Toy Systems and Quantum Master Equations

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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, Kossakowski, 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 $(A, B) \equiv \operatorname{tr}\left(A^\dagger B\right)$ 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 $\operatorname{tr}\rho = 1$. 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**

$$\dot{\rho} = [H, \rho]/\mathrm{i}\hbar\,. \tag{2.1}$$

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

$$\langle O(t)\rangle_{\rho(t)} = \operatorname{tr}\Big(O(t)U(t)\rho U^\dagger(t)\Big) \tag{2.2}$$

$$= \operatorname{tr}\Big(U^\dagger(t)O(t)U(t)\rho\Big) \equiv \langle O_H(t)\rangle_\rho \tag{2.3}$$

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 $U_0(t) = e^{H_0 t/\mathrm{i}\hbar}$ 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

$$O_I(t) = U_0^\dagger(t)O(t)U_0(t) \tag{2.4a}$$

$$\rho_I(t) = U_I(t)\rho U_I^\dagger(t). \tag{2.4b}$$

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)

$$\begin{aligned}
\mathrm{i}\hbar\,\dot{\rho}_I(t) &= \mathrm{i}\hbar\frac{\mathrm{d}}{\mathrm{d}t}\Big(U_0^\dagger\rho(t)U_0\Big) \\
&= -U_0^\dagger H_0^\dagger \rho(t)U_0 + U_0^\dagger\rho(t)H_0U_0 \\
&+ U_0^\dagger[H_0, \rho(t)]U_0 + U_0^\dagger[H_I, \rho(t)]U_0 \\
&= U_0^\dagger\Big[U_0H_I'U_0^\dagger, \rho(t)\Big]U_0
\end{aligned}$$

$$= \left[H_I', \rho_I(t)\right], \tag{2.5}$$

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

Consider two quantum systems in Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$. The Hilbert space of the composite system is the **tensor product** $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$ (definition 3). 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:

$$\langle O_A \otimes I \rangle_\rho = \langle O_A \rangle_{\rho_A}. \tag{2.6}$$

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

$$\rho = \sum_{jk} A_j \otimes B_k \left(A_j \otimes B_k, \rho\right). \tag{2.7}$$

We may then compute that

$$\begin{aligned}
\rho_A &= \sum_i A_i (A_i, \rho_A) && (2.8)\\
&= \sum_i A_i (A_i \otimes I, \rho) \quad \text{(eq. (2.6))} && (2.9)\\
&= \sum_i A_i \Big(A_i \otimes I, \textstyle\sum_{jk} A_j \otimes B_k \big(A_j \otimes B_k, \rho\big)\Big) \quad \text{(eq. (2.7))} && (2.10)\\
&= \sum_{ijk} A_i \big(A_i \otimes I, A_j \otimes B_k\big)\big(A_j \otimes B_k, \rho\big) && (2.11)
\end{aligned}$$

$$= \sum_{ijk} A_i \big(A_i, A_j\big)(B_k, I)\big(A_j \otimes B_k, \rho\big) \tag{2.12}$$

$$= \sum_{ijk} A_i \delta_{ij} \operatorname{tr} B_k \big(A_j \otimes B_k, \rho\big) \tag{2.13}$$

$$= \sum_{jk} A_j \operatorname{tr} B_k \big(A_j \otimes B_k, \rho\big). \tag{2.14}$$

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

$$\operatorname{tr}_B (A \otimes B) = A \operatorname{tr} B \tag{2.15}$$

and extending linearly.

With this definition, we continue from eq. (2.14) to find that

$$\rho_A = \sum_{jk} \operatorname{tr}_B \big(A_j \otimes B_k\big)\big(A_j \otimes B_k, \rho\big) \tag{2.16}$$

$$= \operatorname{tr}_B \Big(\textstyle\sum_{jk} A_j \otimes B_k \big(A_j \otimes B_k, \rho\big)\Big) \tag{2.17}$$

$$= \operatorname{tr}_B \rho. \tag{2.18}$$

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

$$S(\rho \| \rho_A \otimes \rho_B) \tag{2.19}$$

$$\equiv \operatorname{tr} \rho(\ln \rho - \ln(\rho_A \otimes \rho_B)) \tag{2.20}$$

$$= \operatorname{tr}(\rho \ln \rho) - \operatorname{tr}_A \operatorname{tr}_B (\rho \ln(\rho_A \otimes I)) - \operatorname{tr}_B \operatorname{tr}_A (\rho \ln(I \otimes \rho_B)) \tag{2.21}$$

$$= S(\rho_A) + S(\rho_B) - S(\rho). \tag{2.22}$$

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

$$S(\rho) \le S(\rho_A) + S(\rho_B), \tag{2.23}$$

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), or that the relative entropy between subsystems is less than that between combined systems (theorem 2.9.3).

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

$$H_{SB}(t) = H_S \otimes I + I \otimes H_B + H_I(t) \tag{2.24}$$

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

$$\rho_S(t) = \mathrm{tr}_B\left(U(t)(\rho_S(0) \otimes \rho_B)U^\dagger(t)\right). \tag{2.25}$$

Whatever eq. (2.25) 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

$$\mathcal{V}(t_1)\mathcal{V}(t_2) = \mathcal{V}(t_1 + t_2) \quad \text{for} \quad t_1, t_2 \geq 0. \tag{2.26}$$

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. (2.25) and theorems theorems 2.9.2 and 2.9.3):

$$\begin{aligned} S(\mathcal{V}(t)\rho \| \mathcal{V}(t)\rho_0) &= S\Big(\mathrm{tr}_B\left[U(t)(\rho \otimes \rho_B)U^\dagger(t)\right] \| \rho_0\Big) && (2.27)\\ &\leq S\Big(U(t)(\rho \otimes \rho_B)U^\dagger(t) \| \rho_0 \otimes \rho_B\Big) && (2.28)\\ &= S(\rho \otimes \rho_B \| \rho_0 \otimes \rho_B) && (2.29) \end{aligned}$$

$$= S(\rho \| \rho_0). \tag{2.30}$$

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 CTCP 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. (2.42). 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. (2.25) becomes (writing ρ_S as ρ)

$$\rho(t) = \sum_{ij} \langle\phi_i|U(t)\big(\rho(0) \otimes \lambda_j |\phi_j\rangle\langle\phi_j|\big)U^\dagger(t)|\phi_i\rangle \tag{2.31}$$

$$= \sum_{ij} \lambda_j \left\langle\phi_i\middle|U(t)\middle|\phi_j\right\rangle \rho(0) \left\langle\phi_j\middle|U^\dagger(t)\middle|\phi_i\right\rangle \tag{2.32}$$

$$= \sum_{ij} M_{ij}(t)\rho(0)M_{ij}^\dagger(t), \tag{2.33}$$

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). 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. (2.33) becomes

$$\rho(t) = \sum_{mn} c_{mn}(t) F_m \rho(0) F_n^\dagger, \tag{2.34}$$

where

$$c_{mn}(t) \equiv \sum_{ij} \left\langle F_m\middle|M_{ij}(t)\right\rangle \left\langle M_{ij}(t)\middle|F_n\right\rangle. \tag{2.35}$$

