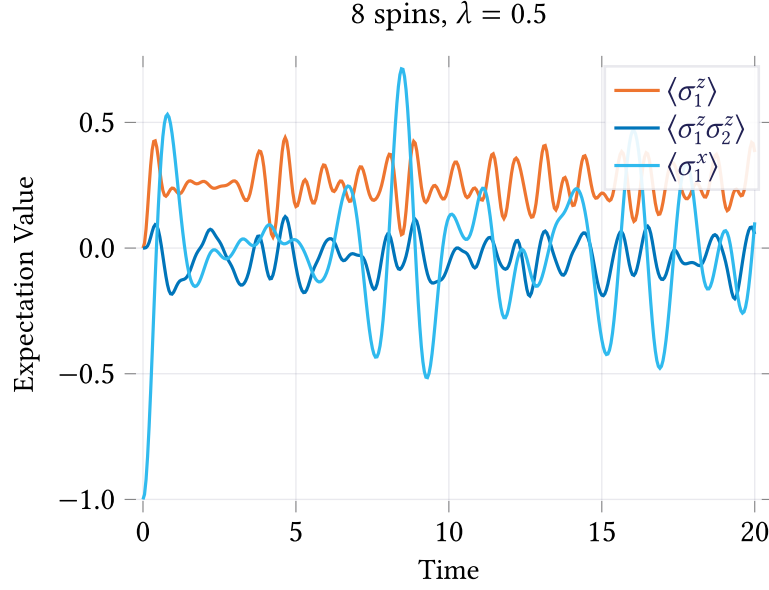


Figure 3.13: Isolated Ising time evolution.

3.3 Previous calculations

Note that for c_i and d_i from an orthonormal basis for \mathcal{L}_i ,

$$\langle \bigotimes_i a_i c_i | \bigotimes_i b_i d_i \rangle = \text{tr} \left(\bigotimes_i a_i^* b_i c_i^\dagger d_i \right) \quad (3.139)$$

$$= \prod_i \text{tr} (a_i^* b_i c_i^\dagger d_i) \quad (3.140)$$

$$= \prod_i a_i^* b_i \langle c_i | d_i \rangle \quad (3.141)$$

$$= \begin{cases} \prod_i a_i^* b_i & c_i = d_i \\ 0 & \text{otherwise.} \end{cases} \quad (3.142)$$

Thus

$$\langle \sigma_i^x | \eta_k \rangle = - \left\langle c_i^\dagger + c_i \left| \sum_j a_{jk} c_j + b_{jk} c_j^\dagger \right. \right\rangle \quad (3.143)$$

$$= a_{ik} + b_{ik} \quad (3.144)$$

$$\langle \sigma_i^x | \eta_k^\dagger \rangle = \langle \eta_k | \sigma_i^x \rangle \quad (3.145)$$

$$= a_{ik}^* + b_{ik}^* \quad (3.146)$$

$$\langle \sigma_i^x | \eta_k^\dagger \eta_k \rangle = 0 \quad \text{since trace } i \text{ vanishes} \quad (3.147)$$

$$\langle \sigma_i^x | \eta_k \eta_k^\dagger \rangle = \langle \eta_k^\dagger \eta_k | \sigma_i^x \rangle \quad (3.148)$$

$$= 0. \quad (3.149)$$

Thus

$$\sigma_i^x = \sum_k A_{ik} + A_{ik}^\dagger = 2 \text{He} \sum_k A_{ik}, \quad (3.150)$$

where

$$A_{ik} = (a_{ik} + b_{ik})\eta_k. \quad (3.151)$$

According to Pfeuty, if $\lambda \neq 0$ then

$$a_{ik} + b_{ik} = \sqrt{\frac{2}{N}} \begin{cases} \sin(ki) & k > 0 \\ \cos(ki) & k \leq 0, \end{cases} \quad (3.152)$$

and if $\lambda = 0$ then $a_{ik} + b_{ik} = 1/\sqrt{N}$.

