Steepest-Entropy-Ascent Quantum Thermodynamic Modeling of Quantum Information and Quantum Computing Systems

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(ABSTRACT)

Quantum information and quantum computing (QIQC) systems offer the potential for vast improvements in certain computations. A practical QC realization requires maintaining the stored information for time-scales long enough to implement algorithms. One primary cause of information loss is decoherence, i.e., the loss of coherence between two energy levels in a quantum system. This work attributes decoherence to dissipation and uses steepest-entropy-ascent quantum thermodynamics (SEAQT) to predict the evolution of system state. SEAQT asserts that, at any instant of time, the system state evolves such that the rate of system entropy change is maximized while conserving system energy. With this principle, SEAQT is applicable to systems in any state, near or far from stable equilibrium, making it particularly well suited for predicting the dissipation occurring as quantum algorithms are implemented. In the present research, the dynamics of qubits (quantum-bits) are first examined during common quantum gates. This is then extended to modeling a nuclear-magnetic-resonance (NMR) QC implementing Shor’s algorithm. Additionally, SEAQT is used to predict experimentally observed dissipation occurring in a two-qubit NMR QC. Further, a density operator perturbation method incorporating sets of any expectation value constraints is presented, which is then used as the basis for randomly generating states used in analyzing the dynamics of entangled, non-interacting systems within SEAQT. Finally, a reservoir interaction model and decoherence control scheme are developed for general quantum systems where each system locally experiences a heat interaction with an external reservoir. This control scheme is employed in modeling an NMR QC and shown to eliminate nearly all of the noise caused by dissipation.
Quantum computers (QCs) have the potential to perform certain tasks much more efficiently than today’s supercomputers. One primary challenge in realizing a practical QC is maintaining the stored information, the loss of which is known as decoherence. This work attributes decoherence to dissipation (a classical analogue being heat generated due to friction) occurring while an algorithm is run on the QC. Standard quantum modeling approaches assume that for any dissipation to occur, the QC must interact with its environment. However, in this work, steepest-entropy-ascent quantum thermodynamics (SEAQT) is used to model the evolution of the QC as it runs an algorithm. SEAQT, developed by Hatsopolous, Gyftopolous, Beretta, and others over the past 40 years, supplements the laws of quantum mechanics with those of thermodynamics and in contrast to the standard quantum approaches does not require the presence of an environment to account for the dissipation which occurs. This work first applies the SEAQT framework to modeling single qubits (quantum bits) to characterize the effect of dissipation on the information stored on the qubit. This is later extended to a nuclear-magnetic-resonance (NMR) QC of 7 qubits. Additionally, SEAQT is used to predict experimentally observed dissipation in a two-qubit NMR QC. Afterwards, several methods for constrained perturbations of a QC’s state are presented. These methods are then used with SEAQT to analyze the effect of dissipation on the entanglement of two qubits. Finally, a model is derived within the SEAQT framework accounting for a qubit interacting with its environment, which is at a constant temperature. This model is then used to develop a method for limiting the decoherence and shown to significantly lowering the resulting error due to decoherence.
Dedication

This work is dedicated to all of my friends and family who have helped me reach this point. I share this accomplishment with all of you. Mom and Dad, thank you for your constant love and support. Without the values you instilled in me none of this would have been possible.

To my grandparents, thank you for all of your love, encouragement, and support throughout my academic career. I would also like to thank the middle and high-school teachers whose encouragement and guidance first helped develop my curiosity and passion for math and science. Thank you to all my friends for your support and always being available anytime I need to relieve stress. And finally to my wife, without your influence in my life I would not be where I am today. You’ve kept me grounded and focused as I’ve finished school and have helped me through challenging times. Thank you for all the compromises and sacrifices you’ve made so that I could finish and for all your love and support.
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Contents

List of Figures xiv

List of Tables xxiii

1 Introduction 1

1.1 Background: Quantum Information and Computing and Steepest-Entropy-Ascent Quantum Thermodynamics 1

1.1.1 QIQC Introduction 2

1.1.2 SEAQT Background 6

1.2 Motivation, Goals, and Work to be Completed 8

1.3 Original Contributions 10

1.4 Dissertation Outline 12

2 Model Dynamics for Single Qubit Gates and Heat Interactions for Simple Quantum Systems 16

2.1 Introduction 16

2.1.1 Preliminary Review of Quantum Computing 18

2.2 Model Development 23

2.2.1 Hamiltonian Evolution and Quantum Gate Implementation 23
2.2.2 An Equation of Motion Consisting of Multiple Dissipative Models . . 27
2.2.3 SEAQT Equation of Motion for a Simple System Interacting with a Reservoir . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 29
2.3 Model Results . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 36
2.3.1 Free Evolution . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 37
2.3.2 Free Evolution and Not Gate . . . . . . . . . . . . . . . . . . . . . . . 39
2.3.3 Free Evolution under Reservoir Interactions . . . . . . . . . . . . . . 42
2.4 Conclusions . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 45

Appendix A Additional Unitary Evolutions 49
A.1 Hadamard Gate and Free Evolution about the Z-Axis . . . . . . . . . . . 49
A.2 Hadamard Gate and Free Evolution about the X-Axis . . . . . . . . . . . 50
A.3 Hadamard-Not-Hadamard Gate Pulse Sequence . . . . . . . . . . . . . . 51

3 Modeling the Entropy Generation and the Effects of a varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System 53
3.1 Introduction . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 53
3.2 Model Development . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 56
3.2.1 SEAQT Equation of Motion in a Rotating Reference Frame . . . . . . . 56
3.2.2 Hamiltonian Development . . . . . . . . . . . . . . . . . . . . . . . . . . 60
3.2.3 Transition Probability Based Relaxation Time . . . . . . . . . . . . . . 65
3.3 Results ............................................................................. 66

3.3.1 Generation of the Initial State from a Set of Pseudo-Pure States ... 67

3.3.2 von-Neumann-Experimental Data Comparison ......................... 69

3.3.3 SEAQT $\tau_{D,H(C)} = \tau_{Matthiessen,H(C)}$ - Experimental Data Comparison . 72

3.3.4 SEAQT $\tau_D = \tau_{Matthiessen}/100$-Experimental Data Comparison .... 74

3.4 Discussion and Conclusion .................................................. 76

Appendix B Rotating Reference Frame Derivation Details .................. 80

4 A Method for Generating Random Perturbed Density Operators Subject to an Arbitrary Set of Constraints 83

4.1 Introduction .................................................................. 83

4.2 Model Development ...................................................... 85

4.2.1 General Perturbation Approach and “Closeness” of Quantum States . 85

4.2.2 Example Constant Energy and Entropy Perturbations .................. 88

4.2.3 Review of State Distance and Entanglement Measures ................ 89

4.3 Results ........................................................................ 91

4.3.1 Perturbations with No Constraints ................................... 92

4.3.2 Perturbations under the Constant Energy Constraint ................. 94

4.3.3 Perturbations under Constant Entropy Constraint ..................... 96

4.3.4 Perturbations under Constant Energy and Entropy Constraints ... 99
5 Modeling the Effects of Perturbations and Steepest-Entropy-Ascent on the Time Evolution of Entanglement

5.1 Introduction ...................................................... 103

5.2 Model Development .............................................. 105

5.2.1 Entanglement Measures ..................................... 106

5.2.2 SEAQT Equation of Motion for a General Quantum System and Stationary States ........................................ 108

5.2.3 Perturbation Approaches .................................... 114

5.3 Results ............................................................. 118

5.3.1 Entanglement Evolution using Weighted-Average Perturbations . . . 120

5.3.2 Entanglement Evolution using the General Bipartite Constant Energy Constrained Perturbations with $\epsilon = 10^{-1}$ ........................................ 123

5.3.3 Entanglement Evolution using the General Bipartite Constant Energy and Entropy Constrained Perturbations with $\epsilon = 10^{-1}$ ............... 126

5.3.4 Entanglement Evolution using the General Bipartite Constant Energy and Entropy Constrained Perturbations with $\epsilon = 10^{-2}$ ............... 130

5.4 Conclusions ...................................................... 135

6 Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer ...................................................... 137
6.1 Introduction ................................................................. 137
6.2 Model Development ..................................................... 139
   6.2.1 NMR Hamiltonian and Shor Algorithm Development ........ 139
   6.2.2 SEAQT Equation of Motion for a General Quantum System ...... 151
   6.2.3 SEAQT Equation of Motion for a General Quantum System Interacting with One or More Reservoirs ......................... 154
   6.2.4 Reservoir Heat Interaction Based Decoherence Control Scheme .. 163
6.3 Results ........................................................................... 166
   6.3.1 Thermal Equilibrium Spectra ........................................ 167
   6.3.2 Ground State Spectra ................................................ 169
   6.3.3 End State Spectra ..................................................... 172
   6.3.4 Reservoir Energy and Entropy Transfer Analysis .............. 175
6.4 Conclusions ................................................................. 181

Appendix C Composite System Reservoir Interaction Dissipation Operator
   Evaluation ................................................................. 184
   C.1 Dissipation Operator .................................................... 184
      C.1.1 $J^{th}$ Subsystem Dissipation Operator ......................... 185
   C.2 Dissipation Operator Simplification .................................. 189
      C.2.1 Evaluation of the Gram Determinant ............................ 190
      C.2.2 Evaluation of $\Gamma^J$ .............................................. 190
C.2.3 Definitions of $B^I_1$ and $B^I_2$ ........................................ 191
C.2.4 Evaluation of $B^I_3$ .................................................. 191
C.2.5 Evaluation of $B^I_3 / \Gamma^J$ ......................................... 191

Appendix D Evaluation of Perceived Quantities for the Generators of the Motion

D.0.1 General Operator $\hat{F}$ ............................................ 193
D.0.2 Evaluation of $(\hat{B} \ln(\hat{\rho}))^J$ ............................ 195
D.0.3 Evaluation of $(\hat{I}_{a,J} \oplus \hat{\theta}_{b,J} \oplus \hat{\theta}_{a,J})^J$ ........................................ 196
D.0.4 Evaluation of $(\hat{\theta}_{a,J} \oplus \hat{\theta}_{b,J} \oplus \hat{I}_{b,J})^J$ ........................................ 196
D.0.5 Evaluation of $(H)^J$ .................................................. 196

Appendix E Evaluation of Inner Products of the Perceived Quantities

E.0.1 General Definition of the Inner Product between Two Perceived Quantities 198
E.0.2 Evaluation of $(\hat{I}_{a,J} \oplus \hat{\theta}_{a,J} \oplus \hat{I}_{b,J})^J$ ........................................ 200
E.0.3 Evaluation of $(\hat{\theta}_{a,J} \oplus \hat{\theta}_{b,J} \oplus \hat{\theta}_{a,J} \oplus \hat{\theta}_{b,J})^J$ .......................... 200
E.0.4 Evaluation of $(\hat{I}_{a,J} \oplus \hat{\theta}_{a,J} \oplus \hat{I}_{b,J} \oplus \hat{\theta}_{b,J})^J$ and
$(\hat{\theta}_{a,J} \oplus \hat{\theta}_{b,J} \oplus \hat{I}_{b,J} \oplus \hat{\theta}_{b,J})^J$ ........................................ 201
E.0.5 Evaluation of $(\hat{I}_{a,J} \oplus \hat{\theta}_{a,J} \oplus \hat{\theta}_{b,J}, \hat{H})^J$ ........................................ 201
E.0.6 Evaluation of $(\hat{\theta}_{a,J} \oplus \hat{\theta}_{b,J} \oplus \hat{I}_{b,J}, \hat{H})^J$ ........................................ 202
E.0.7 Evaluation of $(\hat{I}_{a,J} \oplus \hat{\theta}_{a,J} \oplus \hat{\theta}_{b,J}, \hat{B} \ln(\hat{\rho}))^J$ .......................... 202
E.0.8 Evaluation of \( \left( \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb}, \hat{B} \ln(\hat{\rho}) \right)^J \) . . . . . . . . . . . . . . . 203

E.0.9 Evaluation of \( \left( \hat{H}, \hat{\mathcal{B}} \ln(\hat{\rho}) \right)^J \) . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 203

E.0.10 Evaluation of \( \left( \hat{H}, \hat{H} \right)^J \) . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . . 204

Bibliography 206
List of Figures

2.1 Bloch sphere representation of a two-level system [45] .......................... 20

2.2 Polarization vector and density operator eigenvalue evolution; the X, Y, and Z polarization components of the results generated here are red, blue, and black, respectively. The polarization components generated by Tabakin are green for the unitary dynamics and light blue for the dynamics of the SEAQT equation of motion and generally lie on top of the unitary and SEAQT results generated in the present work. A similar color scheme is applied to the evolution of the two density operator eigenvalues. ......................................................... 38

2.3 Entropy and energy evolution; both the energy and entropy predicted by Tabakin are green for the unitary dynamics and light blue for the dynamics of the SEAQT equation of motion and generally lie on top of the SEAQT results generated here. ................................................................. 39

2.4 Polarization vector and density operator eigenvalue evolution; the X, Y, and Z polarization components of the results generated here are red, blue, and black, respectively. The polarization components generated by Tabakin are green for the unitary dynamics and light blue for the dynamics of the SEAQT equation of motion and generally lie on top of the SEAQT results generated here. A similar color scheme is applied to the evolution of the two density operator eigenvalues. The evolutions of the unitary dynamics end at $t \approx 50$ ns as this is where the published data ends. .............................................. 40
2.5 Entropy and energy evolutions; both the energy and entropy predicted by Tabakin are dashed green for the unitary dynamics and dotted light blue for the dynamics of the SEAQT equation of motion. The evolutions of the reversible dynamics end at $t \approx 50$ ns as this is where the published data ends.

2.6 Polarization vector and density operator eigenvalue evolution; the X, Y, and Z polarization components of the SEAQT results generated here are red, blue, and black, respectively. The polarization components generated by Tabakin are dashed green for the Korsch-type bath and dashed black for the Beretta-type bath. The Tabakin eigenvalues plotted in dashed green correspond to those of the Korsch bath evolution.

2.7 Entropy and energy evolution. Both the energy and entropy predicted by Tabakin are dashed green for the Korsch-type bath and dashed black for the Beretta-type bath.

2.8 System-reservoir energy and entropy transfer. The left plot shows the overall rate of entropy change in red, and the entropy generation rate of the system state under the Beretta equation in dark blue. The system-reservoir entropy transfer, computed as the difference of the two aforementioned quantities, is shown in black and finally, the rate of the system’s change in energy is shown in light blue. The right plot shows the ratio of the rate of change of the system’s energy to its total entropy.

A.1 Polarization vector evolution.

A.2 Eigenvalue and energy evolution.