For convenience, we may choose $F_{d^2} = I/\sqrt{d}$, where $d = \dim(\mathcal{H}_S)$. With an eye towards simplifying eq. (2.39), we eliminate the explicit time dependence of eq. (2.35) by defining

$$a_{mn} \equiv \lim_{t\to 0^+} \frac{c_{mn}(t) - d\delta_{d^2 d^2}}{t} \tag{2.36}$$

and introduce the sum of Kraus operators

$$
\begin{aligned}
F &= \frac{1}{\sqrt{d}} \sum_{n=1}^{d^2-1} a_{nd^2} F_n && (2.37)\\
&= \frac{F+F^\dagger}{2} + \mathrm{i}\frac{F-F^\dagger}{2\mathrm{i}} \equiv G + H/\mathrm{i}\hbar, && (2.38)
\end{aligned}
$$

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

$$
\begin{aligned}
\dot{\rho} &= \lim_{\Delta t \to 0^+} \frac{\mathcal{V}(\Delta t)\rho - \rho}{\Delta t}\\
&= \lim_{\Delta t \to 0^+} \left(\frac{c_{d^2 d^2} - d}{d \Delta t}\rho + \sum_{m,n=1}^{d^2-1} \frac{c_{mn}(\Delta t)}{\Delta t} F_m \rho F_n^\dagger \right.\\
&\left. + \frac{1}{\sqrt{d}} \sum_{n=1}^{d^2-1} \left(\frac{c_{nd^2}(\Delta t)}{\Delta t} F_n \rho + \frac{c_{d^2 n}(\Delta t)}{\Delta t} \rho F_n^\dagger \right) \right) && (2.39)\\
&= \frac{a_{d^2 d^2}}{d}\rho + F\rho + \rho F^\dagger + \sum_{m,n=1}^{d^2-1} a_{mn} F_m \rho F_n^\dagger\\
&= \frac{a_{d^2 d^2}}{d}\rho + \{G, \rho\} + \frac{[H,\rho]}{\mathrm{i}\hbar} + \sum_{m,n=1}^{d^2-1} a_{mn} F_m \rho F_n^\dagger\\
&= \{G', \rho\} + \frac{[H,\rho]}{\mathrm{i}\hbar} + \sum_{m,n=1}^{d^2-1} a_{mn} F_m \rho F_n^\dagger, && (2.40)
\end{aligned}
$$

where $G' = G + a_{d^2 d^2} I/d$. Since $\mathcal{V}(t)$ is trace-preserving, $\operatorname{tr}\dot{\rho} = 0$. Applying this condition to eq. (2.40) and cycling the trace gives

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

so $G' = -\sum_{m,n=1}^{d^2-1} a_{mn} F_n^\dagger F_m / 2$. This allows us to write eq. (2.40) as

$$
\dot{\rho} = \frac{[H,\rho]}{\mathrm{i}\hbar} + \sum_{m,n=1}^{d^2-1} a_{mn}\left(F_m \rho F_n^\dagger - \frac{1}{2}\left\{ F_n^\dagger F_m, \rho \right\} \right), \qquad (2.41)
$$

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. (2.35) to be Hermitian, and eq. (2.36) 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

$$\dot{\rho} = \frac{[H,\rho]}{\mathrm{i}\hbar} + \sum_{k=1}^{d^2-1} \gamma_k \Big(L_k \rho L_k^\dagger - \frac{1}{2}\Big\{ L_k^\dagger L_k, \rho \Big\} \Big) \equiv \mathcal{L}\rho, \tag{2.42}$$

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), 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. (2.24) to give rise to Markovian dynamics. While there are several different regimes where this is true, we will consider the **weak-coupling** limit which we justify by supposing that the environment is similar to a **harmonic bath** of many harmonic oscillators.

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

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

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

$$[H_S, A_{\alpha\omega}] = -\omega A_{\alpha\omega}. \tag{2.43}$$

Using eq. (2.43) to commute past the exponential in eq. (2.4a) gives $A'_{\alpha\omega} = e^{-\mathrm{i}\omega t} A_{\alpha\omega}$ in the interaction picture. Thus the interaction Hamiltonian in the interaction picture is

$$H_I' = \sum_{\alpha\omega} e^{-\mathrm{i}\omega t} A_{\alpha\omega} \otimes B_\alpha', \tag{2.44}$$

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

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

$$\langle B_\alpha^\dagger(t) B_\beta(t-s)\rangle_{\rho_B} \tag{2.45}$$

and their one-sided Fourier transform

$$\Gamma_{\alpha\beta}(\omega) \equiv \int_0^\infty \mathrm{d}s\, e^{\mathrm{i}\omega s} \left\langle B_\alpha^\dagger(t) B_\beta(t-s)\right\rangle_{\rho_B} \tag{2.46}$$

$$\equiv \mathrm{i} S_{\alpha\beta}(\omega) + \gamma_{\alpha\beta}(\omega)\big/2, \tag{2.47}$$

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

$$\gamma_{\alpha\beta}(\omega) \equiv \int_{-\infty}^\infty \mathrm{d}s\, e^{\mathrm{i}\omega s} \left\langle B_\alpha^\dagger(t) B_\beta(t-s)\right\rangle_{\rho_B} \tag{2.48}$$

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

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

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

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

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

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

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

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

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

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

$$\dot{\rho}_S = -\int_0^\infty \mathrm{d}s\, \mathrm{tr}_B \left[H_I(t), \left[H_I(t-s), \rho_S(t) \otimes \rho_B\right]\right]. \tag{2.49}$$

This is justified when the reservoir correlation functions in eq. (2.46) vanish quickly over a time τ_B that is smaller than the relaxation time τ_R (see section 2.7). Substituting eq. (2.44) into eq. (2.49) and using eq. (2.46) gives

$$\dot{\rho}_S = 2\,\mathrm{He} \sum_{\alpha\beta\omega\omega'} e^{\mathrm{i}(\omega'-\omega)t} \Gamma_{\alpha\beta}(\omega) \Big(A_{\beta\omega}\rho_S A^\dagger_{\alpha\omega'} - A^\dagger_{\alpha\omega'} A_{\beta\omega}\rho_S \Big), \tag{2.50}$$

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

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

for system evolution are large compared to the relaxation time τ_R, then the contribution from the fast-oscillating terms of eq. (2.50) where $\omega' \neq \omega$ may be neglected. This **rotating wave** or **secular approximation** is analogous to how we consider the high-energy position distribution in the infinite square well to be uniform, even though it is actually a fast-oscillating function. By coarse-graining in this sense, we obtain

$$\dot{\rho}_S = 2\,\mathrm{He} \sum_{\alpha\beta\omega} \Gamma_{\alpha\beta}(\omega) \Big(A_{\beta\omega}\rho_S A^\dagger_{\alpha\omega} - A^\dagger_{\alpha\omega} A_{\beta\omega}\rho_S \Big). \tag{2.51}$$

Now applying the decomposition eq. (2.47) gives the interaction picture Lindblad equation

$$\dot{\rho}_S = \mathrm{i}[H_{LS}, \rho_S] + \mathcal{D}\rho_S, \tag{2.52}$$

where the **Lamb shift Hamiltonian** is

$$H_{LS} = \sum_{\alpha\beta\omega} S_{\alpha\beta}(\omega) A^{\dagger}_{\alpha\omega} A_{\beta\omega}, \tag{2.53}$$

and the *dissipator* is

$$\mathcal{D}\rho_S = \sum_{\alpha\beta\omega} \gamma_{\alpha\beta}\Big(A_{\beta\omega}\rho_S A^{\dagger}_{\alpha\omega} - \frac{1}{2}\Big[A^{\dagger}_{\alpha\omega}A_{\beta\omega}, \rho_S\Big]\Big). \tag{2.54}$$

The Lamb shift (or environment renormalization) Hamiltonian commutes with the system Hamiltonian since eq. (2.43) implies that $[H_S, A^{\dagger}_{\alpha\omega}A_{\beta\omega}] = 0$. Adding the system's Hamiltonian H_S to H_{LS} and diagonalizing gives the Schrödinger picture Lindblad equation eq. (2.42).