Now since η_k is an eigenoperator of the Hamiltonian with eigenvalue $\omega_k = -E_k$, and η_k^\dagger similarly has $\omega_k = E_k$, we may use eqs. (2.79), (2.127) and (2.134)^o to find that the dissipator is

$$\begin{aligned} \mathcal{D}\rho &= \sum_{ik} \frac{2L}{c} C(-E_k)^2 n_B(E_k) \left(A_{ik} \rho A_{ik}^\dagger - \frac{1}{2} \{A_{ik}^\dagger A_{ik}, \rho\} \right) \\ &\quad + \sum_{ik} \frac{2L}{c} C(E_k)^2 (n_B(E_k) + 1) \left(A_{ik}^\dagger \rho A_{ik} - \frac{1}{2} \{A_{ik} A_{ik}^\dagger, \rho\} \right) \end{aligned} \quad (3.153)$$

$$\begin{aligned} &= \sum_{ik} \frac{2L}{c} C(-E_k)^2 n_B(E_k) |a_{ik} + b_{ik}|^2 \left(\eta_k \rho \eta_k^\dagger - \frac{1}{2} \{\eta_k^\dagger \eta_k, \rho\} \right) \\ &\quad + \sum_{ik} \frac{2L}{c} C(E_k)^2 (n_B(E_k) + 1) |a_{ik} + b_{ik}|^2 \left(\eta_k^\dagger \rho \eta_k - \frac{1}{2} \{\eta_k \eta_k^\dagger, \rho\} \right) \end{aligned} \quad (3.154)$$

$$\begin{aligned} &= \sum_k \frac{2L}{Nc} C(-E_k)^2 n_B(E_k) \left(\eta_k \rho \eta_k^\dagger - \frac{1}{2} \{\eta_k^\dagger \eta_k, \rho\} \right) \\ &\quad + \sum_k \frac{2L}{Nc} C(E_k)^2 (n_B(E_k) + 1) \left(\eta_k^\dagger \rho \eta_k - \frac{1}{2} \{\eta_k \eta_k^\dagger, \rho\} \right), \end{aligned} \quad (3.155)$$

since

$$\sum_i |a_{ik} + b_{ik}|^2 = \frac{2}{N} \sum_i \sin^2(ki) = \frac{1}{N}. \quad (3.156)$$

If $\rho_0 = |0\rangle\langle 0| = \otimes_k \eta_k \eta_k^\dagger$, then at $t = 0$

$$\mathcal{D}\rho = \sum_{ik} \frac{2L}{c} C(E_k)^2 (n_B(E_k) + 1) A_{ik}^\dagger A_{ik} \neq 0, \quad (3.157)$$

so the ground state of the closed system is not stationary?

3.4 Characterization of two-level dissipators

If we have a two-level system with density operator ρ , a general form of the dissipator is

$$\begin{aligned}\mathcal{D}\rho &= \gamma_- |h_-|^2 \left(\sigma^- \rho \sigma^+ - \frac{1}{2} \{ \sigma^+ \sigma^-, \rho \} \right) \\ &+ \gamma_+ |h_+|^2 \left(\sigma^+ \rho \sigma^- - \frac{1}{2} \{ \sigma_- \sigma^+, \rho \} \right) \\ &+ \gamma_z |h_z|^2 (\sigma^z \rho \sigma^z - \rho),\end{aligned}\tag{3.I58}$$

where each of the Pauli operators σ^a is assumed to be an eigenoperator of some Hamiltonian with eigenvalue ω_a , and $\gamma_a = \gamma(\omega_a)$. We also have coefficients from expressing part of an interaction Hamiltonian as $\sum_a h_a \sigma^a$.

We evaluate eq. (3.I58)^{*} by substituting

$$\rho = \rho_{00} \sigma^- \sigma^+ + \rho_{01} \sigma^- + \rho_{10} \sigma^+ + \rho_{11} \sigma^+ \sigma^-.\tag{3.I59}$$

This gives

$$\begin{aligned}\mathcal{D}\rho &= \gamma_+ |h_+|^2 (\sigma^+ \sigma^- - \sigma_- \sigma^+) \rho_{00} + \gamma_- |h_-|^2 (\sigma^- \sigma^+ - \sigma^+ \sigma^-) \rho_{11} \\ &+ \gamma_- |h_-|^2 \left(-\frac{1}{2} \{ \sigma^+ \sigma^-, \sigma^- \} \right) \rho_{01} + \gamma_+ |h_+|^2 \left(-\frac{1}{2} \{ \sigma_- \sigma^+, \sigma^- \} \right) \rho_{01} \\ &+ \gamma_- |h_-|^2 \left(-\frac{1}{2} \{ \sigma^+ \sigma^-, \sigma^+ \} \right) \rho_{10} + \gamma_+ |h_+|^2 \left(-\frac{1}{2} \{ \sigma_- \sigma^+, \sigma^+ \} \right) \rho_{10}\end{aligned}\tag{3.I60}$$