A.3 Polarization vector and eigenvalue evolution.
A.4 Entropy and energy evolution. ................................................................. 51
A.5 Polarization vector and eigenvalue evolution. .............................................. 52
A.6 Energy evolution during the first Hadamard gate (A.6a) and the Not gate. (A.6b). ................................................................. 52

3.1 Kullback-Leibler relative entropy evolution; evolutions for quench times of 100 $\mu$s and 500 $\mu$s using the von Neumann equation are shown in addition to experimental values; the so-called “mean entropy production”, $\langle \Sigma \rangle$, predicted using the Tasaki-Crooks equation is shown as well. .................................................. 71

3.2 So-called “mean entropy production”, $\langle \Sigma \rangle$, vs. quench time; the evolution of $\langle \Sigma \rangle$ as predicted by the von Neumann equation for quench times between 20 $\mu$s and 800 $\mu$s are shown in addition to the Tasaki-Crooks “mean entropy production” and experimental values. .................................................. 72

3.3 Kullback-Leibler relative entropy evolution; evolutions for quench times of 100 $\mu$s and 500 $\mu$s using the SEAQT equation of motion are shown in addition to experimental values; the so-called “mean entropy production”, $\langle \Sigma \rangle$, predicted using the Tasaki-Crooks equation is shown as well. .................................................. 73

3.4 So-called “mean entropy production”, $\langle \Sigma \rangle$, vs. quench time; the evolution of $\langle \Sigma \rangle$ as predicted by the SEAQT equation of motion for quench times between 20 $\mu$s and 800 $\mu$s are shown in addition to the Tasaki-Crooks “mean entropy production” and experimental values. .................................................. 74
3.5 Kullback-Leibler relative entropy evolution; evolutions for quench times of 100 \( \mu s \) and 500 \( \mu s \) using the SEAQT equation of motion are shown in addition to experimental values; the so-called “mean entropy production”, \( \langle \Sigma \rangle \), predicted using the Tasaki-Crooks equation is shown as well. .......................... 75

3.6 So-called “mean entropy production”, \( \langle \Sigma \rangle \), vs. quench time; the evolution of \( \langle \Sigma \rangle \) as predicted by the SEAQT equation of motion for quench times between 20 \( \mu s \) and 800 \( \mu s \) are shown in addition to the Tasaki-Crooks “mean entropy production” and experimental values. .......................... 76

4.1 Perturbed state energy-entropy diagram and distance measure \( \theta_d \) vs fidelity. 92

4.2 Perturbed state entropy vs. mutual information and mutual information vs. concurrence. .......................... 93

4.3 Perturbed state mutual information vs. maximum CHSH operator expectation value and maximum CHSH operator expectation value vs. concurrence. .......................... 94

4.4 Perturbed state energy-entropy diagram and distance measure \( \theta_d \) vs fidelity. 95

4.5 Perturbed state entropy vs. mutual information and mutual information vs. concurrence. .......................... 95

4.6 Perturbed state mutual information vs. maximum CHSH operator expectation value and maximum CHSH operator expectation value vs. the concurrence. .......................... 96

4.7 Perturbed state energy-entropy diagram and distance measure \( \theta_d \) vs fidelity. 97

4.8 Perturbed state entropy vs. mutual information and mutual information vs. concurrence. .......................... 98
<table>
<thead>
<tr>
<th>Section</th>
<th>Description</th>
<th>Page</th>
</tr>
</thead>
<tbody>
<tr>
<td>4.9</td>
<td>Perturbed state mutual information vs. maximum CHSH operator expectation value and maximum CHSH operator expectation value vs. concurrence.</td>
<td>98</td>
</tr>
<tr>
<td>4.10</td>
<td>Perturbed state energy-entropy diagram and distance measure $\theta_d$ vs fidelity.</td>
<td>99</td>
</tr>
<tr>
<td>4.11</td>
<td>Perturbed state entropy vs. mutual information and mutual information vs. concurrence.</td>
<td>100</td>
</tr>
<tr>
<td>4.12</td>
<td>Perturbed state mutual information vs. maximum CHSH operator expectation value and maximum CHSH operator expectation value vs. concurrence.</td>
<td>100</td>
</tr>
<tr>
<td>5.1</td>
<td>Theoretical and experimental concurrence and $\left\langle \hat{B}<em>{CHSH} \right\rangle</em>{Max}$ evolutions for the Bell diagonal state characterized by the parameters $c_1 = 1$, $c_2 = 0.4$, and $c_3 = -0.4$, presented in [44]; the theoretical results were generated using a quantum optics experiment and the theoretical results were produced using the Kraus-Operator-Sum approach.</td>
<td>120</td>
</tr>
<tr>
<td>5.2</td>
<td>Concurrence and $\left\langle \hat{B}<em>{CHSH} \right\rangle</em>{Max}$ evolutions for values of the weighting parameter $\zeta = 1$, 0.96, 0.92, 0.88, 0.84, 0.8, 0.76, 0.72, and 0.68 where $\zeta = 1$ corresponds to the uppermost solid orange line and each lower solid line corresponds to the next lower value of $\zeta$.</td>
<td>121</td>
</tr>
<tr>
<td>5.3</td>
<td>Perturbed and stationary state Bell diagonal parameters $c_1 \pm c_2$ vs. the weighting parameter $\zeta$ and perturbed and stationary state entropy correlation.</td>
<td>122</td>
</tr>
<tr>
<td>5.4</td>
<td>Correlations between the entanglement operator $\hat{\xi}$, the stationary state entropy, and the total entropy production (or generation).</td>
<td>123</td>
</tr>
<tr>
<td>5.5</td>
<td>Concurrence and $\left\langle \hat{B}<em>{CHSH} \right\rangle</em>{Max}$ evolutions for nine random perturbations.</td>
<td>124</td>
</tr>
<tr>
<td>5.6</td>
<td>Perturbed and stationary state concurrence and $\left\langle \hat{B}<em>{CHSH} \right\rangle</em>{Max}$ values.</td>
<td>124</td>
</tr>
</tbody>
</table>
5.7 Correlations of change in concurrence and $\left< \hat{B}_{CHSH} \right>_{\text{Max}}$ vs. the total entropy production (or generation) 125

5.8 Correlations between $|\hat{\xi}|$, the stationary state entropy, and the total entropy production (or generation) 126

5.9 Concurrence and $\left< \hat{B}_{CHSH} \right>_{\text{Max}}$ evolutions for nine random perturbations 127

5.10 Perturbed and stationary state concurrence and $\left< \hat{B}_{CHSH} \right>_{\text{Max}}$ values 128

5.11 Correlations of change in concurrence and $\left< \hat{B}_{CHSH} \right>_{\text{Max}}$ vs. the total entropy production (or generation) 128

5.12 Correlations between $|\hat{\xi}|$, the stationary state entropy, and the total entropy production (or generation) 129

5.13 Correlation between the total entropy generation and the state distance measure $\theta_d$ and the initial entropy production (or generation) rate vs. the maximum entropy production (or generation) rate 130

5.14 Concurrence and $\left< \hat{B}_{CHSH} \right>_{\text{Max}}$ evolutions for nine random perturbations 131

5.15 Perturbed and stationary state concurrence and $\left< \hat{B}_{CHSH} \right>_{\text{Max}}$ values 132

5.16 Correlations of change in concurrence and $\left< \hat{B}_{CHSH} \right>_{\text{Max}}$ vs. the total entropy production (or generation) 133

5.17 Correlations between $|\hat{\xi}|$, the stationary state entropy, and the total entropy production (or generation) 133

5.18 Correlation between the total entropy generation and the state distance measure $\theta_d$ and the initial entropy production (or generation) rate vs. the maximum entropy production (or generation) rate 134
6.1 Quantum computing algorithm to compute the modular exponentiation with a base $a = 11$ and the associated system state through the algorithm (adapted from [58]). .......................................................... 143

6.2 Thermal equilibrium spectra of qubits 1, 2, and 3; all frequencies are relative to those given in Table 6.2. .......................................................... 168

6.3 Ground state spectra of qubits 1, 2, and 3; experimental results are shown in addition to the theoretical spectra and those obtained from the pseudo-pure state using the von Neumann equation; all frequencies are relative to those given in Table 6.2 .......................................................... 170

6.4 Ground state spectra of qubits 1, 2, and 3; experimental results are shown in addition to the pseudo-pure state spectra obtained from the Beretta and Beretta+Reservoir equations; all frequencies are relative to those given in Table 6.2 and $\tau_{D,J} = \tau_{Matthisien,J}/100$. .......................................................... 171

6.5 End state spectra of qubits 1, 2, and 3; experimental results are shown in addition to the theoretical spectra and those obtained from the pseudo-pure state using the von Neumann equation; all frequencies are relative to those given in Table 6.2. .......................................................... 173

6.6 End state spectra of qubits 1, 2, and 3; experimental results are shown in addition to theoretical results predicted under the evolution of the Kraus/Operator-Sum approach [58] and the pseudo-pure state spectra obtained from the Beretta equation, all frequencies are relative to those given in Table 6.2. .......................................................... 174
6.7 End state spectra of qubits 1, 2, and 3; experimental results are shown in addition to the theoretical results predicted under the evolution of the Kraus/Operator-Sum approach [58] and the pseudo-pure state spectra obtained from the Beretta+Reservoir equation; all frequencies are relative to those given in Table 6.2.

6.8 Composite system entropy evolution; (a) shows the rate of entropy change for the composite system as predicted by the Beretta equation, which is equivalent to the entropy generation rate, while (b) shows the rate of entropy change for the composite system as predicted by the Beretta+Reservoir equation, which is equivalent to the difference of the entropy generation rate of the qubits and the rate of entropy transferred from the qubits to their respective reservoirs. The rate of entropy change predicted by the Beretta+Reservoir is significantly smaller than that predicted by the Beretta equation alone.

6.9 Energy evolution of qubit 1 after the preparation sequence has taken place; (a) shows that as the state of qubit 1 is manipulated during the algorithm, energy is either transferred to or from the reservoir, while (b) shows that the sharp changes in energy are not discontinuous but happen relatively very rapidly in time compared to the length of the algorithm.

6.10 Energy evolution of qubits 2 and 3 after the preparation sequence has taken place; (a) shows that, like qubit 1, there is energy transfer both to and from the reservoir to qubit 2, while (b) shows that there is primarily energy transfer from the reservoir to qubit 3 throughout the algorithm.
6.11 Energy evolution of qubits 4 and 5 after the preparation sequence has taken place; (a) and (b) show that there is negligible energy transfer to/from qubits 4 and 5, respectively, and their respective reservoirs during the algorithm. . . . 179

6.12 Energy evolution of qubits 6 and 7 after the preparation sequence has taken place; (a) shows that, like qubit 1, there is energy transfer both to and from the reservoir to qubit 6, while (b) shows that there is negligible energy transfer to/from qubit 7 and its reservoir during the algorithm. . . . . . . . . . . . . . . . . . . . . . 180
List of Tables

6.1 Pseudo-pure ground state preparation scheme taken from [54]; note that time proceeds from left to right and $N_j$ denotes a NOT gate on qubit $j$ and $C_{ij}$ denotes a controlled-NOT gate where qubit $i$ is the control qubit and qubit $j$ is the target. * A correction from the original document reading $S_{14} = S_5 N_6 N_7 C_{61}$ was made here. .......................................................... 149

6.2 Physical properties of the NMR quantum computer adapted from [58]; the values given for $\omega_{0,i}/2\pi$ are in Hz and relative to 470 MHz for qubits 1-5 and 125 MHz for qubits 6 and 7; the spin-lattice, or longitudinal, relaxation time and the spin-spin, or transverse, relaxation time are given by $T_1$ and $T_2$, respectively, in units of seconds, while $J_{i,j}$ is the J-coupling coefficient between qubits $i$ and $j$ given in units of Hz. .......................................................... 151
Chapter 1

Introduction

This dissertation details the use of Steepest-Entropy-Ascent Quantum Thermodynamics (SEAQT) for modeling various applications related to quantum information and quantum computing (QIQC) systems as well as some theoretical extensions within the SEAQT framework itself that are broadly applicable. This chapter introduces and outlines the remainder of the dissertation, first providing (in Section 1.1) a brief background into the field of QIQC and into SEAQT, which sets the context for the following chapters.

Using this background, Section 1.2 provides the motivation for undertaking this work, the general goals and objectives that are met in the remaining chapters, and details of the tasks necessary to meet these goals. Section 1.3 then describes the original contributions dissertation made in the process of meeting these goals. Finally, Section 1.4 provides a more detailed outline of the dissertation and the content presented in each chapter.

1.1 Background: Quantum Information and Computing and Steepest-Entropy-Ascent Quantum Thermodynamics

This section presents background information on the fields of quantum information, quantum computing, and steepest-entropy-ascent quantum thermodynamics (SEAQT). First, Section
1.1.1 provides an overview of QIQC, briefly explaining the quantum phenomena on which QIQC systems are based, the challenges facing the development of practical quantum computers, and a few of the impacts that this field can have on society. Following that, Section 1.1.2 provides an overview of SEAQT, including some previous applications, and explains how it is well suited for use in the analysis of quantum information and quantum computing systems.

### 1.1.1 QIQC Introduction

QIQC systems rely on quantum mechanical phenomena to store, transfer, and process information. The two primary quantum phenomena available in QIQC that classical systems lack are 1) the ability of a system to be in a superposition state (i.e., to simultaneously be in multiple quantum states at a given instant of time) and 2) the allowance of multiple quantum systems to be entangled, meaning that the state of any individual system cannot be described independently of the others (i.e., it is not possible to separate the state of system A from system B and, thus, both must be described together).

The possibility of superposition states in quantum mechanical systems allows for the number of states (corresponding to input values) that a quantum algorithm can simulate simultaneously to scale exponentially with the number of qubits (i.e., a quantum bit represented by a two-level quantum system) in the quantum computer, leading to the potential for vast parallelization. For example, a quantum computer consisting of 300 quantum bits (qubits) could simultaneously simulate roughly as many states ($2^{300}$) as there are atoms in the observable universe [20]. This exponential scaling could have great impact in applications that require large-scale parallelization to perform meaningful computations. For example, this scaling could allow for the simulation of more complex quantum systems [47] and lead,
for example, to the design of new molecules for pharmaceutical purposes, the beginnings of which are already underway [32]. Additionally, factoring large numbers, a hard problem for classical computers to solve (i.e., one that can only be solved with algorithms that scale poorly with the size of the problem), can be done efficiently on quantum computers through the use of Shor’s algorithm [50, 51]. This will have a great impact on commonly used cryptography systems, which rely on the difficulty of factoring large numbers to keep information secure. Thus the ability to de-encrypt data could affect sectors where information security is required.

The other phenomenon on which QIQC systems rely, entanglement, allows for the manipulation of systems that may be spatially separated. In addition to being a fundamental resource used in quantum computing, entanglement has numerous other applications, some of which include superdense coding (the ability to transfer two bits of classical information using a single quantum bit or qubit), quantum teleportation [6, 8], quantum cryptography, [7], and improved radar detection systems [2].

Though superposition and entanglement offer vast potential for a variety of new technologies, there exist numerous challenges to effectively utilizing these phenomena in developing practical systems. A well-known set of requirements for the development of a quantum computer was first laid out by DiVincenzo in [22, 23]. These are briefly summarized as follow:

1) The necessity of the Hilbert space associated with the quantum computer to grow exponentially with the size of the system: this implies that each qubit in a quantum computer must be formed using independent, distinguishable particles and not by the various levels that may be present in a single particle that happens to have multiple energy eigenstates (e.g., a quantum harmonic oscillator).