2.5 Relaxation to thermal equilibrium

The system will generally relax from its initial configuration to a stationary solution of eq. (2.42) (see section 2.7). We expect that the thermal state

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

would be the equilibrium state. This is true when the reservoir correlation functions obey the KMS condition [10, 11]

$$\Big\langle B^{\dagger}_{\alpha}(t) B_{\beta}(0)\Big\rangle_{\rho_B} = \Big\langle B_{\beta}(0) B^{\dagger}_{\alpha}(t + \mathrm{i}\beta)\Big\rangle_{\rho_B}, \tag{2.55}$$

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

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. (2.43). 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 [12]. Ignoring the Lamb shift (which only offsets) and considering only the effects at ω, eq. (2.52) becomes

$$\begin{aligned}\dot{\rho} &= \gamma_0(N+1)\Big(\sigma_-\rho\sigma_+ - \frac{1}{2}\{\sigma_+\sigma_-, \rho\}\Big) \\ &\quad + \gamma_0 N\Big(\sigma_+\rho\sigma_- - \frac{1}{2}\{\sigma_-\sigma_+, \rho\}\Big) \equiv \mathcal{D}\rho,\end{aligned} \tag{2.56}$$

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

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

This is consistent with what we observe in atomic spectra: an exponential decay to an equilibrium level which gives Lorentzian peaks. At low temperatures ($N \to 0$) 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 [13] (*Cf.* [1]).

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. (2.45) 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].

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

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

This induces an extension of Dirac notation where all pairs $f \otimes x$ of dual and usual vectors from the same space are evaluated as $\langle f|x\rangle = f(x)$ and extended linearly. For example, given a linear operator $U : V \otimes W \to V \otimes W$ and a basis $|\phi_i\rangle$ for W, the partial trace over W may be expressed as $\operatorname{tr}_W U = \langle \phi_i|U|\phi_i\rangle$. This forms the justification of the step from eq. (2.31) to eq. (2.32) 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

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

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

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

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

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

which evaluates to

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

Theorem 2.9.2. *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

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

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

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

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

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

Theorem 2.9.4 (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)

$$H = \left(-J\sum_i \sigma_{zi}\sigma_{z(i+1)} - h\sum_i \sigma_{xi}\right) + \sum_{ik}\omega_{ik}a_{ik}^\dagger a_{ik} + \sum_{ik}C_k\left(a_{ik}^\dagger + a_{ik}\right)\sigma_{zi} \tag{2.57}$$

$$\equiv H_S \otimes I + I \otimes H_B + H_I. \tag{2.58}$$

The Schrodinger picture operators of the interaction Hamiltonian

$$H_I = \sum_i A_i \otimes B_i \tag{2.59}$$

are

$$A_i = \sigma_{zi} \tag{2.60}$$

$$B_i = \sum_k C_k\left(a_{ik}^\dagger + a_{ik}\right) \equiv \sum_k B_{ik}. \tag{2.61}$$

In the interaction picture,

$$A_i(t) = \sigma_{zi} \tag{2.62}$$

and

$$B_{ik}(t) = C_k\left(e^{\mathrm{i}\omega_{ik}t}a_{ik}^\dagger + e^{-\mathrm{i}\omega_{ik}t}a_{ik}\right). \tag{2.63}$$

Proof. Consider an observable A which satisfies

$$[H, A] = \omega A \tag{2.64}$$

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

$$H^n A = H^{n-1}AH + H^{n-1}[H, A] \tag{2.65}$$

$$= H^{n-1}A(H + \omega I) \tag{2.66}$$

$$= A(H + \omega I)^n. \tag{2.67}$$

Then

$$e^H A = \sum_{n\geq 0} \frac{H^n A}{n!} \tag{2.68}$$

$$= A \sum_{n\geq 0} \frac{(H+\omega I)^n}{n!} \tag{2.69}$$

$$= Ae^{H+\omega I} \tag{2.70}$$

$$= Ae^{\omega} e^{H}, \quad \text{(BCH)} \tag{2.71}$$

so the interaction picture operator is

$$A(t) = e^{\mathrm{i}Ht} A e^{-\mathrm{i}Ht} \tag{2.72}$$

$$= e^{\mathrm{i}\omega t} A e^{\mathrm{i}Ht} e^{-\mathrm{i}Ht} \tag{2.73}$$

$$= e^{\mathrm{i}\omega t} A. \tag{2.74}$$

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

$$\left[H_B, a_{jl}\right] = \sum_{ik} \left[a_{ik}^\dagger a_{ik}, a_{jl}\right] \quad \text{(definition of } H_B\text{)} \tag{2.75}$$

$$= -\sum_{ik} \delta_{ij}\delta_{kl} a_{jl} \quad \text{(commutation relations)} \tag{2.76}$$

$$= -a_{jl}, \tag{2.77}$$

which follows from the commutation relations

$$\left[a^\dagger a, a\right] = a^\dagger aa - aa^\dagger a \tag{2.78}$$

$$= a^\dagger aa - a^\dagger aa - a\left[a, a^\dagger\right] \tag{2.79}$$

$$= -a \tag{2.80}$$

and

$$\left[a^\dagger a, a^\dagger\right] = a^\dagger aa^\dagger - a^\dagger a^\dagger a \tag{2.81}$$

$$= a^\dagger aa^\dagger - a^\dagger aa^\dagger - a^\dagger\left[a^\dagger, a\right] \tag{2.82}$$

$$= a^\dagger. \quad \square$$

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

1. $\mathrm{tr}_B\left[H_I(t), \rho_0\right] = 0$, 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 $\left\langle B_{ik}^\dagger(t) B_{jl}(t-s) \right\rangle_{\rho_B^{(I)}(t)}$ 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

$$\rho_{\text{th}} = \frac{e^{-\beta H_B}}{\operatorname{tr} e^{-\beta H_B}}, \tag{2.83}$$

the reservoir correlation functions are

$$\begin{aligned} \left\langle B_{ik}^\dagger(t) B_{jl}(t-s) \right\rangle &= \left\langle B_{ik}^\dagger(s) B_{jl}(0) \right\rangle && (2.84) \\ &= \delta_{ij}\delta_{kl} C_k C_l \big(e^{-\mathrm{i}\omega_{ik} s} (n_B(\omega_{ik}) + 1) + e^{\mathrm{i}\omega_{ik} s} n_B(\omega_{ik}) \big). && (2.85) \end{aligned}$$