$$\begin{aligned}&+ \gamma_z |h_z|^2 (\sigma^z \sigma^- \sigma^z - \sigma^-) \rho_{01} + \gamma_z |h_z|^2 (\sigma^z \sigma^+ \sigma^z - \sigma^+) \rho_{10} \\ &= \gamma_+ |h_+|^2 (\sigma^+ \sigma^- - \sigma_- \sigma^+) \rho_{00} + \gamma_- |h_-|^2 (\sigma^- \sigma^+ - \sigma^+ \sigma^-) \rho_{11} \\ &- \gamma_- |h_-|^2 \frac{1}{2} \sigma^- \rho_{01} - \gamma_+ |h_+|^2 \frac{1}{2} \sigma^- \rho_{01} - \gamma_z |h_z|^2 2 \sigma^- \rho_{01} \\ &- \gamma_- |h_-|^2 \frac{1}{2} \sigma^+ \rho_{10} - \gamma_+ |h_+|^2 \frac{1}{2} \sigma^+ \rho_{10} - \gamma_z |h_z|^2 2 \sigma^+ \rho_{10}.\end{aligned}\tag{3.I61}$$

Ignoring the Lamb shift, the entries of the density matrix in the interaction picture are then given by

$$\dot{\rho}_{00} = -\gamma_+ |h_+|^2 \rho_{00} + \gamma_- |h_-|^2 \rho_{11}\tag{3.I62a}$$

$$\dot{\rho}_{01} = -\frac{1}{2} (\gamma_- |h_-|^2 + \gamma_+ |h_+|^2 + 4\gamma_z |h_z|^2) \rho_{01}\tag{3.I62b}$$

$$\dot{\rho}_{10} = -\frac{1}{2} (\gamma_- |h_-|^2 + \gamma_+ |h_+|^2 + 4\gamma_z |h_z|^2) \rho_{10}\tag{3.I62c}$$

$$\dot{\rho}_{11} = \gamma_+ |h_+|^2 \rho_{00} - \gamma_- |h_-|^2 \rho_{11}.\tag{3.I62d}$$

In the case where $h_z = 0$ and $h_- = h_+ =: h$, eq. (3.I62)^{*} reduces to

$$\dot{\rho}_{00} |h|^{-2} = -\gamma_+ \rho_{00} + \gamma_- \rho_{11}\tag{3.I63a}$$

$$\dot{\rho}_{01} |h|^{-2} = -\frac{1}{2} (\gamma_- + \gamma_+) \rho_{01}\tag{3.I63b}$$

$$\dot{\rho}_{10}|h|^{-2} = -\frac{1}{2}(\gamma_- + \gamma_+)\rho_{10} \quad (3.163c)$$

$$\dot{\rho}_{11}|h|^{-2} = \gamma_+\rho_{00} - \gamma_-\rho_{11}. \quad (3.163d)$$

Thus as $t \rightarrow \infty$, ρ approaches a pure state with both levels fractionally occupied? (Wait, this neglects the unitary evolution. Will do in full.) If so, compare to canonical occupations?

3.5 Pfeuty scratch work

I have

$$\lambda = -\frac{1}{\lambda_{\text{Pf}}} = -\frac{2\Gamma}{J}, \quad (3.164)$$

and my Hamiltonian eq. (3.2)^o should have

$$H \mapsto \frac{4}{J}H \quad (3.165)$$

to be correctly nondimensionalized and match Pfeuty's results. Then

$$E_k = \frac{\Lambda_k}{\lambda_{\text{Pf}}} = -\Lambda_k\lambda. \quad (3.166)$$

Pfeuty defines:

$$\lambda = \frac{J}{2\Gamma} \quad (3.167)$$

$$a_i = S_{xi} - iS_{yi} \quad (3.168)$$

$$a_i^\dagger = S_{xi} + iS_{yi} \quad (3.169)$$

$$c_i = \exp\left(\pi i \sum_{j=1}^{i-1} a_j^\dagger a_j\right) a_i \quad (3.170)$$

$$c_i^\dagger = a_i^\dagger \exp\left(-\pi i \sum_{j=1}^{i-1} a_j^\dagger a_j\right) \quad (3.171)$$