2) The ability to prepare the system in some standard, known state (e.g., the ground energy state) typically used at the beginning of an algorithm: without this ability, it is not possible
to properly interpret the output of an algorithm.

3) The ability to sufficiently isolate the quantum computing system from its environment, thus, minimizing unintended interactions that would otherwise lead to decoherence: as a consequence, the lifetime of the qubit (i.e., how long information can be stored on the qubit before it is degraded by decoherence below some threshold) must be long enough to implement algorithms.

4) The ability to implement a set of universal operations in a controlled fashion on the quantum computer: it has been shown [21] that two-qubit gates in combination with single qubit operations are all that is necessary to preform any quantum algorithm. Implementing two-qubit gates requires that the two qubits interact either directly or indirectly, and, thus, any physical realization of a quantum computer must have a means of doing this.

5) The ability to reliably perform strong measurements on individual qubits in the quantum computer (i.e., a measurement that determines in which eigenstate a system is): this is necessary not only to obtain the results of the algorithm, but since quantum measurements are probabilistic in nature, this is also necessary to ensure the reliability of said measurement.

There are many possible physical realizations of quantum computers meeting DiVincenzo’s requirements. Each has its strengths and weaknesses. For example, liquid state nuclear magnetic resonance quantum computers, where the qubits are realized by the nuclei of the various atoms forming a molecule and information is stored via their spin orientation, experience relatively weak interactions with their environment, leading to long decoherence times compared to the time it takes to implement an algorithm. However, to make larger quantum computers using NMR requires making larger molecules whose qubits (nuclei) can be easily distinguished from one another during measurement. This turns out to be a prohibitive feature for scaling NMR quantum computers to sizes that would make them
1.1. Background: Quantum Information and Computing and Steepest-Entropy-Ascent Quantum Thermodynamics

useful in practical applications but lead to their success in the early development of prototype quantum computers [57, 58].

Another physical realization of a quantum computer is based on optical photons, where information is stored in the location of the photon or via the photon’s polarization. These states can be relatively well controlled, but photons only indirectly interact with one another through optical media, which is an inefficient process. Thus, while single-qubit operations can be done, this makes implementing multi-qubit operations difficult, and, thus, there is difficulty in meeting DiVincenzo’s requirement of the ability to perform a set of universal operations [47].

In ion traps, the hyperfine states associated with the nuclear spin of the ion as well as the ground state vibrational modes (phonons) between adjacent pairs of ions are used to store information and perform interactions. The lifetimes associated with the nuclear spin states can be very long relative to the time it takes to implement an algorithm, and single-qubit operations can be implemented relatively straightforwardly through the use of laser pulses. However, the lifetime of the phonon states shared between two qubits, which are necessary for their interactions and, thus, multiqubit gates, is relatively short. This results in decoherence occurring when implementing multi-qubit gates. Further, ion traps require that the series of ions all be in their motional ground states, which is difficult to prepare [47].

The final realizations mentioned here are spin- and charge-based quantum dots. In spin-based quantum dots, the qubits are realized by the orientation of the spin of an extra electron in a quantum dot, whereas in the charge-based approach, a qubit is realized by the presence or absence of an electron in a quantum dot. While it is easy to detect the presence of charge using current technology, the motion of distant charges as well as the presence of unwanted phonon interactions leads to relatively short decoherence times for charge-based quantum dots. Spin-based qubits suffer the opposite problem, while it is easier to control the state
of the spin using localized pulsed magnetic fields, it is difficult to reliably measure spin orientation (and, thus, the qubit’s state) in semiconductor devices [47].

As discussed above, different physical realizations have certain advantages over others, though none have yet been proven feasible enough to build a practical quantum computer. Thus far, it seems as though superconducting circuits provide the best physical realization for meeting DiVincenzo’s criteria, as Google, IBM, and Intel have all recently announced quantum processors consisting of 72, 50, and 49 qubits based on this model [31, 33, 46].

Though some physical realizations may inherently be more successful at minimizing decoherence than others, it is still always a factor that must be considered not only when designing the quantum computer itself but also when developing the algorithms to be run on them. Though decoherence can be caused by other mechanisms (e.g., unintended interactions with other qubits), the focus of the following work is on the decoherence caused by dissipation. While dissipation is commonly modeled as being caused by an interaction of the system with its environment, in this work it is instead attributed to irreversibilities within the system itself.

1.1.2 SEAQT Background

SEAQT, first proposed by Hatsopoulos and Gyftopoulos [25, 26, 27, 28] and then completed with the dynamics proposed by Beretta [12], is a mathematical modeling approach that supplements the postulates of quantum mechanics with those of thermodynamics, forming a single, unified theory [9]. Specifically, SEAQT asserts that a system evolves such that the increase of the system’s entropy (i.e., the von Neumann entropy) is maximized at any given time (otherwise known as the principle of steepest entropy ascent (SEA)). This principle allows for an equation of motion to be developed governing the dynamics of a system in any
state (both near and far from stable equilibrium), and, thus, can provide the system state’s evolution as it evolves from some non-equilibrium state to stable thermodynamic equilibrium. This principle, along with recent modeling advances (e.g., [39]), permits the effects of non-unitary, dissipative dynamics under SEA to be modeled across all temporal and spatial scales and further permits the macroscopic behavior of systems to be directly related to the microscopic processes that are occurring. In addition, because there is no need to track the mechanical properties (i.e., position and velocity) associated with the system of interest, SEAQT also enjoys a much smaller computational burden compared to commonly used methods (e.g., molecular dynamics) that do require this information.

Since its inception, several theoretical extensions of SEAQT have been made in modeling various types of systems and interactions, including the development of a framework for modeling chemical reaction kinetics [11, 39], models of systems experiencing heat and mass interactions with and without a reservoir [40], and the development of methods to model systems from microscopic, quantum scales through mesoscopic scales and up to macroscopic scales. The generality of the SEAQT mathematical framework allows it to be applied to any quantum mechanical as well as classical system with some select previous applications being

- Predicting chemical reaction kinetics [1, 11, 36, 37, 39, 42, 43, 59]
- Modeling decoherence in bipartite quantum systems [15, 16]
- Modeling the heat and mass diffusion of both fermionic and bosonic Helium [41, 66, 67]
- Modeling electron and phonon transport [39]
- Modeling thermal expansion, magnetization, and continuous and discontinuous phase transitions [61, 62, 63, 64, 65]
- Modeling the adsorption of hydrogen onto a carbon nanotube [52, 53]
Additionally, recent work has been completed or is currently underway in modeling the diffusion of lipid species in cell membranes using an Ising-based model as well as the chemical reaction rates associated with hypersonic flows. Because SEAQT is capable of modeling the change in a system’s state through time, while capturing the dissipation occurring within the system at any given instant in time, it is an ideal candidate for modeling the dissipation and, thus, the resulting decoherence exhibited in quantum systems.

1.2 Motivation, Goals, and Work to be Completed

The motivation for this work stems from the potential societal benefits quantum computers have and the current challenges preventing their realization, i.e., in particular, the need to control and minimize the decoherence occurring during their operation. Because SEAQT inherently accounts for the dissipation occurring in a system at any given state and time, it is well suited for addressing this problem. Thus, the goal of this work is to use SEAQT to predict how and when dissipation occurs over the course of a quantum algorithm, characterize how this dissipation leads to decoherence and information loss, and use this to develop a thermodynamics based control strategy for reducing the decoherence and subsequent information loss.

To meet this overall goal, SEAQT is first used to model the dissipation experienced in a single qubit as it undergoes common quantum computing operations, examining when dissipation is most rapidly occurring and how it affects the system state. An extended form of the SEAQT equation of motion is then used to account for heat interactions between the qubit and a thermal reservoir. This allows one to show how the dynamics experienced under environmental interactions of the Lindblad form can be modeled via an interaction with a thermal reservoir. This examination provides an intuitive understanding of how a system’s
state changes and decoherence occurs during single qubit operations, providing the basis for what needs to be done in developing a method to control the decoherence.

Next, the entropy generation of a system modeled in a rotating reference frame (a frame commonly used in quantum computing) during a nuclear magnetic resonance experiment is examined as are the effects of the SEAQT relaxation time on system state evolution. The original experimental work was done in an effort to show that irreversibilities exist at a microscopic level [3], and this modeling work attempts to explain these irreversibilities using SEAQT.

This doctoral work also addresses the goal of understanding how dissipation occurs in quantum systems. It does so by illuminating how various rates of change of a system’s Hamiltonian as well as the SEAQT relaxation time affect the the entropy generation rate (dissipation) in a system at a given instant of time and the properties (i.e., energy and entropy) of the stable equilibrium state that the system approaches.

To understand the sensitivity of various quantum state measures, specifically those related to the entanglement of two quantum systems, on system state, a general perturbation procedure is developed and used to generate randomly perturbed density operators. This procedure is then used to quantify changes in the system concurrence, CHSH operator maximum expectation value, and mutual information (all measures of system entanglement) for perturbations of various magnitudes under various constraints. This work addresses the aforementioned goals by quantifying how differences between a system’s expected state and the system’s actual state can affect the measurement statistics seen in a quantum computing algorithm. In addition, as is seen when addressing entanglement, certain entangled states of non-interacting qubits can be non-dissipative, yet not-stable-equilibrium states under SEA. Thus a perturbation method is needed to observe the dynamics of states in the neighborhood of these non-dissipative states.
With an understanding of the sensitivity of various system state measures, specifically those related to entanglement, SEAQT is used to quantify how a composite system state itself changes under SEA with a specific focus on the entanglement of two non-interacting qubits. Understanding this provides insight into the effects of dissipation on entanglement, and how particular states may be used to limit the loss of entanglement, a key component of any quantum computation algorithm.

Finally, to address the goal of controlling decoherence in a quantum algorithm, a methodology utilizing a generalized form of the previously discussed reservoir interactions is developed and applied during Shor’s algorithm for factoring 15. The results obtained from this work are compared with experimental results, theoretical and numerical results for unitary dynamics, and also with those of the SEAQT equation of motion where no reservoir interactions are present.

1.3 Original Contributions

In performing the above tasks, several original contributions are made to the theory of SEAQT, including

- Generalizing system-reservoir heat interactions to systems in arbitrary states (i.e. not limited to those in hypo-equilibrium states) and to systems where unitary dynamics and coherences are present

- Deriving the SEAQT equation of motion and its associated operators for an arbitrary rotating reference frame and showing its relation to the lab-frame equation of motion

- Developing and implementing a method for perturbating a given density operator by a specified magnitude subject to any set of desired constraints
1.3. Original Contributions

• Developing a relation between the entanglement characteristics of a non-equilibrium state and the stationary state to which it evolves

• Developing an equation of motion based on Beretta’s original formulation for a general quantum system where each subsystem experiences a local heat interaction with a reservoir

• Developing a decoherence control scheme utilizing time varying reservoir heat interactions and a rotating reference frame

These original theoretical contributions are then applied to

• Modeling the state evolution of a general spin 1/2 system experiencing a heat interaction

• Modeling the evolution of a two qubit system in an NMR experiment

• Developing sets of perturbed density operators under energy and entropy constraints

• Using the entanglement characteristics of a bipartite system density operator to predict the stationary, not stable equilibrium states to which entangled, but non-interacting states, evolve

• Predicting the magnitude of the noise (arising from dissipation) associated with an NMR quantum computing experiment

• Applying the control scheme to minimize the decoherence due to dissipation in the NMR quantum computer
1.4 Dissertation Outline

This dissertation is organized into chapters where each specific chapter is in the form of an independent paper. Roughly speaking, Chapters 2 through 5 address different aspects and features of the SEAQT equation of motion and the dissipation, which causes decoherence in QIQC applications. Chapter 6 then combines these various aspects in implementing a control scheme to limit decoherence.

Chapter 2

Chapter 2 first presents the replication of the system state dynamics during common single qubit quantum computing gates under reversible dynamics (the von-Neumann equation) as well as under the irreversible dynamics of the SEAQT equation of motion. In both cases, these quantum computing gates are implemented via time-dependent Hamiltonians.

Next, a brief derivation of the equation of motion for a simple quantum system experiencing a heat interaction with a constant temperature reservoir is presented. Here, no assumptions of system state are made, allowing this equation of motion to be applied to systems where coherences between the energy eigenlevels may be present.

This extension to the SEAQT equation of motion is then used to predict the system state dynamics during the same quantum computing gates, while a heat interaction is present, and the results are compared with 3 other theoretical models.

Chapter 3

Chapter 3 first presents a brief derivation of the SEAQT equation of motion in a rotating reference frame (i.e., in the Heisenberg picture). In addition to converting all relevant
operators from the lab frame to the rotating frame, the resulting operators producing the reversible and irreversible dynamics are also explored. Also included in Chapter 3 is the description of a method that utilizes the transition rate probability (of which a brief derivation is provided) to compute a value for the SEAQT relaxation time $\tau_D$.

These theoretical results are then applied to examining the system state evolution of a single qubit realized in a nuclear magnetic resonance (NMR) experiment and undergoing a “fast-quenching” process. The fast-quenching process is achieved by a time-varying Hamiltonian operator consisting of a strong, static longitudinal component, and a transverse component whose orientation and magnitude change with time.

**Chapter 4**

Chapter 4 presents a general method for producing randomly perturbed density operators under any set of desired constraints. The density operators are a specified “distance” away from the state described by the original density operator. This approach is then applied to a bipartite system of qubits and used to examine the sensitivity of other metrics (such as various entanglement measures) to the perturbation magnitude. The constraint sets used include constant energy, constant entropy, and both constant energy and entropy.

**Chapter 5**

Chapter 5 presents an analysis of the evolution of perturbed Bell diagonal states under the SEAQT equation of motion and analyzes their loss of entanglement using various measures. First, a brief derivation is presented showing that Bell diagonal states are stationary, not-stable-equilibrium states relative to the SEAQT equation of motion, highlighting the need for the development of perturbation methods to study evolutions of nearby states.
Next three perturbation methods are presented, the first being the general method described in Chapter 4. The second is a method based on a set of unitary operations that are constrained to hold the system energy constant (and that also inherently hold the system entropy constant), and the third is a weighted average with an uncorrelated bipartite state of zero energy. Sets of density operators are randomly generated with each method and the resulting time-varying characteristics of the system’s entanglement are analyzed.

Chapter 6

Chapter 6 presents the application of SEAQT to a 7-qubit NMR quantum computer that implements Shor’s factoring algorithm. First, an overview of quantum computing using NMR and Shor’s factoring algorithm is presented, including the development of the algorithm to be implemented and the need for generating pseudo-pure states to start the algorithm.

Next, the development of the SEAQT equation of motion for a general quantum system where each system experiences a local heat interaction with a reservoir is presented. The resulting equation, in combination with the use of a rotating reference frame and an adjustment to the system Hamiltonian, is then used to develop a methodology for using reservoir interactions to limit the decoherence present within a system. For a given relaxation time constant, results are generated using both the SEAQT equation of motion with and without reservoir heat interaction. The former in effect implements the decoherence control methodology. These results are compared with published data as well as those produced using the reversible dynamics of the von-Neumann equation.