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

$$\begin{aligned} \langle a_{ik} a_{jl} \rangle &= 0 && (2.86) \\ \left\langle a_{ik}^\dagger a_{jl}^\dagger \right\rangle &= 0 && (2.87) \\ \left\langle a_{ik}^\dagger a_{jl} \right\rangle &= \delta_{ij}\delta_{kl}\, n_B(\omega_{ik}) && (2.88) \\ \left\langle a_{ik} a_{jl}^\dagger \right\rangle &= \delta_{ij}\delta_{kl} (n_B(\omega_{ik}) + 1), && (2.89) \end{aligned}$$

where

$$n_B(\omega) = \frac{1}{e^{\beta\omega} - 1} \tag{2.90}$$

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

$$\begin{aligned} &\left\langle B_{ik}^\dagger(t) B_{jl}(t-s) \right\rangle && (2.91) \\ &= C_k C_l \left\langle \left(e^{-\mathrm{i}\omega_{ik} t} a_{ik} + e^{\mathrm{i}\omega_{ik} t} a_{ik}^\dagger \right) \left(e^{\mathrm{i}\omega_{jl}(t-s)} a_{jl}^\dagger + e^{-\mathrm{i}\omega_{jl}(t-s)} a_{jl} \right) \right\rangle && (2.92) \\ &= C_k C_l \left(e^{-\mathrm{i}\omega_{ik} t + \mathrm{i}\omega_{jl}(t-s)} \left\langle a_{ik} a_{jl}^\dagger \right\rangle + e^{-\mathrm{i}\omega_{ik} t - \mathrm{i}\omega_{jl}(t-s)} \langle a_{ik} a_{jl} \rangle \right. && (2.93) \\ &\quad \left. + e^{\mathrm{i}\omega_{ik} t + \mathrm{i}\omega_{jl}(t-s)} \left\langle a_{ik}^\dagger a_{jl}^\dagger \right\rangle + e^{\mathrm{i}\omega_{ik} t - \mathrm{i}\omega_{jl}(t-s)} \left\langle a_{ik}^\dagger a_{jl} \right\rangle \right). && (2.94) \end{aligned}$$

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

Thus the **spectral correlation tensor** is

$$\Gamma_{ij}(\omega) \equiv \sum_{kl}\int_0^\infty \mathrm{d}s\, e^{i\omega s}\left\langle B_{ik}^\dagger(t)B_{jl}(t-s)\right\rangle_{\rho_B} \tag{2.95}$$

$$= \delta_{ij}\sum_k \int_0^\infty \mathrm{d}s\, C_k^2\Big(e^{i(\omega-\omega_{ik})s}(n_B(\omega_{ik})+1) + e^{i(\omega+\omega_{ik})s}n_B(\omega_{ik})\Big) \tag{2.96}$$

$$= \delta_{ij}\sum_k C_k^2\left(\pi\delta(\omega_{ik}-\omega) - i\mathscr{P}\frac{1}{\omega_{ik}-\omega}\right)(n_B(\omega_{ik})+1) \tag{2.97}$$

$$+\left(\pi\delta(-\omega_{ik}-\omega) + i\mathscr{P}\frac{1}{\omega_{ik}+\omega}\right)n_B(\omega_{ik}) \tag{2.98}$$

$$\equiv \delta_{ij}\left(\frac{\gamma(\omega)}{2} + iS(\omega)\right), \tag{2.99}$$

where we have used that

$$\int_0^\infty \mathrm{d}s\, e^{-i\omega s} = \pi\delta(\omega) - i\mathscr{P}\frac{1}{\omega}, \tag{2.100}$$

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

$$\sum_k \mapsto \frac{L}{\pi}\int_0^\infty \mathrm{d}k = \frac{L}{\pi c}\int_0^\infty \mathrm{d}\omega \tag{2.101}$$

so that we have[3]

$$\gamma(\omega) = \frac{2L}{c}C(\omega)^2(n_B(\omega)+1) \tag{2.102}$$

and

$$S(\omega) = \mathscr{P}\int_0^\infty \mathrm{d}\omega_k\, \frac{L}{c}C(\omega_k)^2\left(\frac{n_B(\omega_{ik})+1}{\omega-\omega_{ik}} + \frac{n_B(\omega_{ik})}{\omega+\omega_{ik}}\right). \tag{2.103}$$

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

$$\gamma(0) = \lim_{\omega\to 0}\frac{2L}{c}C(\omega)^2(n_B(\omega)+1) \tag{2.104}$$

[2]We 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.

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

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

$$S(0) = \mathcal{P} \int_0^\infty \mathrm{d}\omega_k \, \frac{L}{c} C(\omega_k)^2 \left(\frac{n_B(\omega_{ik}) + 1}{-\omega_{ik}} + \frac{n_B(\omega_{ik})}{\omega_{ik}} \right) \tag{2.105}$$

$$= -\frac{L}{c} \mathcal{P} \int_0^\infty \mathrm{d}\omega_k \, \frac{C(\omega_k)^2}{\omega_k} \quad (\text{let } \omega_{ik} := \omega_k) \tag{2.106}$$

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**

$$J(\omega) \equiv \frac{2\alpha}{\pi} \int_0^\infty \mathrm{d}\omega_k \, C(\omega_k)^2 \delta(\omega - \omega_k) \tag{2.107}$$

$$= \frac{2\alpha}{\pi} C(\omega)^2 \tag{2.108}$$

be

$$J(\omega) = \frac{2\alpha}{\pi} \frac{\omega}{1 + (\omega/\Omega)^2}. \tag{2.109}$$

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

$$S(0) = -\frac{2\alpha}{\pi} \mathcal{P} \int_0^\infty \frac{\mathrm{d}\omega_k}{1 + (\omega_k/\Omega)^2} \tag{2.110}$$

$$= -\frac{\Omega}{\alpha}. \tag{2.111}$$

Thus the Lamb shift Hamiltonian

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

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

$$\gamma(0) = \lim_{\omega \to 0} \frac{4\alpha L}{\pi c} \frac{\omega}{1 + (\omega/\Omega)^2} (n_B(\omega) + 1) \tag{2.112}$$

$$= \frac{2L}{c} \frac{1}{\beta}, \tag{2.113}$$

so the dissipator is

$$\mathcal{D}\rho_S = \frac{4L}{\pi c}\frac{\alpha}{\beta}\sum_i (\sigma_{zi}\rho_S\sigma_{zi} - \rho_S). \tag{2.114}$$

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

$$\dot{\rho}_S(t) = \frac{\alpha}{\beta}\sum_i (\sigma_{zi}\rho_S(t)\sigma_{zi} - \rho_S(t)) \tag{2.115}$$

$$= \frac{\alpha}{\beta}\sum_i [\sigma_{zi}, \rho_S(t)]\sigma_{zi}. \tag{2.116}$$

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

$$\dot{\rho}_{00} = 0 \tag{2.117}$$

$$\dot{\rho}_{11} = 0 \tag{2.118}$$

$$\dot{\rho}_{01} = -\frac{2\alpha}{\beta}\rho_{01} \tag{2.119}$$

$$\dot{\rho}_{01} = -\frac{2\alpha}{\beta}\rho_{10}. \tag{2.120}$$

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

$$H = \sum_i h_i A_i, \tag{2.121}$$

we want to find eigenoperators

$$A = \sum_j a_j A_j, \tag{2.122}$$

of $H\angle$. If

$$\left[A_i, A_j\right] = \sum_k s_{ijk} A_k \tag{2.123}$$

$$s_{ijk} = \left\langle \left[A_i, A_j\right] \middle| A_k \right\rangle, \tag{2.124}$$

then the eigenvalue equation is

$$[H, A] = \omega A \tag{2.125}$$

$$\sum_{ijk} h_i a_j s_{ijk} A_k = \sum_j \omega a_j A_j \tag{2.126}$$

$$\sum_{jk} S_{jk} a_j A_k = \sum_j \omega a_j A_j, \tag{2.127}$$

where the matrix $\boldsymbol{S}$ has coefficients

$$S_{jk} = \sum_i h_i s_{ijk} = \left\langle A_j \middle| H\angle \middle| A_k \right\rangle. \tag{2.128}$$