$$\eta_k = \sum_i \left(\frac{\varphi_{ki} + \psi_{ki}}{2} c_i + \frac{\varphi_{ki} - \psi_{ki}}{2} c_i^\dagger \right) \quad (3.172)$$

$$\varphi_{ki} = \sqrt{\frac{2}{N}} \begin{cases} \sin(ki) & k > 0 \\ \cos(ki) & k \leq 0 \end{cases} \quad (3.173)$$

$$\psi_{ki} = -\Lambda_k^{-1}((1 + \lambda \cos k)\varphi_{ki} + (\lambda \sin k)\varphi_{-ki}) \quad (3.174)$$

$$\Lambda_k^2 = 1 + \lambda^2 + 2\lambda \cos k \quad (3.175)$$

$$k = \frac{2\pi m}{N} \quad \text{for } m = -\frac{N}{2}, \dots, \frac{N}{2} - 1, \quad N \text{ even.} \quad (3.176)$$

We would like to express the S_{xi} in terms of eigenoperators of the system Hamiltonian

$$H = \Gamma \sum_k \Lambda_k \eta_k^\dagger \eta_k - \frac{\Gamma}{2} \sum_k \Lambda_k. \quad (3.177)$$

$$\{\eta_k, \eta_k^\dagger\} = \sum_{ij} \frac{\varphi_{ki} + \psi_{ki}}{2} \frac{\varphi_{kj} - \psi_{kj}}{2} \{c_i, c_j\} + \sum_{ij} \frac{\varphi_{ki} + \psi_{ki}}{2} \frac{\varphi_{kj} + \psi_{kj}}{2} \{c_i, c_j^\dagger\} \quad (3.178)$$

$$+ \sum_{ij} \frac{\varphi_{ki} - \psi_{ki}}{2} \frac{\varphi_{kj} - \psi_{kj}}{2} \{c_i^\dagger, c_j\} + \sum_{ij} \frac{\varphi_{ki} - \psi_{ki}}{2} \frac{\varphi_{kj} + \psi_{kj}}{2} \{c_i^\dagger, c_j^\dagger\} \\ = \frac{I}{4} \sum_i (\varphi_{ki} + \psi_{ki})^2 + (\varphi_{ki} - \psi_{ki})^2 \quad (3.179)$$

$$= \frac{I}{2} \sum_i \varphi_{ki}^2 + \psi_{ki}^2 \quad (3.180)$$

$$= I? \quad (3.181)$$

According to Mathematica, no? But [I6, pp. 452–454] is probably right.

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

Computer details

A.1 Julia version information

```
versioninfo()
```

```
Julia Version 1.4.0
```

```
Commit b8e9a9ecc6 (2020-03-21 16:36 UTC)
```

```
Platform Info:
```

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

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

```
  WORD_SIZE: 64
```

```
  LIBM: libopenlibm
```

```
  LLVM: libLLVM-8.0.1 (ORCJIT, haswell)
```

```
using Pkg
```

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

```
Activating environment at
```

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

```
Pkg.status()
```

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

```
[7d9fca2a] Arpack v0.4.0
```

```
[b964fa9f] LaTeXStrings v1.2.0
```

```
[eff96d63] Measurements v2.3.0
```

```
[3b7a836e] PGFPlots v3.3.2
```

```
[91a5bcdd] Plots v1.6.6
```

```
[6e0679c1] QuantumOptics v0.8.2
```

```
[1986cc42] Unitful v1.4.1
```

```
[37e2e46d] LinearAlgebra
```

A.2 Notebook Preamble

```
using Plots, LaTeXStrings
```

```
using Unitful, Measurements
```

```
using LinearAlgebra, Arpack, QuantumOptics
```

```
import PGFPlots: pushPGFPlotsPreamble, popPGFPlotsPreamble
```

```
popPGFPlotsPreamble() # If reevaluating, so no duplicates
```

```
pushPGFPlotsPreamble(")
```

```
    \usepackage{siunitx}
```

```
    \usepackage[semibold,osf]{libertinus}
```

```
    \usepackage[scr=boondoxo,cal=esstix]{mathalfa}
```

```
    \usepackage{bm}
```

```
    \input{latexdefs}
```

```
")
```

```
pgfplots();
```

```
using PlotThemes
```

```
theme(:vibrant,
```

```
    size=(400, 300),
```

```
    dpi=300,
```

```
    titlefontsize=12,
```

```
    tickfontsize=12,
```

```
    legendfontsize=12,
```

```
)
```

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