Generally speaking, the content presented in this chapter extends what is first presented in simpler forms in the previous chapters. Time-varying Hamiltonian operators (which were encountered in Chapters 2 and 3) are widely used in Chapter 6 and the composite
system equation of motion for two qubits seen in Chapter 5 is now extended to seven qubits. Furthermore, the composite system reservoir interaction model draws from and extends the derivation presented in Chapter 2, and the decoherence control scheme using reservoir interactions utilizes the rotating reference frame presented in Chapter 3. Thus, for an introduction into each of these topics, it is recommended to first refer to one of the earlier chapters.
Chapter 2

Model Dynamics for Single Qubit Gates and Heat Interactions for Simple Quantum Systems

2.1 Introduction

The ability to reliably store and manipulate information contained within a computing system is key to successfully obtaining results. While this has long been achieved on classical computing systems, these requirements, in particular the ability to reliably store information, present formidable challenges in the development of quantum computing systems. The loss of information in quantum systems typically comes from the loss of coherence between two energy eigenlevels, a process otherwise known as decoherence. One cause of decoherence (at least in the steepest-entropy-ascent quantum thermodynamics (SEAQT) picture of physical reality) is the dissipation that occurs within a quantum system, and, thus, understanding how and when this dissipation occurs can help improve the design and control of quantum computers and quantum algorithms.

To gain insight into the dissipation, which occurs during quantum algorithms, this work builds upon that done by Tabakin [55], which focuses on the state evolution of a general
two-level quantum system (which is henceforth be referred to as a qubit). Specifically, because single qubit operations form the building blocks of all quantum algorithms, it is during these processes that the system state evolution is examined.

In addition, these evolutions are examined under a variety of model dynamics, including the unitary dynamics of standard quantum mechanics where no dissipation occurs as well as the non-unitary dynamics of two-different models that lead to dissipation. Specifically, the latter two models include the dynamics resulting from the standard SEAQT equation of motion and that resulting from the reservoir/bath heat interaction model within the SEAQT framework. Additionally, it is also shown that previous phenomenological descriptions of system-reservoir interactions can be derived starting from fundamental principles using the SEAQT framework.

To accomplish these tasks, a review of a qubit’s state representation is first discussed along with its visualization on a Bloch sphere. Then some common quantum computing operations are reviewed along with how they are represented mathematically and how they change the system’s state as represented on the Bloch sphere.

With this review in mind, the ideal unitary time evolution of state (i.e., evolution with no dissipation) of quantum systems is discussed in terms of a time varying Hamiltonian with this time evolution being related to the common quantum computing operations discussed above.

Following the discussion of the ideal unitary evolution and gate implementations, models for the non-unitary dynamics are discussed. These include the SEAQT equation of motion and a fundamentally derived equation of motion for system-reservoir interactions within the SEAQT mathematical framework, which happens to reproduce phenomenological-based equations for system-reservoir interactions. This equation generalizes previous work modeling
system-reservoir heat interactions within the SEAQT framework \[40\] in that 1) reversible dynamics are now included and 2) relaxations on the assumptions of system state are made relative to previous developments. Specifically, it is no longer required that the composite system-reservoir state form a so-called hypo-equilibrium state.

Next, using the time-varying forms of the Hamiltonian as is done for the unitary dynamics, the same gates are then applied using the aforementioned non-unitary models, examining how the system state changes in each case, how dissipation occurs, and, thus, how information may be lost. Finally, it is shown that the same dynamics from previous phenomenological descriptions of system-reservoir interactions can be obtained using the system-reservoir interaction model as derived within the SEAQT framework. Knowledge of the effects of reservoir interactions on a system’s state then allow for the design of reservoir interactions to control decoherence.

\[2.1\] Preliminary Review of Quantum Computing

Quantum State Representation and the Bloch Sphere

Quantum systems in pure states are typically represented by a wave function $\psi(t)$, which describes the probability amplitude of a system at time $t$. In addition to being functions of time, wave functions are also commonly functions of position, or as will be the case in this work, a function of particle spin. Assuming we are examining a spin-1/2 particle (having only two possible spin states such as, e.g., an electron), neglecting spatial dependence, and adopting bra-ket notation, the state of this quantum system can be represented as

\[
|\psi(t)\rangle = \alpha(t) |0\rangle + \beta(t) |1\rangle = \alpha(t) \begin{bmatrix} 1 \\ 0 \end{bmatrix} + \beta(t) \begin{bmatrix} 0 \\ 1 \end{bmatrix} = \begin{bmatrix} \alpha(t) \\ \beta(t) \end{bmatrix}
\] (2.1)
where on the two right-most equalities specific vector representations are assigned for $|0\rangle$ and $|1\rangle$. This constitutes a choice of a set of basis vectors used to represent the system state and relevant operators. In general this choice is arbitrary, but certain choices can simplify the analysis of a problem. Here the choice of basis vectors correspond to the eigenvectors of the Pauli-Z matrix. This choice of basis is commonly known as the computational basis and is used throughout this work unless otherwise stated. $\alpha$ and $\beta$ are in general complex numbers representing the probability amplitudes of the system being in a spin-up state, $|0\rangle$, or a spin-down state, $|1\rangle$, respectively. If both $\alpha$ and $\beta$ are non-zero, the system is said to be in a superposition state, which is commonly the case in quantum computing. Requiring that the wavefunction is normalized implies that $|\alpha| + |\beta| = 1$. For present purposes, an additional useful representation is to use spherical coordinates, allowing the state vector to be represented as

$$
|\psi(t)\rangle = \cos\left(\frac{\theta(t)}{2}\right) |0\rangle + e^{i\phi(t)} \sin\left(\frac{\theta(t)}{2}\right) |1\rangle
$$

(2.2)

where the wavefunction normalization implies that the radius of the Bloch sphere $r$ is equal to one and the assumption that the coefficient multiplying $|0\rangle$ is real implies that a global phase has been factored out of the state of the system. This is a common assumption since global phases are generally unobservable and all that is of interest in quantum computing applications is the relative phase between states. This allows any state $|\psi(t)\rangle$ of any qubit to be represented as a unique point on the surface of a sphere of radius $r = 1$, which is known as the Bloch sphere, illustrated in Figure 2.1.

In addition to the pure states already discussed, it is often necessary to work with a more general set of quantum states, otherwise known as mixed states, which are represented with what is known as the density operator $\hat{\rho}(t)$. The density operator corresponding to a pure state can be computed by a projector such that $\hat{\rho}(t) = |\psi(t)\rangle \langle \psi(t)|$, and in general for both
pure and mixed states, the density operator can be represented with respect to a basis as

$$\hat{\rho}(t) = \begin{bmatrix} \rho_{00}(t) & \rho_{01}(t) \\ \rho_{10}(t) & \rho_{11}(t) \end{bmatrix} \tag{2.3}$$

To map the broader class of states represented by the density matrix to the Bloch sphere, the cartesian components of the so called Bloch vector, $\vec{r}$, (also sometimes referred to as the Polarization vector $\vec{P}$) are calculated as functions of the density operator elements as

$$r_x(t) = \rho_{01}(t) + \rho_{10}(t) \tag{2.4}$$
$$r_y(t) = i (\rho_{01}(t) - \rho_{10}(t)) \tag{2.5}$$
$$r_z(t) = \rho_{00}(t) - \rho_{11}(t) \tag{2.6}$$
where it can be seen that for pure states $|\vec{r}| = 1$ so that the corresponding points lie on the surface of the Bloch sphere and for mixed states $|\vec{r}| < 1$, indicating that the points lie in the interior of the Bloch sphere. This relation of the density operator elements to points on the Bloch sphere permits the visual representation of any state of a two-level system and provides a useful tool in analyzing a qubit’s change of state during a quantum algorithm, which will be analyzed next.

**Single Qubit Operations**

As is true for classical algorithms, quantum computing algorithms require the manipulation of specific bits to perform useful tasks. Two common operations used in quantum algorithms are reviewed here. The first is the Not gate, whose action is to rotate the Bloch vector $\pi$ radians about the $\hat{x}$ axis of the Bloch sphere and is regularly used throughout algorithms. The second gate that is reviewed here is known as the Hadamard gate, whose action is to rotate the Bloch vector by $\pi$ radians about the $(\hat{x} + \hat{z})/\sqrt{2}$ axis of the Bloch sphere. Among other uses, this gate is commonly used at the beginning of algorithms, when a qubit is in a spin-up state, to put the system in a superposition of states where there is no relative phase between the probability amplitudes of the states. This allows for the use of multiple input values to be run in parallel with a single algorithm. Mathematically, the Not and Hadamard gates are, respectively, defined in the computational basis as

$$X \equiv \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad H \equiv \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \quad (2.7)$$

To illustrate their effect on a system’s state, assume that the system is in a spin-up state $|\psi\rangle = |0\rangle$, whose corresponding density operator is then operated on by the gates as

\[ X\hat{\rho}X^\dagger = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix} \]  
(2.8)

and

\[ H\hat{\rho}H^\dagger = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} \begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \]  
(2.9)

In general, all single qubit operations (Not and Hadamard gates included) can be thought of as a rotation of a system’s Bloch vector through some angle \( \theta \) and about some specified axis \( \hat{n} \). This general rotation operator can be written as

\[ \hat{R}_{\vec{n}}(\theta) = e^{-i\frac{\theta}{2} \vec{n} \cdot \vec{\sigma}} = e^{-i\frac{\theta}{2}(n_x\hat{\sigma}_x+n_y\hat{\sigma}_y+n_z\hat{\sigma}_z)} \]  
(2.10)

where \( \vec{n} = [n_x, n_y, n_z] \) is a vector of unit norm specifying the \( x \), \( y \), and \( z \) components of the axis about which to rotate, \( \theta \) represents the angle through which to rotate, and \( \vec{\sigma} = [\hat{\sigma}_x, \hat{\sigma}_y, \hat{\sigma}_z] \) is a vector of the X, Y, and Z Pauli spin matrices. Specifying \( \theta = \pi \) and \( \vec{n} = [1, 0, 0] \) gives the Not gate and \( \theta = \pi \) and \( \vec{n} = [1, 0, 1]/\sqrt{2} \) gives the Hadamard gate, up to an unimportant global phase factor. Though these operations are useful for studying the states of qubits after single qubit operations, they do not govern the dynamics of the system, and, thus, it is necessary to relate the time evolution of the Hamiltonian to rotation operations of this form, which is done in Section 2.2.
2.2 Model Development

This section first discusses the use of a time-dependent Hamiltonian and the corresponding unitary evolution to implement specific single qubit operations, i.e., those specifically discussed in Section 2.1.1. Next, because the aim of this work is to model the decoherence caused by dissipation during the course of an algorithm, three models for the system’s equations of motion are presented, including an original derivation for system-reservoir heat interactions within the SEAQT framework.

2.2.1 Hamiltonian Evolution and Quantum Gate Implementation

The von Neumann equation, governing the unitary dynamics of systems in both pure and mixed states, is used as the basis for relating a system’s evolution under a specified Hamiltonian to the desired quantum gates to be implemented. The von Neumann equation is given as

$$\frac{d\hat{\rho}(t)}{dt} = -\frac{i}{\hbar} \left[ \hat{H}(t), \hat{\rho}(t) \right]$$ (2.11)

where $\hat{\rho}$ is the density operator and $\hat{H}$ is the system Hamiltonian. The solution to the von Neumann equation in terms of the unitary time evolution operator is

$$\hat{\rho}(t) = \hat{U}(t, t_0)\hat{\rho}(t_0)\hat{U}^\dagger(t, t_0)$$ (2.12)

where the unitary time evolution operator, $\hat{U}(t, t_0)$ is given as

$$\hat{U}(t, t_0) = \hat{T}e^{-\frac{i}{\hbar} \int_{t_0}^{t} \hat{H}(t')dt'}$$ (2.13)
and \( \hat{T} \) is the time-ordering operator. The time-ordering operator accounts for the fact that the Hamiltonian, \( \hat{H}(t) \), at two instances of time may not commute, thus, making it not possible to analytically evaluate the exponential involved in the unitary time evolution operator. However, for the cases where the Hamiltonian at different instants of time does not commute, the effect of the time ordering operator on the unitary evolution of the system can be easily numerically approximated as in [49]

\[
\hat{T} e^{-(i/\hbar) \int_{t_0}^{t} \hat{H}(t') dt'} = \lim_{N \to \infty} \prod_{n=0}^{N-1} e^{-(i/\hbar) \hat{H}(n\Delta) \Delta} \tag{2.14}
\]

where \( \Delta \equiv (t - t_0)/N \), which is equivalent to considering the Hamiltonian as constant over a short enough interval of time. To study the implementation of single-qubit quantum gates, the Hamiltonian of a spin 1/2 particle in an externally applied magnetic field is considered such that

\[
\hat{H}(t) = \hbar \frac{P(t)}{2} (n_x \hat{\sigma}_x + n_y \hat{\sigma}_y + n_z \hat{\sigma}_z) \tag{2.15}
\]

where \( P(t) \) is a scalar corresponding to the strength of the externally applied field, \( \vec{n} \) corresponds to the orientation of the field, and \( \hat{\sigma}_x, \hat{\sigma}_y, \) and \( \hat{\sigma}_z \) correspond to the components of the particle’s spin angular momentum in the X, Y, and Z directions, respectively. So long as the values of \( \vec{n} \) remain constant through time, this Hamiltonian will commute with itself at all instances of time and, thus, the time-ordering operator is not needed. The corresponding unitary time evolution operator is expressed as

\[
\hat{U}(t, t_0) = \exp \left\{ \frac{-i}{2} (n_x \hat{\sigma}_x + n_y \hat{\sigma}_y + n_z \hat{\sigma}_z) \int_{t_0}^{t} P(t') dt' \right\} \tag{2.16}
\]
2.2. Model Development

which is equivalent to the rotation operator given by equation (2.10) when \( \int_{t_0}^{t} P(t')dt' = \theta \). Thus to implement arbitrary single qubit rotations, it is sufficient to apply an external field to a spin 1/2 particle in a specific direction for a given length of time.

To maintain the level splitting of the energy eigenvalues (i.e., the difference in energy between a spin oriented along the direction of the externally applied field and that oriented in the opposite direction of the field) during the course of a particle’s evolution, a static external field is typically applied whose orientation is considered to be along the Z-axis corresponding to a Hamiltonian of the form

\[
\hat{H}(t) = \frac{\hbar \omega}{2} \sigma_z
\]  

(2.17)

where \( \omega \) is the Larmor frequency of the particle, which is related to the strength of the externally applied field as well as the magnetic moment of the particle itself. While the above is sufficient for inducing rotations about the longitudinal axis (Z-axis), it is also necessary to introduce time-dependent external fields in the X and Y (transverse) directions to implement arbitrary rotations. Assuming the magnetic moment of the particle is isotropic, the resulting Hamiltonian then takes the form

\[
\hat{H}(t) = \frac{\hbar \omega}{2} (\sigma_z + P_x(t)\hat{\sigma}_x + P_y(t)\hat{\sigma}_y)
\]  

(2.18)

where now it may be possible that the Hamiltonian does not commute at two different instants of time, and, thus, the time-ordering operator needs to be used or the evolution needs to be numerically approximated.