Thus eigenoperators may be found by solving the ordinary eigenvalue problem

$$\boldsymbol{S}^{\mathsf{T}} \boldsymbol{a} = \omega \boldsymbol{a}. \tag{2.129}$$

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

$$H = -\sum_{i\in\mathbb{Z}_N} \sigma_i^x \sigma_{i+1}^x + \lambda \sum_{i\in\mathbb{Z}_N} \sigma_i^z \tag{3.1}$$

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

$$\sigma_i^{\pm} = \frac{\sigma_i^x \pm \mathrm{i}\sigma_i^y}{2} \tag{3.2}$$

satisfy

$$\sigma_i^z = 2\sigma_i^+\sigma_i^- - I \tag{3.3}$$

and have commutators

$$\begin{aligned}
\left[\sigma_i^+, \sigma_j^-\right] &= \frac{1}{4}\left[\sigma_i^x + \mathrm{i}\sigma_i^y, \sigma_j^x - \mathrm{i}\sigma_j^y\right] && (3.4)\\
&= \frac{1}{4}\left(\left[\sigma_i^x, \sigma_j^x\right] + \left[\sigma_i^y, \sigma_j^y\right] + \mathrm{i}\left[\sigma_i^y, \sigma_j^x\right] - \mathrm{i}\left[\sigma_i^x, \sigma_j^y\right]\right) && (3.5)\\
&= \delta_{ij}\sigma_i^z. && (3.6)
\end{aligned}$$

Thus their anticommutators are

$$\begin{aligned}
\left\{\sigma_i^+, \sigma_j^-\right\} &= 2\sigma_i^+\sigma_j^- - \left[\sigma_i^+, \sigma_j^-\right] && (3.7)\\
&= 2\sigma_i^+\sigma_j^- - \delta_{ij}\sigma_i^z && (3.8)\\
&= \delta_{ij} I + 2\sigma_i^+\sigma_j^-(1-\delta_{ij}). && (3.9)
\end{aligned}$$

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

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

$$|\boldsymbol{n}\rangle = \prod_{i\in\mathbb{Z}_N} \left(c_i^\dagger\right)^{n_i} |\boldsymbol{0}\rangle, \tag{3.10}$$

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

$$\begin{aligned}
c_i |\boldsymbol{n}\rangle &= -n_i(-1)^{n_{<i}} |\boldsymbol{n}_{i\leftarrow 0}\rangle && (3.11)\\
c_i^\dagger |\boldsymbol{n}\rangle &= -(1-n_i)(-1)^{n_{<i}} |\boldsymbol{n}_{i\leftarrow 1}\rangle, && (3.12)
\end{aligned}$$

where

$$\begin{aligned}
\boldsymbol{n}_{i\leftarrow m} &= \boldsymbol{n} \quad \text{with} \quad n_i = m && (3.13)\\
n_{<i} &= \sum_{j<i} n_j. && (3.14)
\end{aligned}$$

Then consider

$$c_i = -\left(\prod_{j<i}\sigma_j^z\right)\sigma_j^- \tag{3.15}$$

acting on the states

$$|\boldsymbol{n}\rangle = \prod_{i\in\mathbb{Z}_N} \left(\sigma_i^+\right)^{n_i} |\boldsymbol{0}\rangle, \tag{3.16}$$

where $|\boldsymbol{0}\rangle = |{\uparrow}\rangle^{\otimes N}$ is the state with all z-spins up, or all zero qubits.

Double-check up/down and make so that 1 bit is 1 occupied. I get the z-eigenstate conventions confused.

This gives the same result as eq. (3.11), so the c_i satisfy the CARs. This change from spin-1/2 sites to (non-local) fermions is known as the **Jordan-Wigner transformation**. We may then compute that the inverse transformations are

$$\sigma_i^+\sigma_i^- = c_i^\dagger c_i \tag{3.17}$$

$$\sigma_i^z = 2c_i^\dagger c_i - I \tag{3.18}$$

$$\sigma_i^x = -\left(\prod_{j<i}\left(2c_j^\dagger c_j - I\right)\right)\left(c_i^\dagger + c_i\right) \tag{3.19}$$

$$\sigma_i^y = \mathrm{i}\left(\prod_{j<i}\left(2c_j^\dagger c_j - I\right)\right)\left(c_i^\dagger - c_i\right). \tag{3.20}$$

While σ_i^x remains complicated, the product $\sigma_i^x\sigma_{i+1}^x$ does not:

$$\sigma_i^x\sigma_{i+1}^x = \left(\prod_{j<i}\left(2c_j^\dagger c_j - I\right)\right)\left(c_i^\dagger + c_i\right)\left(\prod_{j<i+1}\left(2c_j^\dagger c_j - I\right)\right)\left(c_{i+1}^\dagger + c_{i+1}\right) \tag{3.21}$$

$$= \left(c_i^\dagger + c_i\right)\left(I - 2c_i^\dagger c_i\right)\left(c_{i+1}^\dagger + c_{i+1}\right) \tag{3.22}$$

$$= \left(c_i^\dagger - c_i\right)\left(c_{i+1}^\dagger + c_{i+1}\right). \tag{3.23}$$

We may now perform the Jordan-Wigner transformation of eq. (3.1) to obtain

Where is the boundary term in Pfeuty (2.4)? I think it is gone since I have defined the c_i for $i \in \mathbb{Z}_N$, so that c_N is automatically correct and you do not need to add a correction term due to applying the Jordan-Wigner transform with $i = N \in \mathbb{Z}$?

$$H = \sum_i \left(c_i - c_i^\dagger\right)\left(c_{i+1}^\dagger + c_{i+1}\right) + \lambda\sum_i 2c_i^\dagger c_i - \lambda N I. \tag{3.24}$$

We now Fourier transform with

$$c_i = \frac{1}{\sqrt{N}}\sum_k e^{\mathrm{i}ki}C_k \tag{3.25}$$

and

$$c_i^\dagger = \frac{1}{\sqrt{N}}\sum_k e^{-\mathrm{i}ki}C_k^\dagger, \tag{3.26}$$

where

$$k = \frac{2\pi n}{N} - \frac{N-1}{N}\pi, \quad n \in \mathbb{Z}_N. \tag{3.27}$$

(I like this choice of k since it is parity-symmetric. Inverting k gives a different C_k except at zero if N is odd, unlike the usual convention for Brillouin zones where the C_k at the boundary must be identified. The drawback is that even N has no $k = 0$.)

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

$$C_k^\dagger = \sum_i U_{ik} c_i^\dagger. \tag{3.28}$$

Then

$$\begin{aligned} \left\{C_k, C_{k'}^\dagger\right\} &= \sum_{ij} U_{ik}^* U_{jk'} \left\{c_i, c_j^\dagger\right\} &(3.29)\\ &= \sum_i U_{ik}^* U_{ik'} &(3.30)\\ &= \left(\boldsymbol{U}^\dagger \boldsymbol{U}\right)_{kk'} &(3.31)\\ &= \delta_{kk'}, &(3.32) \end{aligned}$$

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

Proof. For the Fourier transform,

$$F_{ik} = \frac{1}{\sqrt{N}} e^{\mathrm{i}ki}. \tag{3.33}$$

We may then confirm that

$$\begin{aligned} \left(\boldsymbol{F}^\dagger \boldsymbol{F}\right)_{kk'} &= \sum_i \frac{1}{N} e^{\mathrm{i}(k'-k)i} &(3.34)\\ &= \delta_{kk'}. &(3.35) \end{aligned}$$

Thus the Fourier transform is unitary. □

Now since

$$\frac{1}{N} \sum_{i \in \mathbb{Z}_N} e^{\mathrm{i}(k'-k)i} = \delta_{kk'}, \tag{3.36}$$

and also

$$C_{-k} = C_k^* \tag{3.37}$$

$$= \frac{1}{\sqrt{N}} \sum_i e^{-\mathrm{i}(-k)i} c_i \tag{3.38}$$

$$= \frac{1}{N} \sum_{ik'} e^{\mathrm{i}(k'+k)i} C_{k'}, \tag{3.39}$$

we have that

$$\sum_i c_i^\dagger c_i = \frac{1}{N} \sum_{ikk'} e^{\mathrm{i}(k'-k)i} C_k^\dagger C_{k'} \tag{3.40}$$

$$= \sum_k C_k^\dagger C_k, \tag{3.41}$$

$$\sum_i \left(c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i\right) = \frac{1}{N} \sum_{ikk'} e^{\mathrm{i}(k'-k)i} \left(e^{\mathrm{i}k'} + e^{-\mathrm{i}k}\right) C_k^\dagger C_{k'} \tag{3.42}$$

$$= \sum_k 2\cos k\, C_k^\dagger C_k, \tag{3.43}$$

$$\sum_i \left(c_{i+1} c_i + c_i^\dagger c_{i+1}^\dagger\right) = \frac{1}{N} \sum_{ikk'} \left(e^{\mathrm{i}(k'+k)i} e^{\mathrm{i}k} C_k C_{k'} + e^{-\mathrm{i}(k'+k)i} e^{-\mathrm{i}k'} C_k^\dagger C_{k'}^\dagger\right) \tag{3.44}$$

$$= \sum_k \left(e^{-\mathrm{i}k} C_{-k} C_k + e^{\mathrm{i}k} C_k^\dagger C_{-k}^\dagger\right). \tag{3.45}$$

Thus eq. (3.24) is now

$$H = -\sum_k 2\cos k\, C_k^\dagger C_k + \sum_k \left(e^{-\mathrm{i}k} C_{-k} C_k + e^{\mathrm{i}k} C_k^\dagger C_{-k}^\dagger\right) + \sum_k 2\lambda C_k^\dagger C_k - \lambda N I \tag{3.46}$$

$$= \sum_k (\lambda - \cos k)\left(C_k^\dagger C_k + C_{-k}^\dagger C_{-k}\right) + \sum_k \mathrm{i} \sin k \left(C_{-k} C_k - C_k^\dagger C_{-k}^\dagger\right) - \lambda N I \tag{3.47}$$

$$= \sum_k (\lambda - \cos k)\left(C_k^\dagger C_k - C_{-k} C_{-k}^\dagger\right) + \sum_k \mathrm{i} \sin k \left(C_{-k} C_k - C_k^\dagger C_{-k}^\dagger\right) - I \sum_k \cos k \tag{3.48}$$

$$= \sum_k \boldsymbol{v}_k^\dagger \boldsymbol{H}_k \boldsymbol{v}_k - I \sum_k \cos k, \tag{3.49}$$

where

$$\boldsymbol{H}_k = \begin{bmatrix} \lambda - \cos k & -\mathrm{i} \sin k \\ \mathrm{i} \sin k & \cos k - \lambda \end{bmatrix} \tag{3.50}$$

and

$$\boldsymbol{v}_k = \begin{bmatrix} C_k \\ C_{-k}^\dagger \end{bmatrix}. \tag{3.51}$$

Instead of halving the sums by using parity symmetry, we can use weighting functions of k:

$$\sum_k C_k^\dagger C_k = \sum_k \left(\alpha_k C_k^\dagger C_k + \beta_k C_{-k}^\dagger C_{-k}\right) \tag{3.52}$$
$$= \sum_k \left(\alpha_k C_k^\dagger C_k - \beta_k C_{-k} C_{-k}^\dagger\right) + I \sum_k \beta_k, \tag{3.53}$$

where $\alpha_k + \beta_{-k} = 1$.
Can this be used to make $\boldsymbol{H}_k$ singular, or otherwise help so that we ultimately have one term like $\eta^\dagger \eta$?

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

$$E_k^\pm = \pm\sqrt{-\det \boldsymbol{H}_k} \tag{3.54}$$
$$= \pm\sqrt{\lambda^2 - 2\lambda\cos k + \cos^2 k + \sin^2 k} \tag{3.55}$$
$$= \pm\sqrt{\lambda^2 - 2\lambda\cos k + 1}. \tag{3.56}$$

The eigenvectors are then

$$\boldsymbol{q}_k^\pm = \begin{bmatrix} -\mathrm{i}\sin k \\ E_k^\pm - (\lambda - \cos k) \end{bmatrix}, \tag{3.57}$$

except if $k = 0$, in which case

$$\boldsymbol{H}_k = \begin{bmatrix} \lambda - 1 & 0 \\ 0 & 1 - \lambda, \end{bmatrix} \tag{3.58}$$
$$\boldsymbol{q}_0^+ = \begin{bmatrix} 1 \\ 0 \end{bmatrix}, \quad \text{and} \quad \boldsymbol{q}_0^- = \begin{bmatrix} 0 \\ 1 \end{bmatrix}. \tag{3.59}$$

To disregard this, we consider N even going forward. To construct the unitary transformation, we must normalize the $\boldsymbol{q}_k^\pm$. We find that

$$\left\|\boldsymbol{q}_k^\pm\right\|^2 = \left(E_k^\pm - (\lambda - \cos k)\right)^2 + \sin^2 k \tag{3.60}$$
$$= \left(E_k^\pm\right)^2 + \lambda^2 + \cos^2 k - 2\lambda\cos k - 2E_k^\pm(\lambda - \cos k) + 1 - \cos^2 k \tag{3.61}$$
$$= 2E_k^\pm\left(E_k^\pm - (\lambda - \cos k)\right). \tag{3.62}$$

Now

$$\frac{(\boldsymbol{q}_k^{\pm})_1}{\|\boldsymbol{q}_k^{\pm}\|} = \frac{-\mathrm{i}\sin k}{\sqrt{2E_k^{\pm}\left(E_k^{\pm} - (\lambda - \cos k)\right)}} \tag{3.63}$$

$$= \frac{-\mathrm{i}\sin k}{\sqrt{2\left|E_k^{\pm}\right|\left(\left|E_k^{\pm}\right| \mp (\lambda - \cos k)\right)}} \tag{3.64}$$

and

$$\frac{(\boldsymbol{q}_k^{\pm})_2}{\|\boldsymbol{q}_k^{\pm}\|} = \sqrt{\frac{E_k^{\pm} - (\lambda - \cos k)}{2E_k^{\pm}}} \tag{3.65}$$

$$= \sqrt{\frac{\left|E_k^{\pm}\right| \mp (\lambda - \cos k)}{2\left|E_k^{\pm}\right|}} \tag{3.66}$$

$$\boldsymbol{U}_k^{\dagger} = \begin{bmatrix} \left(\hat{\boldsymbol{q}}_k^{+}\right)^{\dagger} \\ \left(\hat{\boldsymbol{q}}_k^{-}\right)^{\dagger} \end{bmatrix}. \tag{3.67}$$