Finally, because the rotation operator requires that precession takes place about a specified axis, it is necessary to stop the precession of the particle due to the static field applied in the
Z direction. This is commonly taken into account by examining the evolution of the system state in a rotating reference frame with an angular velocity equal to that of the Larmor frequency for the particle. However, for the purposes of comparing these results with those presented in [55], for the remainder of this chapter this will be accomplished using so-called bias gates, whose action is to cancel out the static externally applied field and, thus, the associated precession. The resulting Hamiltonian is then given by

$$\hat{H}(t) = \frac{\hbar \omega}{2} \left( (1 - P_{\text{Bias}}(t)) \hat{\sigma}_z + P_x(t)\hat{\sigma}_x + P_y(t)\hat{\sigma}_y + P_z(t)\hat{\sigma}_z \right)$$  \hspace{1cm} (2.19)$$

where a pulsed field in the Z direction has been included in addition to the bias gate to allow for rotations about an arbitrary axis while the bias gate is being applied. This is the general form of the Hamiltonian used in the remainder of this chapter. To implement the $P_x(t)$, $P_y(t)$, and $P_z(t)$ pulses, a piecewise function is used in combination with a pulse amplitude following the form of a normal distribution centered around time $t_0$ and having a total duration of $\Delta t_{\text{pulse}}$. Thus,

$$P_{x,y,z}(t) = \begin{cases} 
0 & t < t_0 - \Delta t_{\text{pulse}}/2 \\
\frac{1}{\sqrt{2\pi}\sigma} \exp\left(-\left(\frac{t-t_0}{\sqrt{2}\sigma}\right)^2\right) & t_0 - \Delta t_{\text{pulse}}/2 \leq t \leq t_0 + \Delta t_{\text{pulse}}/2 \\
0 & t > t_0 + \Delta t_{\text{pulse}}/2 
\end{cases}$$  \hspace{1cm} (2.20)$$

where the standard deviation characterizing the pulse is $\sigma = \Delta t_{\text{pulse}}/8$. This choice ensures that 4 standard deviations occur between the beginning of the pulse and the mid-point of the pulse, implying that the pulse function when integrated over time is accurate to within $10^{-2}\%$ (i.e., the cumulative distribution function is $> 0.9999$). The corresponding bias pulse used when implementing these gates is given by
2.2. Model Development

\[ P_{Bias}(t) = \frac{1}{2} \left( \text{erf} \left( \frac{t - (t_0 - \frac{\Delta t_{\text{pulse}}}{2})}{a} \right) - \text{erf} \left( \frac{t - (t_0 + \frac{\Delta t_{\text{pulse}}}{2})}{a} \right) \right) \]  

(2.21)

where the parameter \( a = 0.05 \) ns is chosen to give an approximately similar gate implementation to that of Tabakin [55]. The specific values used for \( t_0 \) and \( \Delta t_{\text{pulse}} \) are presented in the results section.

2.2.2 An Equation of Motion Consisting of Multiple Dissipative Models

To capture the dynamics of the system state under various dissipative models as specific gates are being applied, Tabakin [55] utilizes the following general equation of motion:

\[ \frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] + \mathcal{L}_1 + \mathcal{L}_2 + \mathcal{L}_3 \]  

(2.22)

where \( \mathcal{L}_1 \) represents the dynamics produced by the Lindblad equation and is given by

\[ \mathcal{L}_1 = \gamma_1 \left[ \hat{L}(t)\hat{\rho}\hat{L}^\dagger(t) - \frac{\hat{L}^\dagger(t)\hat{L}(t)\hat{\rho} + \hat{\rho}\hat{L}^\dagger(t)\hat{L}(t)}{2} \right] \]  

(2.23)

and \( \hat{L}(t) \) is the Lindblad spin-space operator, while \( \gamma_1 \) sets the rate of the Lindblad contribution in units of per second. \( \mathcal{L}_2 \) in equation (2.22) represents the dynamics of a simple quantum system under the principle of steepest entropy ascent and is given by

\[ \mathcal{L}_2 = \gamma_2 \left[ \hat{\rho} \left( \tilde{S} - \langle \tilde{S} \rangle \right) - \beta_2(t) \left( \frac{\hat{\rho}\hat{H}(t) + \hat{H}(t)\hat{\rho}}{2} - \hat{\rho} \langle \hat{H}(t) \rangle \right) \right] \]  

(2.24)

where \( \tilde{S} \equiv -\log_e(\hat{\rho}(t)) \) and \( \beta_2(t) \) is expressed as
\[ \beta_2(t) = \frac{\langle (\hat{H} - \langle \hat{H} \rangle)(\tilde{S} - \langle \tilde{S} \rangle) \rangle}{\langle (\hat{H} - \langle \hat{H} \rangle)^2 \rangle} \quad (2.25) \]

\( L_2 \) corresponds to the dissipation operator of SEAQT although here it is written in a notation different from what is used in subsequent chapters. Finally \( L_3 \) represents a system-reservoir interaction written as

\[ L_3 = \gamma_3 \left[ \dot{\rho} \left( \tilde{S} - \langle \tilde{S} \rangle \right) - \beta_3(t) \left( \frac{\dot{\rho} \hat{H}(t) + \hat{H}(t) \dot{\rho}}{2} - \dot{\rho} \langle \hat{H}(t) \rangle \right) \right] \quad (2.26) \]

where two cases for \( \beta_3(t) \) are are considered. The first is when \( \beta_3(t) \) is held constant, and the second is when \( \beta_3(t) \) is computed as

\[ \beta_3(t) = \frac{\langle \Delta E \Delta \tilde{S} \rangle - k_B T_Q \langle \Delta \tilde{S} \Delta \tilde{S} \rangle}{\langle \Delta \tilde{S} \Delta \tilde{S} \rangle - k_B T_Q \langle \Delta E \Delta \tilde{S} \rangle} \quad (2.27) \]

where \( \Delta E = \langle \hat{H} - \langle \hat{H} \rangle \rangle \) and \( \Delta \tilde{S} = \langle \tilde{S} - \langle \tilde{S} \rangle \rangle \). Equation (2.27) is derived by enforcing the condition that the ratio of the rate of heat transfer to the rate of entropy transfer with the heat reservoir is \( \dot{Q}/\dot{\tilde{S}} = k_B T_Q \) where \( T_Q \) is a fixed parameter associated with the temperature of the system-reservoir heat interaction. In equations (2.24) and (2.26), \( \gamma_2 \), and \( \gamma_3 \) correspond to the inverse relaxation times associated with each mechanism. In Section 2.2.3, it is shown that the above system-reservoir interaction model can be derived from fundamental principles within the SEAQT framework.

The two SEAQT based models in combination with the unitary dynamics are used to study the dissipation occurring as single-qubit operations are applied. The results shown in Section 2.3 primarily focus on accurate gate implementation as well as on the dissipation captured by the SEAQT equation of motion both with and without reservoir interactions present.
2.2. Model Development

2.2.3 SEAQT Equation of Motion for a Simple System Interacting with a Reservoir

To derive an equation of motion under the principle of SEA for a simple quantum system, $S$, experiencing a heat interaction with a single reservoir, $R$, it is first necessary to reduce the overall Hilbert space $\mathcal{H} = \mathcal{H}_S \otimes \mathcal{H}_R$, which is of dimension $\dim(S) \cdot \dim(R)$, to a simpler form of dimension $\dim(S) + \dim(R)$. In the following work, it will be assumed that the system $S$, which will encapsulate the qubit, is a two-level system, implying that there are $\dim(S) = 2$ degrees of freedom.

It will further be assumed that the degrees of freedom representing the reservoir, $R$, are orthogonal and independent to the degrees of freedom of $S$. This permits the two sets of energy levels (i.e., those of $S$ and those of $R$) to be broken into two independent, unentanglable subsystems of energy levels. This could, for example, perhaps be realized by a quantum harmonic oscillator where the ground state and first excited state serve as qubit $S$ and all higher states serve as the reservoir $R$. Although no specific physical realization is assumed in this chapter, one is suggested in Chapter 6. These assumptions allow the composite Hilbert space to be simplified as follows:

$$\mathcal{H} = \mathcal{H}_S \oplus \mathcal{H}_R \quad (2.28)$$

where $\oplus$ represents the direct sum of the two subspaces, $\mathcal{H}_S$ represents the subspace corresponding to subsystem $S$, and likewise $\mathcal{H}_R$ represents the subspace of the reservoir $R$. It is also noted that now $\dim(\mathcal{H}) = \dim(\mathcal{H}_S) + \dim(\mathcal{H}_R)$, as desired. Next, the assumption is made that the density operator, $\hat{\rho}$, and the Hamiltonian, $\hat{H}$, can both be written as block-diagonal matrices over each of the two subspaces, i.e., $\hat{\rho} = \hat{\rho}_S \oplus \hat{\rho}_R$ and $\hat{H} = \hat{H}_S \oplus \hat{H}_R$, respectively, where $\oplus$ represents the so-called matrix direct sum. This implies that all of
the projectors in $\mathcal{H}_R$ are orthogonal to the projectors in $\mathcal{H}_S$ for both the density operator and the Hamiltonian. The eigenvalues of each operator in subspace $S$ can then be computed solely by the components of the operator in $\mathcal{H}_S$ and likewise for subspace $R$. This allows any function of these operators such as, for example, the square root, exponential, or logarithm, to be written as a block-diagonal matrix as well. Further, standard matrix multiplication of block-diagonal matrices whose "blocks" are the same size (such as $\hat{H}$ and $\hat{\rho}$ above) can be written in terms of standard matrix multiplication of each of the individual blocks (i.e., $(\hat{\rho}_S \oplus \hat{\rho}_R)(\hat{H}_S \oplus \hat{H}_R) = (\hat{\rho}_S \hat{H}_S) \oplus (\hat{\rho}_R \hat{H}_R)$). This allows the reversible dynamics of the von Neumann equation to be written as

$$\frac{d\hat{\rho}}{dt} = \frac{d}{dt} (\hat{\rho}_S \oplus \hat{\rho}_R) = \frac{d\hat{\rho}_S}{dt} \oplus \frac{d\hat{\rho}_R}{dt} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] = -\frac{i}{\hbar} [\hat{H}_S \oplus \hat{H}_R, \hat{\rho}_S \oplus \hat{\rho}_R]$$

or

$$\frac{d\hat{\rho}_S}{dt} \oplus \frac{d\hat{\rho}_R}{dt} = -\frac{i}{\hbar} \left( [\hat{H}_S, \hat{\rho}_S] \oplus [\hat{H}_R, \hat{\rho}_R] \right)$$

Now considering the dissipation operator of SEAQT, $D(\hat{\rho})/Dt$, it is written as

$$\frac{D(\hat{\rho})}{Dt} = -\frac{1}{2\tau_D} \left( \sqrt{\hat{\rho}} \hat{D} + \left( \sqrt{\hat{\rho}} \hat{D} \right)^\dagger \right)$$

With the assumption that $\hat{\rho} = \hat{\rho}_S \oplus \hat{\rho}_R$, it can be shown that $\sqrt{\hat{\rho}} = \sqrt{\hat{\rho}_S} \oplus \sqrt{\hat{\rho}_R}$ and all that remains to form an equation of motion on each subspace (i.e., the subspace corresponding to the system of interest $S$ and the subspace corresponding to the reservoir $R$) is to show that the dissipation operator of SEAQT can be decomposed into components acting on each of these subspaces. This is done by first examining the ratio of determinants that define $\hat{D}$, namely,
2.2. Model Development

\[
\tilde{D} = \sqrt{\rho} \begin{vmatrix}
\tilde{B} \ln(\tilde{\rho}) & \tilde{R}_0 & \tilde{R}_1 & \cdots & \tilde{R}_n \\
(\tilde{R}_0, \tilde{B} \ln(\tilde{\rho})) & (\tilde{R}_0, \tilde{R}_0) & (\tilde{R}_0, \tilde{R}_1) & \cdots & (\tilde{R}_0, \tilde{R}_n) \\
(\tilde{R}_1, \tilde{B} \ln(\tilde{\rho})) & (\tilde{R}_1, \tilde{R}_0) & (\tilde{R}_1, \tilde{R}_1) & \cdots & (\tilde{R}_1, \tilde{R}_n) \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
(\tilde{R}_n, \tilde{B} \ln(\tilde{\rho})) & (\tilde{R}_n, \tilde{R}_0) & (\tilde{R}_n, \tilde{R}_1) & \cdots & (\tilde{R}_n, \tilde{R}_n)
\end{vmatrix}
\]

where \( \Gamma \) is a Gram determinant defined later in the chapter. To enforce that there is only energy transfer between the two subsystems (i.e., a heat interaction), it is noted that \( \tilde{I} = \tilde{I}_S \oplus \tilde{I}_R = \tilde{I}_S \oplus \hat{0}_R + \hat{0}_S \oplus \tilde{I}_R \) and the generators of the motion, which operate on the overall system Hilbert space, are chosen as \( \tilde{R}_0 = \tilde{I}_S \oplus \hat{0}_R, \tilde{R}_1 = \hat{0}_S \oplus \tilde{I}_R, \) and \( \tilde{R}_2 = \tilde{H}_S \oplus \tilde{H}_R. \) Here \( \tilde{I} \) and \( \hat{0} \) are the identity and null operators, respectively. With this choice, \( \tilde{D} \) reduces to

\[
\tilde{D} = \sqrt{\rho} \begin{vmatrix}
\tilde{B} \ln(\tilde{\rho}) & \tilde{I}_S \oplus \hat{0}_R & \hat{0}_S \oplus \tilde{I}_R & \tilde{H}_S \oplus \tilde{H}_R \\
(\tilde{I}_S \oplus \hat{0}_R, \tilde{B} \ln(\tilde{\rho})) & (\tilde{I}_S \oplus \hat{0}_R, \tilde{I}_S \oplus \hat{0}_R) & (\tilde{I}_S \oplus \hat{0}_R, \hat{0}_S \oplus \tilde{I}_R) & (\tilde{I}_S \oplus \hat{0}_R, \tilde{H}_S \oplus \tilde{H}_R) \\
(\hat{0}_S \oplus \tilde{I}_R, \tilde{B} \ln(\tilde{\rho})) & (\hat{0}_S \oplus \tilde{I}_R, \tilde{I}_S \oplus \hat{0}_R) & (\hat{0}_S \oplus \tilde{I}_R, \hat{0}_S \oplus \tilde{I}_R) & (\hat{0}_S \oplus \tilde{I}_R, \tilde{H}_S \oplus \tilde{H}_R) \\
(\tilde{H}_S \oplus \tilde{H}_R, \tilde{B} \ln(\tilde{\rho})) & (\tilde{H}_S \oplus \tilde{H}_R, \tilde{I}_S \oplus \hat{0}_R) & (\tilde{H}_S \oplus \tilde{H}_R, \hat{0}_S \oplus \tilde{I}_R) & (\tilde{H}_S \oplus \tilde{H}_R, \tilde{H}_S \oplus \tilde{H}_R)
\end{vmatrix}
\]