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

$$\eta_k^{\pm} = \frac{\mathrm{i}\sin k}{\sqrt{2E_k(E_k \mp (\lambda - \cos k))}} C_k + \sqrt{\frac{E_k \mp (\lambda - \cos k)}{2E_k}} C_{-k}^{\dagger}, \tag{3.68}$$

so that

$$E_k^{\pm}\left(\eta_k^{\pm}\right)^{\dagger}\eta_k^{\pm} = E_k^{\pm}\left(\frac{-\mathrm{i}\sin k}{\sqrt{2E_k(E_k \pm (\cos k - \lambda))}} C_k^{\dagger} + \sqrt{\frac{E_k \pm (\cos k - \lambda)}{2E_k}} C_{-k}\right) \tag{3.69}$$

$$\left(\frac{\mathrm{i}\sin k}{\sqrt{2E_k(E_k \pm (\cos k - \lambda))}} C_k + \sqrt{\frac{E_k \pm (\cos k - \lambda)}{2E_k}} C_{-k}^{\dagger}\right) \tag{3.70}$$

$$= \frac{\sin^2 k}{2\left(E_k^{\pm} + (\cos k - \lambda)\right)} C_k^{\dagger} C_k + \frac{E_k^{\pm} + (\cos k - \lambda)}{2} C_{-k} C_{-k}^{\dagger} \tag{3.71}$$

$$- \frac{\mathrm{i}\sin k}{2} C_k^{\dagger} C_{-k}^{\dagger} + \frac{\mathrm{i}\sin k}{2} C_{-k} C_k. \tag{3.72}$$

and

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

$$= E_k^{\pm} I \tag{3.74}$$

$$E_k^{\pm}\left\{\left(\eta_k^{\pm}\right)^{\dagger}, \eta_k^{\mp}\right\} = \frac{\sin^2 k}{2\sqrt{E_k \pm (\cos k - \lambda)}\sqrt{E_k \mp (\cos k - \lambda)}} + \frac{\sqrt{E_k \pm (\cos k - \lambda)}\sqrt{E_k \mp (\cos k - \lambda)}}{2} \tag{3.75}$$

$$= |\sin k| I \tag{3.76}$$

Thus eq. (3.49) becomes

$$H = \sum_k E_k^{+}\left(\eta_k^{+}\right)^{\dagger}\eta_k^{+} + \sum_k E_k^{-}\left(\eta_k^{-}\right)^{\dagger}\eta_k^{-} - I\sum_k \cos k. \tag{3.77}$$

While the $\eta_k^{\pm}$ are individually fermionic, they are not compatible with each other.

3.2 Eigenoperators for the transverse Ising Hamiltonian

Pfeuty defines:

$$\lambda = \frac{J}{2\Gamma} \tag{3.78}$$

$$a_i = S_{xi} - \mathrm{i}S_{yi} \tag{3.79}$$

$$a_i^{\dagger} = S_{xi} + \mathrm{i}S_{yi} \tag{3.80}$$

$$c_i = \exp\left(\pi\mathrm{i}\sum_{j=1}^{i-1} a_j^{\dagger} a_j\right) a_i \tag{3.81}$$

$$c_i^{\dagger} = a_i^{\dagger}\exp\left(-\pi\mathrm{i}\sum_{j=1}^{i-1} a_j^{\dagger} a_j\right) \tag{3.82}$$

$$\eta_k = \sum_i \left(\frac{\varphi_{ki} + \psi_{ki}}{2} c_i + \frac{\varphi_{ki} - \psi_{ki}}{2} c_i^{\dagger}\right) \tag{3.83}$$

$$\varphi_{ki} = \sqrt{\frac{2}{N}}\begin{cases}\sin(ki) & k > 0\\ \cos(ki) & k \leq 0\end{cases} \tag{3.84}$$

$$\psi_{ki} = -\Lambda_k^{-1}((1 + \lambda\cos k)\varphi_{ki} + (\lambda\sin k)\varphi_{-ki}) \tag{3.85}$$

$$\Lambda_k^2 = 1 + \lambda^2 + 2\lambda\cos k \tag{3.86}$$

$$k = \frac{2\pi m}{N} \quad \text{for} \quad m = -\frac{N}{2}, \ldots, \frac{N}{2} - 1, \quad N \text{ even}. \tag{3.87}$$

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

$$H = \Gamma \sum_k \Lambda_k \eta_k^\dagger \eta_k - \frac{\Gamma}{2} \sum_k \Lambda_k. \tag{3.88}$$

We see that I, η_k, $\eta_k^\dagger$, and $\eta_k^\dagger \eta_k$ are all eigenoperators of H. Since these operators form an orthonormal complete basis for the Liouville space, we then seek out the coefficients $\langle S_{xi} | \eta_k \rangle$.

I don't think this is true! (I.e. the η_k do not satisfy the fermionic CARs.) All the inner products below are pointless.

$$\psi_{ki}^2 = -\Lambda_k^{-2}\Big((1 + \lambda \cos k)^2 \varphi_{ki}^2 + (1 + \lambda \cos k)(\lambda \sin k) \varphi_{ki} \varphi_{-ki} + \lambda^2 \sin^2 k \varphi_{-ki}^2 \Big) \tag{3.89}$$

$$= -\Lambda_k^{-2}\Big((1 + 2\lambda \cos k + \lambda^2 \cos^2 k) \varphi_{ki}^2 + (1 + \lambda \cos k)(\lambda \sin k) \varphi_{ki} \varphi_{-ki} + \lambda^2 \sin^2 k \varphi_{-ki}^2 \Big) \tag{3.90}$$

For $k > 0$:

$$\psi_{ki}^2 = -\frac{2}{N} \sin^2(ki) + \frac{2}{N} \Lambda_k^{-2}\Big((1 + \lambda \cos k)(\lambda \sin k) \sin^2(ki) - \lambda^2 \sin^2 k \sin^2(ki) \Big) \tag{3.91}$$

$$= -\frac{2}{N} \sin^2(ki) + \frac{2}{N} \Lambda_k^{-2}\Big((\Lambda_k^2 - \lambda \cos k - \lambda^2 + \lambda^2 \sin^2 k)(\lambda \sin k) \sin^2(ki) - \lambda^2 \sin^2 k \sin^2(ki) \Big) \tag{3.92}$$

$$= -\frac{2}{N} \sin^2(ki) + \frac{2}{N} \Lambda_k^{-2}\Big((\Lambda_k^2 - \lambda \cos k - \lambda^2)(\lambda \sin k) \sin^2(ki) + (\lambda \sin k - 1)\lambda^2 \sin^2 k \sin^2(ki) \Big) \tag{3.93}$$

$$\tag{3.94}$$

For $k \leq 0$:

$$\psi_{ki}^2 = -\frac{2}{N} \cos^2(ki) - \frac{2}{N} \Lambda_k^{-2}\Big((1 + \lambda \cos k)(\lambda \sin k) \cos^2(ki) + \lambda^2 \sin^2 k \cos^2(ki) \Big) \tag{3.95}$$

$$\begin{aligned} \left\{ \eta_k, \eta_k^\dagger \right\} = &\sum_{ij} \frac{\varphi_{ki} + \psi_{ki}}{2} \frac{\varphi_{kj} + \psi_{kj}}{2} \left\{ c_i, c_j \right\} + \sum_{ij} \frac{\varphi_{ki} + \psi_{ki}}{2} \frac{\varphi_{kj} - \psi_{kj}}{2} \left\{ c_i, c_j^\dagger \right\} \\ &+ \sum_{ij} \frac{\varphi_{ki} - \psi_{ki}}{2} \frac{\varphi_{kj} + \psi_{kj}}{2} \left\{ c_i^\dagger, c_j \right\} + \sum_{ij} \frac{\varphi_{ki} - \psi_{ki}}{2} \frac{\varphi_{kj} - \psi_{kj}}{2} \left\{ c_i^\dagger, c_j^\dagger \right\} \end{aligned} \tag{3.96}$$

$$= \frac{I}{2} \sum_i (\varphi_{ki} + \psi_{ki})(\varphi_{ki} - \psi_{ki}) \tag{3.97}$$

$$= \frac{I}{2} \sum_i (\varphi_{ki}^2 - \psi_{ki}^2) \tag{3.98}$$

$$= I? \tag{3.99}$$

According to Mathematica, not in general.