(2.33)

where it is noted that \( \tilde{B} \ln(\tilde{\rho}) = \tilde{B}_S \ln(\tilde{\rho}_S) \oplus \tilde{B}_R \ln(\tilde{\rho}_R) \) allows \( \tilde{D} \) to be written as \( \tilde{D} = \tilde{D}_S \oplus \tilde{D}_R \) so that
\[ \tilde{D}_S = \sqrt{\hat{\rho}_S} \]

\[ (\hat{I}_S \oplus \hat{0}_R, \hat{B} \ln(\hat{\rho})) \quad (\hat{I}_S \oplus \hat{0}_R, \hat{I}_S \oplus \hat{0}_R) \quad (\hat{0}_S \oplus \hat{I}_R, \hat{I}_S \oplus \hat{0}_R) \quad (\hat{0}_S \oplus \hat{I}_R, \hat{0}_S \oplus \hat{I}_R) \quad (\hat{0}_S \oplus \hat{I}_R, \hat{I}_S \oplus \hat{0}_R) \quad (\hat{0}_S \oplus \hat{I}_R, \hat{H}_S \oplus \hat{H}_R) \]

\[ \Gamma \]

(2.34)

and similarly for \( \tilde{D}_R \) where the generators of the motion have been separated into the components that act on each subspace. This permits the dissipation operator for the overall system to be written as

\[ \frac{D(\hat{\rho})}{Dt} = \left( \frac{D(\hat{\rho})}{Dt} \right)_S \oplus \left( \frac{D(\hat{\rho})}{Dt} \right)_R \]

(2.35)

where \( (D(\hat{\rho})/Dt)_S \) is the portion of the dissipation operator acting on the subspace of the system of interest and \( (D(\hat{\rho})/Dt)_R \) the portion acting on the subspace corresponding to the reservoir. Thus, the overall equation of motion can be decomposed into a portion acting on each subspace where the coupling between subspaces enters through the dissipation operator. The equation of motion on the subspace corresponding to the system of interest is then given by

\[ \frac{d\hat{\rho}_S}{dt} = -\frac{i}{\hbar} [\hat{H}_S, \hat{\rho}_S] - \frac{1}{\tau_D} \left( \frac{D(\hat{\rho})}{Dt} \right)_S \]

(2.36)

where the dissipation operator is computed as

\[ \left( \frac{D(\hat{\rho})}{Dt} \right)_S = \frac{1}{2} \left( \sqrt{\hat{\rho}_S} \tilde{D}_S + (\sqrt{\hat{\rho}_S} \tilde{D}_S)^\dagger \right) \]

(2.37)
and the ratio of determinants is expressed as

\[
\tilde{D}_S = \sqrt{\hat{\rho}_S} \begin{vmatrix}
\hat{B}_S \ln(\hat{\rho}_S) & \hat{I}_S & \hat{0}_S & \hat{H}_S \\
\langle s \rangle_S & P_S & 0 & \langle e \rangle_S \\
\langle s \rangle_R & 0 & P_R & \langle e \rangle_R \\
\langle es \rangle_S + \langle es \rangle_R & \langle e \rangle_S & \langle e^2 \rangle_S + \langle e^2 \rangle_R
\end{vmatrix}
\]

Expanding the determinant in the numerator and simplifying yields

\[
\tilde{D}_S = \sqrt{\hat{\rho}_S} \left( \hat{B}_S \ln(\hat{\rho}_S) - \frac{B_1}{\Gamma} \hat{I}_S - \frac{B_3}{\Gamma} \hat{H}_S \right) \tag{2.39}
\]

where

\[
B_1 = \begin{vmatrix}
\langle s \rangle_S & 0 & \langle e \rangle_S \\
\langle s \rangle_R & P_R & \langle e \rangle_R \\
\langle es \rangle_S + \langle es \rangle_R & \langle e \rangle_R & \langle e^2 \rangle_S + \langle e^2 \rangle_R
\end{vmatrix} \tag{2.40}
\]

\[
B_3 = \begin{vmatrix}
\langle s \rangle_S & P_S & 0 \\
\langle s \rangle_R & 0 & P_R \\
\langle es \rangle_S + \langle es \rangle_R & \langle e \rangle_S & \langle e \rangle_R
\end{vmatrix} \tag{2.41}
\]

and

\[
\Gamma = \begin{vmatrix}
P_S & 0 & \langle e \rangle_S \\
0 & P_R & \langle e \rangle_R \\
\langle e \rangle_S & \langle e \rangle_R & \langle e^2 \rangle_S + \langle e^2 \rangle_R
\end{vmatrix} \tag{2.42}
\]

Next, by defining \( \langle e \rangle_{S(R)} = P_{S(R)} \langle e \rangle_{S(R)} \) and likewise for \( \langle s \rangle_{S(R)} \), \( \langle es \rangle_{S(R)} \), and \( \langle e^2 \rangle_{S(R)} \), the probabilities in each subspace are normalized, and it can be shown that the fraction \( B_3/\Gamma \)

reduces to

\[
\frac{B_3}{\Gamma} = \frac{P_S}{P_R} \left( \langle \tilde{e}s \rangle_S - \langle \hat{e} \rangle_S \langle \bar{s} \rangle_S \right) + \left( \langle \tilde{e}s \rangle_R - \langle \hat{e} \rangle_R \langle \bar{s} \rangle_R \right)
\]

\[
\frac{P_S}{P_R} \left( \langle e^2 \rangle_S - \langle \hat{e} \rangle_S^2 \right) + \left( \langle e^2 \rangle_R - \langle \hat{e} \rangle_R^2 \right)
\]

(2.43)

In the limit for \( P_R >> P_S \), the above reduces to

\[
\frac{B_3}{\Gamma} \approx \langle \tilde{e}s \rangle_R - \langle \hat{e} \rangle_R \langle \bar{s} \rangle_R \]

\[
\langle e^2 \rangle_R - \langle \hat{e} \rangle_R^2
\]

(2.44)

Assuming now that the normalized probability distribution in \( \mathcal{H}_R \) (i.e., \( \hat{\rho}_R/P_R \)) follows a canonical distribution characterized by \( \beta_R \) and \( \hat{H}_R \), it can also be shown, regardless of the form of \( \hat{H}_R \), that

\[
\frac{B_3}{\Gamma} \approx -\beta_R
\]

(2.45)

Next, to obtain an equation of motion for the normalized density operator, \( \hat{\rho}_S \), on subspace \( \mathcal{H}_S, \hat{\rho}_S = P_S \hat{\rho}_S \) and the chain rule are used to evaluate the derivative as

\[
\frac{d\hat{\rho}_S}{dt} = P_S \frac{d\hat{\rho}_S}{dt} + \hat{\rho}_S \frac{dP_S}{dt} = -\frac{iP_S}{\hbar} \left[ \hat{H}_S, \hat{\rho}_S \right] - \left( \frac{D(\hat{\rho})}{Dt} \right)_S
\]

(2.46)

Noting that

\[
\frac{dP_S}{dt} = \frac{d\text{Tr}(\rho_S)}{dt} = \text{Tr} \left( \frac{d\hat{\rho}_S}{dt} \right) = -\frac{1}{\tau_D} \text{Tr} \left( \left( \frac{D(\hat{\rho})}{Dt} \right)_S \right)
\]

(2.47)

which can be further reduced to
\[
\frac{dP_S}{dt} = -\frac{1}{\tau_D} \text{Tr} \left( \sqrt{P_S \hat{\rho}_S \hat{D}_S} \right) = -\frac{1}{\tau_D} \text{Tr} \left( P_S \hat{\rho}_S \left( \hat{B}_S \ln(\hat{\rho}_S) - \frac{B_1}{\Gamma} \hat{I}_S - \frac{B_3}{\Gamma} \hat{H}_S \right) \right) \quad (2.48)
\]

and finally to

\[
\frac{dP_S}{dt} = -\frac{P_S}{\tau_D} \left( \langle \tilde{s} \rangle_S + \ln(P_S) - \frac{B_1}{\Gamma} - \frac{B_3}{\Gamma} \langle \tilde{e} \rangle_S \right) \quad (2.49)
\]

where \( \langle \tilde{s} \rangle_S = \hat{\rho}_S \ln(\hat{\rho}_S) \). Substituting this last expression in for \( d\hat{\rho}/dt \) yields

\[
P_S \frac{d\hat{\rho}_S}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_S, \hat{\rho}_S \right] - \left( \frac{D(\hat{\rho})}{Dt} \right)_S - \hat{\rho}_S \frac{dP_S}{dt} \quad (2.50)
\]

Next, substituting \( \hat{\rho}_S = P_S \hat{\rho}_S \) into the dissipation operator on \( \mathcal{H}_S \) and canceling terms gives

\[
\frac{d\hat{\rho}_S}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_S, \hat{\rho}_S \right] - \left( \frac{D(\hat{\rho})}{Dt} \right)_S' \quad (2.51)
\]

where

\[
\left( \frac{D(\hat{\rho})}{Dt} \right)_S' \equiv \frac{1}{2\tau_D} \left( \sqrt{\hat{\rho}_S \hat{D}' + (\sqrt{\hat{\rho}_S \hat{D}'})^\dagger} \right) \quad (2.52)
\]

and

\[
\hat{D}' \equiv \sqrt{\hat{\rho}_S} \left( \hat{B}_S \ln(\hat{\rho}_S) - \langle \tilde{s} \rangle_S \hat{I}_S + \beta_R \left( \hat{H}_S - \langle \tilde{e} \rangle_S \hat{I}_S \right) \right) \quad (2.53)
\]

These final three equations represent the equation of motion for a system experiencing a heat interaction with a reservoir at a temperature \( T_R = 1/k_B \beta_R \). Note that this can be extended to account for multiple reservoir interactions. Furthermore, because the only assumption
regarding the system state is that $P_S << P_R$, it is possible to choose $\beta_R$ such that either of the reservoir models presented in [55] are reproduced. A constant reservoir temperature leads to what is known as the Korsch bath [35] equation, and choosing a value of $\beta_R$ based on the constraint given in equation (2.27) yields the constant $\dot{Q}/\dot{S}$ requirement [14]. With the completion of this derivation, the evolution of a qubit’s state under various dissipation models can be examined during single-qubit gates, the results of which are presented in Section 2.3.

2.3 Model Results

This section presents results for the evolution of the system state during free evolution as well as during the implementation of the Not gate under unitary dynamics, the SEAQT equation of motion, and the SEAQT equation of motion incorporating a reservoir interaction at a constant temperature. First, Section 2.3.1 presents the free evolution under both the reversible dynamics of the von Neumann equation as well as the non-unitary dynamics of the SEAQT equation of motion, and comparisons are made between the published data of Tabakin [55] and the results generated here. Section 2.3.2 then presents the system state evolution during the application of a Not gate, again using the reversible dynamics of the von Neumann equation and the non-unitary dynamics of the SEAQT equation of motion. Finally, the effects of system reservoir interactions on the free evolution are presented in Section 2.3.3 and the results again compared with the published data of Tabakin [55]. Appendix A includes the evolutions of the system state under various pulse sequences.
2.3. Model Results

2.3.1 Free Evolution

This section examines the evolution of the system state under a time-independent Hamiltonian representing a static magnetic field applied in the Z direction, and thus $P_{Bias}(t) = 0$ and $P_{x,y,z}(t) = 0$ in the Hamiltonian given in equation (2.19) throughout the course of the evolution. The initial polarization vector (from which one can compute the elements of the density operator) is $\vec{P} = \vec{r} = [0.5, 0, 0.8]$. Figure 2.2 shows the evolution of the polarization vector and the density operator eigenvalues for both the unitary dynamics and the dynamics of the SEAQT equation of motion for both the published data of Tabakin [55] and the results generated as a part of the current work. Figure 2.3 shows the corresponding system energy and entropy evolutions. In Figure 2.2a, it is seen that for all cases, the Z polarization remains constant throughout the course of the dynamics whereas the X and Y polarization exhibit oscillatory behavior, which is expected since the external field represented by the Hamiltonian is along the Z direction.

The magnitude of the oscillations for the X and Y polarizations remains constant under the unitary dynamics. However for the dynamics of the SEAQT equation of motion, the oscillation magnitude exhibits a decay. This is a result of the dissipation occurring during the evolution and represents decoherence between the two energy eigenlevels of the system. A slight discrepancy can be seen between the results of the published data of Tabakin for the SEAQT equation of motion and the SEAQT results generated here. While the cause of this is not completely clear, it is thought to be caused by a difference in the relaxation time used in the published data and that which is used here.

Figure 2.2b shows the density operator eigenvalue evolution. As expected, both eigenvalues remain constant throughout the evolution for the unitary dynamics. However, for the dynamics of the SEAQT equation of motion, the larger eigenvalue decreases in magnitude.
and the smaller increases by the same amount, corresponding to an increase in system entropy caused by the dissipation.

Figure 2.2: Polarization vector and density operator eigenvalue evolution; the X, Y, and Z polarization components of the results generated here are red, blue, and black, respectively. The polarization components generated by Tabakin are green for the unitary dynamics and light blue for the dynamics of the SEAQT equation of motion and generally lie on top of the unitary and SEAQT results generated in the present work. A similar color scheme is applied to the evolution of the two density operator eigenvalues.

Figure 2.3 shows the system entropy and energy evolution under both the unitary dynamics and the dynamics of the SEAQT equation of motion during free evolution. Figure 2.3a indicates that the system entropy remains constant for the unitary evolution, as expected, but for the dynamics of the SEAQT equation of motion increases until the system has reached stable equilibrium. Figure 2.3b shows that for all cases, the energy remains at a constant value throughout the evolution, as expected.
2.3. Model Results

2.3.2 Free Evolution and Not Gate

This section examines the evolution of the system state under a time-dependent Hamiltonian representing a static magnetic field applied in the Z direction and a Not gate applied at roughly 33 ns. To implement the Not gate, $P_{y,z}(t) = 0$ throughout the evolution, and the pulse parameters used to characterize $P_x(t)$ and $P_{Bias}(t)$ are $\Delta t_{Pulse} = 1$ ns and $t_0 = 33.1$ ns. These parameters and the definitions of the pulses given in Section 2.2 are sufficient to fully characterize the time evolution of the system Hamiltonian. Here the initial polarization vector is again $\vec{P} = [0.5, 0, 0.8]$. Figure 2.4 shows the evolution of the polarization vector and the density operator eigenvalues for both the unitary dynamics and the dynamics of the SEAQT equation of motion for both the published data of Tabakin and the results generated as a part of the current work.

Figure 2.5 shows the corresponding system energy and entropy evolutions. In Figure 2.4a, it is seen that the Z polarization, upon application of the Not gate at 33 ns, flips $P_z = 0.8 \rightarrow -0.8$ and otherwise remains constant for both the unitary dynamics and the dynamics of the
SEAQT equation of motion. The X and Y polarizations again exhibit oscillatory behavior during periods of free evolution, and both experience a phase shift during application of the Not gate, where again the magnitude of the oscillations decay under the dynamics of the SEAQT equation of motion. Figure 2.4b shows the evolution of the density operator eigenvalues where it is again seen that the eigenvalues remain constant under the unitary dynamics and approach a state of higher entropy for the dynamics of the SEAQT equation of motion.

![Polarization Evolution](image1.png) ![Eigenvalue Evolution](image2.png)

Figure 2.4: Polarization vector and density operator eigenvalue evolution; the X, Y, and Z polarization components of the results generated here are red, blue, and black, respectively. The polarization components generated by Tabakin are green for the unitary dynamics and light blue for the dynamics of the SEAQT equation of motion and generally lie on top of the SEAQT results generated here. A similar color scheme is applied to the evolution of the two density operator eigenvalues. The evolutions of the unitary dynamics end at $t \approx 50$ ns as this is where the published data ends.

Figure 2.5 shows the system entropy and energy evolution under both the unitary dynamics and the dynamics of the SEAQT equation of motion during free evolution and the application of the Not gate. In Figure 2.5a, it is again seen that the system entropy remains constant for unitary evolution, as expected, but for the dynamics of the SEAQT equation of motion increases until the system has reached stable equilibrium. Now, however, a small jump in the system entropy can be seen during application of the Not gate at $t \approx 32$ ns. This
happens because during the application of the Not gate, the system is farther from the stable equilibrium state associated with \( \hat{H}(t) \) and its current value of energy, which in this case results in a higher entropy generation rate. Thus, it is concluded that the application of pulsed gates leads to slightly higher entropy generation rates, which for short periods of time increases the rate at which decoherence occurs.

Figure 2.5b shows the details of the energy evolution during the application of the Not gate. Under both dynamical models, the energy exhibits a minimum before approaching the negative of its original value upon completion of the Not gate. The differences in energy evolution between the results generated here and the published data are due to the exact numerical implementation of the bias and gate pulses and could easily be reconciled but are not since that is not of primary focus here.

Figure 2.5: Entropy and energy evolutions; both the energy and entropy predicted by Tabakin are dashed green for the unitary dynamics and dotted light blue for the dynamics of the SEAQT equation of motion. The evolutions of the reversible dynamics end at \( t \approx 50 \) ns as this is where the published data ends.

2.3.3 Free Evolution under Reservoir Interactions

This section examines the free evolution of system state under a time-independent Hamiltonian representing a static magnetic field applied in the Z direction while the system experiences a heat interaction with a reservoir at constant temperature. Thus, as was the case in Section 2.3.1, $P_{\text{Bias}}(t) = 0$ and $P_{x,y,z}(t) = 0$ throughout the course of the evolution. The initial polarization vector (from which one can compute the elements of the density operator) is $\vec{P} = [0.5, 0, 0.8]$. Figure 2.6 shows the evolution of the polarization vector and the density operator eigenvalues for the dynamics of the SEAQT equation of motion incorporating a heat interaction with a reservoir at constant temperature. This figure also shows the data produced by Tabakin’s modeling with a Korsch type reservoir (where the reservoir temperature is constant) and a reservoir proposed by Beretta [14] satisfying the constraint given by equation 2.27. Figure 2.7 shows the corresponding system energy and entropy evolutions.

In Figure 2.6a, it is seen that, contrary to Figure 2.2a, the Z polarization decays toward a value of zero. The X and Y polarizations again exhibit oscillatory behavior of decaying magnitude. It is worth noting that the SEAQT plus reservoir results generated here exactly match those of the Korsch bath. With the lack of constraints on the value of $\beta_R$ in the SEAQT equation of motion incorporating a reservoir interaction, it is also possible to reproduce the dynamics of the Beretta type bath. Figure 2.6b shows the evolution of the density operator eigenvalues where it is seen that both approach the same value $\lambda_{1,2} \approx 0.5$, corresponding to a maximally mixed state. This is to be expected since the reservoir temperature $T_R = 0.273$ K is much higher than the temperature corresponding to the energy of the initial state $T_0 = 0.00093$ K and, thus, energy and entropy flow into the system from the reservoir.

Figure 2.3 shows the corresponding system entropy and energy evolution for the reservoir interaction model. In Figure 2.3a, it is seen that for both reservoir models, the system entropy
2.3. Model Results

![Polarization Evolution](image1)

Figure 2.6: Polarization vector and density operator eigenvalue evolution; the X, Y, and Z polarization components of the SEAQT results generated here are red, blue, and black, respectively. The polarization components generated by Tabakin are dashed green for the Korsch-type bath and dashed black for the Beretta-type bath. The Tabakin eigenvalues plotted in dashed green correspond to those of the Korsch bath evolution.

Figure 2.6 shows that for reservoir interaction types, the system approaches a state of zero energy corresponding to no net Z polarization. Note that the Beretta-type bath reaches stable equilibrium earlier than the Korsch-type bath, indicating that more energy and entropy are transferred into the system early in the interaction with the Beretta bath compared to with the Korsch bath.

Figure 2.8 shows the system-reservoir energy and entropy transfer. Figure 2.8a shows the rate of change of the total system entropy, $\dot{S}$ in red and the entropy generation rate of the system under the Beretta equation (i.e. with no reservoir interaction occurring), $\dot{S}_{Gen}$ in dark blue. The entropy transfer from the reservoir to the system is then computed as the difference $\dot{S}_{in} = \dot{S} - \dot{S}_{Gen}$. Finally, the rate of change of the system energy, which is attributed to the heat interaction, is computed as $\dot{Q} = Tr \left( \dot{H} \rho / dt \right)$ and shown in light blue. Each quantity is shown to reach a maximum value at a unique time before decaying towards zero as the system approaches thermal equilibrium with the reservoir.
Figure 2.7: Entropy and energy evolution. Both the energy and entropy predicted by Tabakin are dashed green for the Korsch-type bath and dashed black for the Beretta-type bath.

Figure 2.8b then shows the ratio of the system’s rate of energy change to its rate of entropy change, $\dot{Q}/\dot{S}$. This ratio varies throughout the evolution, indicating that the temperature associated with the reservoir heat interaction $T_Q = (1/k_B)\dot{Q}/\dot{S}$ also varies. It is noted that by choosing the reservoir temperature $\beta_R$ based on the formulation in [14], that the value of $T_Q$ can be held fixed throughout the evolution.
2.4 Conclusions

This work presents the system state dynamics of three different models: the unitary dynamics of standard quantum mechanics, the non-unitary, dissipative dynamics of the standard SEAQT equation of motion, and dissipative dynamics of a system-reservoir heat interaction model within the SEAQT framework. As expected, no dissipation occurs during the unitary dynamics, and, thus, the system’s eigenvalues and entropy remain constant, and there is no loss of coherence between the two levels of the system. This is in contrast to evolution under the standard SEAQT equation of motion, which accounts for dissipation within the system and, thus, results in an increase in system entropy and decoherence. Finally, the SEAQT reservoir heat interaction model also captures the decoherence occurring within the system. However, now the underlying dissipation is caused by a combination of the dissipation within the system itself and the transfer of energy and entropy from the relatively high-temperature
Comparing the results of the two SEAQT models, it is seen that a larger overall rise in entropy occurs under the reservoir heat interaction than under the standard SEAQT equation of motion. This suggests that by adjusting the reservoir temperature, it may be possible to control the amount of energy and entropy transferred to or from the system. Furthermore, it is noted that for both dissipative models, the dissipation causes the system to approach a state whose eigenvectors are aligned with the eigenvectors of the Hamiltonian, which in this work happens to be along the Z direction during the static evolution. This, in combination with the ability to directly relate a two-level system’s energy to a temperature at stable equilibrium, is used later in developing a system-reservoir interaction scheme for limiting decoherence.

Another aspect to note is the effect of the pulsed Hamiltonian on system state evolution. It is seen that during the application of the Not gate, a slight increase in the entropy generation rate occurs. This suggests that longer pulses exhibiting a less rapid change in the system Hamiltonian lead to less entropy generation than shorter pulses. For certain quantum computing applications, however, this may provide a trade-off when interactions with other qubits or static fields cannot be controlled and, thus, there is undesired precession occurring during the application of a gate. Because this pulsed Hamiltonian approach forms the basis for implementing more complex quantum computing algorithms, it is necessary to have pulses that accurately implement the operation required by the quantum algorithm while minimizing the increase in the entropy generation rate during the algorithm. With knowledge of the effect of a unitary operation representing a gate on the system’s state, a system reservoir interaction can be used to account for and correct the dissipation that occurs during the gate by removing entropy.

Finally, the presentation of a general heat interaction model within the SEAQT framework
for a simple quantum system captures both the dynamics of the Korsch-bath model as well as
the Beretta-bath model (which is to be done as follow up work). Furthermore, this interaction
scheme can be extended to a general quantum system composed of multiple qubits, which
may each be locally interacting with reservoirs at different temperatures. This extension
appears in Chapter 6. Additional follow up work includes showing that an appropriate choice
of $\beta_R(t)$ also replicates the system state dynamics under the Lindblad equation for various
Lindblad operators.
Appendices
Appendix A

Additional Unitary Evolutions

This appendix presents additional unitary evolutions of system state under various free evolution-gate sequence combinations. First, Section A.1 illustrates the evolution during the application of a Hadamard Gate. Next, Section A.2 presents the evolution during the application of a Hadamard Gate followed by free precession about the X-axis (as opposed to the Z-axis as was done previously). Finally, Section A.3 shows the evolutions of the system during a Hadamard-Not-Hadamard gate pulse sequence. In all cases, it is seen that the system’s state evolution matches very well (except for minor deviations during gate implementation due to the numerical implementation) with the results of Tabakin [55].

A.1 Hadamard Gate and Free Evolution about the Z-Axis

This section presents the unitary evolution of the system state during the application of a Hadamard gate. The gate is centered at $t_0 = 33.1$ ns and has a duration of $\Delta t_{\text{pulse}} = 1.4$ ns.
A.2 Hadamard Gate and Free Evolution about the X-Axis

This section presents the unitary evolution of the system state during the application of a Hadamard gate followed by free precession about the X-axis. The gate is centered at \( t_0 = 33.1 \) ns and has a duration of \( \Delta t_{\text{pulse}} = 1.4 \) ns.
A.3 Hadamard-Not-Hadamard Gate Pulse Sequence

This section presents the unitary evolution of the system state during the application of a Hadamard gate, followed by a Not gate, and then followed by another Hadamard gate. The first Hadamard gate is centered at $t_0 = 47.2$ ns and has a duration of $\Delta t_{pulse} = 1.4$ ns. The Not gate is centered at $t_0 = 94.2$ ns and has a duration of $\Delta t_{pulse} = 1.4$ ns. The second Hadamard gate is centered at $t_0 = 142.2$ ns and has a duration of $\Delta t_{pulse} = 1.4$ ns.
Figure A.5: Polarization vector and eigenvalue evolution.

Figure A.6: Energy evolution during the first Hadamard gate (A.6a) and the Not gate (A.6b).
Chapter 3

Modeling the Entropy Generation and the Effects of a varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

3.1 Introduction

Understanding how irreversibilities occur at the quantum level is key to being able to limit their degrading effect on the information stored on quantum computing systems. With a fundamental model of how these irreversibilities occur, it is possible to design better algorithms and control schemes to minimize the decoherence. This work aims to show that steepest-entropy-ascent quantum thermodynamics (SEAQT) can be used to predict irreversibilities that are experimentally observed at the quantum level during a nuclear magnetic resonance (NMR) experiment. SEAQT is well suited for this problem because it inherently predicts irreversibilities within the system and does not rely on the assumption that the system is interacting with an environment. Furthermore, SEAQT predicts the entire system state evolution and dissipation at any given instant of time and not just mean values between the beginning and end states.
To accomplish this, this work attempts to predict the experimental results of Batalhao et al. [3], who observe non-equilibrium entropy production in an isolated system during quenches of an externally applied magnetic field. The system considered is that of a Carbon atom in a CHCl$_3$ molecule in a liquid state NMR experiment. Specifically, these authors define a so-called “mean entropy production”, $\langle \Sigma \rangle$, written in terms of both the von Neumann entropy, $S$, and the Kullback-Leibler relative entropy, $S_{KL}$, between the system’s state in a given process and the corresponding state in a time-reversed process. Thus,

$$\langle \Sigma \rangle = S_{KL} (\hat{\rho}_t^F || \hat{\rho}_{\tau-t}^B) + S (\hat{\rho}_t^F) - S (\hat{\rho}_{\tau-t}^B),$$

(3.1)

where $\hat{\rho}_t^F$ is the density matrix at time $t$ in the forward process, $\hat{\rho}_{\tau-t}^B$ is the density matrix at time $\tau - t$ for the backward process, and the relative entropy is computed as

$$S_{KL} (\hat{\rho}_t^F || \hat{\rho}_{\tau-t}^B) = \text{Tr}(\hat{\rho}_t^F (\ln(\hat{\rho}_t^F) - \ln(\hat{\rho}_{\tau-t}^B)))$$

(3.2)

Here $\tau$ is the total time duration of the forward process otherwise known as the quench time. At the final quench time, the so-called “mean entropy production” defined by Batalhao et al. [3] can equivalently be found from

$$\langle \Sigma \rangle = \sum_{i=1}^{4} P_F(W_i) \Sigma_i$$

(3.3)

where $P_F(W_i)$ is the probability of a particular process $i$ occurring with an associated value of work, $W_i$ and entropy production, $\Sigma_i$. In fact, there are four possible processes for the forward process (and four for the backward) since there are two possible initial states ($|\uparrow\rangle$ and $|\downarrow\rangle$) and two possible final states ($|\uparrow\rangle$ and $|\downarrow\rangle$) for the two-level system considered here.
3.1. Introduction

The entropy production for a given process $i$ is then calculated as

$$\Sigma_i = \beta (W_i - \Delta F_i)$$  \hspace{1cm} (3.4)

where $\Delta F_i$ is the free energy difference between the forward and backward processes, which can be calculated using the Tasaki-Crooks fluctuation relation $[19, 56]$ given by

$$\frac{P^F(W_i)}{P^B(-W_i)} = e^{\beta (W_i - \Delta F_i)}$$  \hspace{1cm} (3.5)

where $P_B(-W_i)$ is the probability that the negative of the value of work done on forward process $i$ is done during the time-reversed process $i$. The probability $P_F(W_i)$ that a given value of work, $W_i$, is done for forward process $i$ is $p^{F_i,\tau}_{m|n} p^{eq,0}_n$ ($i = 1, ..., 4$, $m = 0, 1$, $n = 0, 1$) where

$$p^{eq,0}_n = e^{\beta \epsilon_n} / Z_0$$  \hspace{1cm} (3.6)

corresponds to the probability that the system is in state $n$ at time $t = 0$. $\beta$ corresponds to the initial system temperature, $\epsilon_n$ is the $n^{th}$ energy eigenvalue, and $Z_0$ is the partition function at $t = 0$. Furthermore,

$$p^{F_i,\tau}_{m|n} = \left| \langle m_\tau | \hat{U}(\tau, 0) | n_0 \rangle \right|^2$$  \hspace{1cm} (3.7)

is the conditional transition probability, corresponding to the probability that if the system starts in state $n$, it will be in state $m$ at time $t = \tau$. $\hat{U}(\tau, 0)$ represents the unitary time evolution operator, and the 4 possible values of work that can be done are
Chapter 3. Modeling the Entropy Generation and the Effects of a Varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

\[ W_i = \epsilon_{\tau,m} - \epsilon_{0,n} \]  \hspace{1cm} (3.8)

where $\epsilon_{0,n}$ represents one of the two energy eigenvalues of the system at time $t = 0$ and $\epsilon_{\tau,m}$ represents one of the two energy eigenvalues at $t = \tau$.