$$\begin{aligned} \left\langle \eta_k \middle| \eta_k^\dagger \right\rangle = \sum_{ij} \frac{\varphi_{ki} + \psi_{ki}}{2} \frac{\varphi_{kj} + \psi_{kj}}{2} \langle c_i | c_j \rangle + \sum_{ij} \frac{\varphi_{ki} + \psi_{ki}}{2} \frac{\varphi_{kj} - \psi_{kj}}{2} \left\langle c_i \middle| c_j^\dagger \right\rangle \\ + \sum_{ij} \frac{\varphi_{ki} - \psi_{ki}}{2} \frac{\varphi_{kj} + \psi_{kj}}{2} \left\langle c_i^\dagger \middle| c_j \right\rangle + \sum_{ij} \frac{\varphi_{ki} - \psi_{ki}}{2} \frac{\varphi_{kj} - \psi_{kj}}{2} \left\langle c_i^\dagger \middle| c_j^\dagger \right\rangle \end{aligned} \tag{3.100}$$

$$= \sum_i \left(\frac{\varphi_{ki} + \psi_{ki}}{2} \frac{\varphi_{ki} + \psi_{ki}}{2} + \frac{\varphi_{ki} - \psi_{ki}}{2} \frac{\varphi_{ki} - \psi_{ki}}{2} \right) \tag{3.101}$$

$$= \frac{1}{2} \sum_i (\varphi_{ki}^2 + \psi_{ki}^2) \tag{3.102}$$

Note that the $a_j^\dagger a_j$ commute for different j, so

$$c_i = -\left(\prod_{j=1}^{i-1} \exp\left(a_j^\dagger a_j\right) \right) a_i \tag{3.103}$$

$$= -\left(\bigotimes_{j=1}^{i-1} \exp\left(a_j^\dagger a_j\right) \right) a_i \tag{3.104}$$

$$\tag{3.105}$$

Since $\operatorname{tr}(A \otimes B) = \operatorname{tr} A \operatorname{tr} B$,

$$\langle S_{xi} | c_i \rangle = -\left\langle S_{xi} \middle| \left(\bigotimes_{j=1}^{i-1} \exp\left(a_j^\dagger a_j\right) \right) a_i \right\rangle \tag{3.106}$$

$$= -\prod_{j=1}^{i-1} \left\langle S_{xi} a_i^\dagger \middle| \exp\left(a_j^\dagger a_j\right) \right\rangle \tag{3.107}$$

$$= -\prod_{j=1}^{i-1} \left\langle S_{xi} a_i^\dagger \middle| I - 2a_j^\dagger a_j \right\rangle \tag{3.108}$$

$$= -\prod_{j=1}^{i-1} \left\langle S_{xi} a_i^\dagger \middle| I - 2a_j^\dagger a_j \right\rangle \tag{3.109}$$

$$= -\prod_{j=1}^{i-1} \left(\langle S_{xi} | a_i \rangle + 2 \left\langle S_{xi} \middle| a_j^\dagger a_j a_i \right\rangle \right) \tag{3.110}$$

$$\tag{3.111}$$

OR (note that sign of iπ in eq. (3.81) is different in Leeds, but this makes no difference)

$$\left\langle S_{xi} \middle| c_j \right\rangle = \left\langle a_i + a_i^\dagger \middle| \exp\left(\pi \mathrm{i} \sum_{k=1}^{i-1} a_k^\dagger a_k \right) a_j \right\rangle \tag{3.112}$$

$$= \left\langle \left(a_i + a_i^\dagger \right) a_j^\dagger \middle| \bigotimes_{k=1}^{i-1} \left(I_2 - 2a_k^\dagger a_k \right) \right\rangle \tag{3.113}$$

$$= \delta_{ij} \left\langle a_i a_i^\dagger \middle| \bigotimes_{k=1}^{i-1} \left(I_2 - 2a_k^\dagger a_k \right) \right\rangle \tag{3.114}$$

$$= \delta_{ij} \tag{3.115}$$

$$\left\langle S_{xi} \middle| c_j^\dagger \right\rangle = \delta_{ij} \tag{3.116}$$

$$\left\langle S_{xi} \middle| c_j^\dagger c_k \right\rangle = \left\langle a_i + a_i^\dagger \middle| a_j^\dagger a_k \right\rangle \tag{3.117}$$

$$= (\delta_{ij} + \delta_{jk} + \delta_{ki})(1 - \delta_{ij}\delta_{jk}) \tag{3.118}$$

$$\left\langle S_{xi} \middle| c_j c_k^\dagger \right\rangle = (\delta_{ij} + \delta_{jk} + \delta_{ki})(1 - \delta_{ij}\delta_{jk}). \tag{3.119}$$

Thus

$$\langle S_{xi} | \eta_k \rangle = \frac{\varphi_{ki} + \psi_{ki}}{2} + \frac{\varphi_{ki} - \psi_{ki}}{2} \tag{3.120}$$

$$= \varphi_{ki} \tag{3.121}$$

$$\left\langle S_{xi} \middle| \eta_k^\dagger \right\rangle = \varphi_{ki} \tag{3.122}$$

$$\left\langle S_{xi} \middle| \eta_k^\dagger \eta_k \right\rangle = \sum_{ab} \left(\frac{\varphi_{ka} + \psi_{ka}}{2} c_a^\dagger + \frac{\varphi_{ka} - \psi_{ka}}{2} c_a \right) \left(\frac{\varphi_{kb} + \psi_{kb}}{2} c_b + \frac{\varphi_{kb} - \psi_{kb}}{2} c_b^\dagger \right) \tag{3.123}$$

$$= \sum_{ab} \left(\frac{\varphi_{ka} + \psi_{ka}}{2} \frac{\varphi_{kb} + \psi_{kb}}{2} + \frac{\varphi_{ka} - \psi_{ka}}{2} \frac{\varphi_{kb} - \psi_{kb}}{2} \right) (\delta_{ab} + \delta_{bi} + \delta_{ia})(1 - \delta_{ab}\delta_{bi}) \tag{3.124}$$

$$= \sum_{a} \left(\left(\frac{\varphi_{ka} + \psi_{ka}}{2} \right)^2 + \left(\frac{\varphi_{ka} - \psi_{ka}}{2} \right)^2 \right) (1 - \delta_{ia}) \tag{3.125}$$

$$+ 2\sum_a \left(\frac{\varphi_{ka} + \psi_{ka}}{2}\frac{\varphi_{ki} + \psi_{ki}}{2} + \frac{\varphi_{ka} - \psi_{ka}}{2}\frac{\varphi_{ki} - \psi_{ki}}{2}\right)(1 - \delta_{ia}) \tag{3.126}$$

$$\tag{3.127}$$

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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