To model the dissipation occurring (and hence the entropy production) using SEAQT, its equation of motion must first be converted from the lab frame to a rotating reference frame, since this is the frame used in NMR experiments. From this it is shown that the dissipation which occurs is independent of the frame used, as is expected, and that only the reversible dynamics appear to change upon switching frames. Next, the formulation of the Hamiltonian employed for modeling this experiment is presented along with the associated assumptions. This is followed by a brief presentation of the system’s transition probabilities, which could be related to the relaxation time of SEAQT, $\tau_D$. However, this is left for future work since no suitable results have yet been obtained using this method. With all of these elements in place, the time-varying Kullback-Leibler relative entropy and the so-called “mean entropy production” can be computed. Results are presented using two different constant values of $\tau_D$. Results for the von Neumann equation are also included. Following this, conclusions are drawn regarding the dissipation seen within the system and future modeling is suggested to improve the results.

3.2 Model Development

3.2.1 SEAQT Equation of Motion in a Rotating Reference Frame

To derive the SEAQT equation of motion for a general quantum system in a rotating reference frame (i.e., the Heisenberg picture of quantum mechanics), the following definition is made
relating the density operator as viewed from the rotating frame $\hat{\rho}_R$ and as viewed from the lab frame, $\hat{\rho}_L$, [38]:

$$\dot{\hat{\rho}}_R = \hat{R}_{\vec{n}(t)}(-\phi(t))\hat{\rho}_L\hat{R}_{\vec{n}(t)}^\dagger(-\phi(t))$$ (3.9)

where the rotation operator $\hat{R}_{\vec{n}}(\phi)$ is given as

$$\hat{R}_{\vec{n}(t)}(\phi) = e^{-i\phi(\hat{n}_X I_X + \hat{n}_Y I_Y + \hat{n}_Z I_Z)}$$ (3.10)

$\phi(t) = \omega_{ref} t + \phi_0$ represents the relative angle at time $t$ between the rotating reference frame and the lab frame where $\omega_{ref}$ is the reference frame angular velocity and $\phi_0$ is the initial offset angle, typically (but not always) taken to be zero. Finally $I_{X,Y,Z}$ are the components of the particle’s spin-angular momentum in the X, Y, and Z directions, respectively. Next, expanding the time derivative of $\hat{\rho}_R$ yields

$$\frac{d}{dt}(\hat{\rho}_R) = \frac{d}{dt}\left(\hat{R}_{\vec{n}(t)}(-\phi(t))\hat{\rho}_L\hat{R}_{\vec{n}(t)}^\dagger(-\phi(t))\right)$$ (3.11)

or

$$\frac{d\hat{\rho}_R}{dt} = \hat{R}_{\vec{n}(t)}(-\phi(t))\frac{d\hat{\rho}_L}{dt}\left(\hat{R}_{\vec{n}(t)}(-\phi(t))\right) + \hat{R}_{\vec{n}(t)}(-\phi(t))\frac{d\hat{\rho}_L}{dt}\hat{R}_{\vec{n}(t)}^\dagger(-\phi(t))$$

$$+ \frac{d}{dt}\left(\hat{R}_{\vec{n}(t)}(-\phi(t))\right)\hat{\rho}_L\hat{R}_{\vec{n}(t)}^\dagger(-\phi(t))$$ (3.12)

The time derivative of the rotation operator then is

$$\frac{d}{dt}\hat{R}_{\vec{n}(t)}(-\phi(t)) = \hat{R}_{\vec{n}(t)}(-\phi(t))\frac{d}{dt}\left(i\phi(t)\left(\hat{n}_X I_X + \hat{n}_Y I_Y + \hat{n}_Z I_Z\right)\right)$$ (3.13)
Chapter 3. Modeling the Entropy Generation and the Effects of a varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

or

$$\frac{d}{dt} \hat{R}(\hat{n}(t)) = \hat{R}(\hat{n}(t)) i \left( \left( \omega_{ref} \hat{n}_X + \phi(t) \frac{d\hat{n}_X}{dt} \right) \hat{I}_X + \left( \omega_{ref} \hat{n}_Y + \phi(t) \frac{d\hat{n}_Y}{dt} \right) \hat{I}_Y + \left( \omega_{ref} \hat{n}_Z + \phi(t) \frac{d\hat{n}_Z}{dt} \right) \hat{I}_Z \right)$$ (3.14)

and in the limit as $\omega_{ref} \hat{n}_i >> \phi(t) d\hat{n}_i / dt$, the above expression reduces to

$$\frac{d}{dt} \hat{R}(\hat{n}(t)) = \hat{R}(\hat{n}(t)) i \left( \omega_{ref} \hat{n}_X \hat{I}_X + \omega_{ref} \hat{n}_Y \hat{I}_Y + \omega_{ref} \hat{n}_Z \hat{I}_Z \right)$$ (3.15)

For now, it is assumed that the reference frame rotates solely around the Z-axis so that $\hat{n}_X = \hat{n}_Y = 0$ and the above equation reduces to

$$\frac{d}{dt} \hat{R}_Z(\hat{n}(t)) = \hat{R}_Z(-\hat{n}(t)) i \omega_{ref} \hat{I}_Z$$ (3.16)

Substituting this into equation (3.12) and simplifying results in

$$\frac{d\rho}{dt} = i \hbar \frac{\omega_{ref}}{\hbar} \left[ \hat{I}_Z, \rho \right] + \hat{R}_Z(-\hat{n}) \frac{d\hat{\rho}_L}{dt} \hat{R}_Z^\dagger(-\hat{n})$$ (3.17)

where from the equation of motion in the lab frame, the second term to the right of the equals is written as

$$\hat{R}_Z(-\hat{n}) \frac{d\hat{\rho}_L}{dt} \hat{R}_Z^\dagger(-\hat{n}) = \hat{R}_Z(-\hat{n}) \left( -\frac{i}{\hbar} \left[ \hat{H}_L, \hat{\rho}_L \right] + \frac{D(\hat{\rho}_L)}{Dt} \right) \hat{R}_Z^\dagger(-\hat{n})$$ (3.18)

After some simple algebraic manipulation, this reduces to
\[ \hat{R}_Z(-\phi) \frac{d\hat{\rho}_L}{dt} \hat{R}_Z^\dagger(-\phi) = -\frac{i}{\hbar} \left[ \hat{H}_R, \hat{\rho}_R \right] + \hat{R}_Z(-\phi) \left( \frac{D(\hat{\rho}_L)}{Dt} \right) \hat{R}_Z^\dagger(-\phi) \] (3.19)

where the definition \( \hat{H}_R \equiv \hat{R}_Z(-\phi) \hat{H}_L \hat{R}_Z^\dagger(-\phi) \) is made.

The next step is to evaluate the SEAQT dissipation operator in the rotating frame. Thus,

\[ \hat{R}_Z(-\phi) \left( \frac{D(\hat{\rho}_L)}{Dt} \right) \hat{R}_Z^\dagger(-\phi) = \hat{R}_Z(-\phi) \frac{1}{2\tau_D} \left( \hat{\rho}_L \hat{D}_L + \left( \hat{\rho}_L \hat{D}_L \right)^\dagger \right) \hat{R}_Z^\dagger(-\phi) \] (3.20)

and again after some algebraic manipulation it can be shown that this reduces to

\[ \hat{R}_Z(-\phi) \left( \frac{D(\hat{\rho}_L)}{Dt} \right) \hat{R}_Z^\dagger(-\phi) = \frac{1}{2\tau_D} \left( \hat{\rho}_R \hat{D}_R + \left( \hat{\rho}_R \hat{D}_R \right)^\dagger \right) \] (3.21)

where the definition \( \hat{D}_R \equiv \hat{R}_Z(-\phi) \hat{D}_L \hat{R}_Z^\dagger(-\phi) \) is made. Evaluating this gives yields

\[ \hat{D}_R = \hat{R}_Z(-\phi) \left( \hat{B} \ln(\hat{\rho}_R) - \frac{B_1}{\Gamma} \hat{I} + \frac{B_2}{\Gamma} \hat{H}_R \right) \hat{R}_Z^\dagger(-\phi) \] (3.22)

Here the ratio of determinants found in the definition of \( \hat{D}_L \) has already been expanded to give the terms \( B_1/\Gamma \) and \( B_2/\Gamma \). This straightforwardly reduces to

\[ \hat{D}_R = \hat{B} \ln(\hat{\rho}_R) - \frac{B_1}{\Gamma} \hat{I} + \frac{B_2}{\Gamma} \hat{H}_R \] (3.23)

It is shown in Appendix B that \( B_1, B_2, \) and \( \Gamma \), which are functions of the generators of the motion in the lab frame, can be equivalently evaluated in the rotating reference frame assuming that all of the generators of the motion used to evaluate them have been converted from the lab frame to the rotating frame. With these definitions, it now is possible to write
Chapter 3. Modeling the Entropy Generation and the Effects of a Varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

\[ \hat{R}_Z(-\phi) \left( \frac{D(\hat{\rho}_L)}{Dt} \right) \hat{R}_Z^\dagger(-\phi) = \frac{D(\hat{\rho}_R)}{Dt} \]  

(3.24)

where $D(\hat{\rho}_R)/Dt$ is computed exactly the same way as $D(\hat{\rho}_L)/Dt$, with the exception that now all of the operators involved are those as viewed from a rotating reference frame instead of the lab frame. The evaluation of $d\hat{\rho}_L/dt$ in the rotating frame then becomes

\[ \hat{R}_Z(-\phi) \frac{d\hat{\rho}_L}{dt} \hat{R}_Z^\dagger(-\phi) = -\frac{i}{\hbar} \left[ \hat{H}_R, \hat{\rho}_R \right] + \frac{D(\hat{\rho}_R)}{Dt} \]  

(3.25)

and, thus, the SEAQT equation of motion in the rotating reference frame is

\[ \frac{d\hat{\rho}_R}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_R - \hbar \omega_{ref} \hat{I}_Z, \hat{\rho}_R \right] + \frac{D(\hat{\rho}_R)}{Dt} \]  

(3.26)

3.2.2 Hamiltonian Development

This section follows the presentation given by Levitt [38] for developing the nuclear spin Hamiltonian of a typical NMR experiment. The general Hamiltonian is presented along with the assumptions made in reducing it to the simplified form used in studying the dynamics of the experimental molecule considered here. First, it is assumed that the rapid electronic dynamics take place on much shorter timescales than that of the nuclear spin dynamics (due to their difference in mass) and as a consequence allow the full system Hamiltonian to be approximated by the nuclear spin Hamiltonian for the timescales of interest. Because the systems (nuclei) being analyzed in this work are all of spin $1/2$, there are no contributions to the system’s energy due to electric fields, and, thus, the dynamics are caused solely by the magnetic field that the nuclei experience. With this, the general nuclear spin Hamiltonian due to magnetic fields in the lab frame can be represented as
\[ \hat{H}_L(t) = -\vec{\mu} \cdot \vec{B}(t) = -\vec{\mu} \cdot \left( \vec{B}_{\text{int}}(t) + \vec{B}_{\text{ext}}(t) \right) = \hat{H}_{\text{int},L}(t) + \hat{H}_{\text{ext},L}(t) \] (3.27)

where \( \vec{\mu} \) represents the magnetic moment of the nucleus and \( \vec{B}(t) \) represents the magnetic field it experiences. The second and third equalities are made by decomposing the overall magnetic field into components that originate from within the liquid sample, which cannot be controlled, and those that originate exterior to the liquid sample, which can be controlled. For an NMR experiment, the external component of the magnetic field is typically separated as

\[ \hat{H}_{\text{ext},L}(t) = \hat{H}_{0,L} + \hat{H}_{\text{RF},L}(t) \] (3.28)

where \( \hat{H}_{0,L} \) represents a nuclear Zeeman interaction with the static, longitudinal portion of the external magnetic field and \( \hat{H}_{\text{RF},L}(t) \) represents the time-dependent, transverse, radio-frequency (RF) components of the external magnetic field. This form also assumes that there are no spatial gradients in the externally applied field. \( \hat{H}_{0,L} \), for a system of \( N \) nuclei can be written as

\[ \hat{H}_{0,L} = -\sum_{i=1}^{N} \frac{\hbar \omega_{0,i}}{2} \hat{\sigma}_{Z,i} \] (3.29)

where \( \omega_{0,i} = \mu_{Z,i} B_0 \) is the Larmor angular precession velocity of the \( i^{\text{th}} \) nucleus, \( \mu_{Z,i} \) is the corresponding magnetic moment along the Z direction, \( B_0 \) is the static magnetic field applied along the Z direction, and \( \hat{\sigma}_{Z,i} \) is the Pauli Z matrix for the \( i^{\text{th}} \) nucleus. Neglecting nonresonant and longitudinal effects associated with the pulsed RF field [38], \( \hat{H}_{\text{RF},L}(t) \) can be written as
Chapter 3. Modeling the Entropy Generation and the Effects of a varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

\[ \hat{H}_{RF,L}(t) = -\sum_{i=1}^{N} \frac{\hbar \omega_{Nut,i}}{2} (\cos(\omega_{ref} t + \phi_p)\hat{\sigma}_{X,i} + \sin(\omega_{ref} t + \phi_p)\hat{\sigma}_{Y,i}) \]  

(3.30)

where $\omega_{Nut,i}$ is the nutation frequency of nucleus $i$, $\omega_{ref}$ is the angular velocity of the rotating reference frame, which will be discussed later, $\phi_p$ is the offset phase of the RF field, and $\hat{\sigma}_{X,i}$ and $\hat{\sigma}_{Y,i}$ are the Pauli X and Pauli Y matrices of the $i^{th}$ nucleus.

As to the internal portion of the Hamiltonian, $\hat{H}_{int,L}(t)$, the secular approximation is used, which assumes that the externally applied static magnetic field is the dominant source of the dynamics for spin 1/2 particles, thus, permitting a simplification of the $\hat{H}_{int,L}(t)$. Further, it is also assumed that motionally-averaged values are used, which is a good approximation for room temperature, liquid state NMR experiments [38].

For the experiment being modeled, the effects of chemical shifts on the nuclei (i.e., the influence of a nucleus’ local electronic environment) are assumed to be taken into account in the physical properties of the nuclear spin (which affects the value of $\omega_0,i$). For isotropic fluids, which are used in the relevant experiment, it can be shown that the average effect of so-called direct dipole-dipole coupling is zero, and, thus, this effect is also neglected here.

The next most dominant term in the internal nuclear spin Hamiltonian is due to what is known as through-bond or J-coupling. This effect accounts for the influence one nucleus has on another through the electronic bond(s) connecting them. For isotropic liquids and for heteronuclear coupling, the J-coupling Hamiltonian has the form

\[ \hat{H}_{int,L}(t) = \hat{H}_{J,L} = \sum_{i,j=1,j>i}^{N} 2\pi \hbar J_{ij} \frac{\hat{\sigma}_{Z,i} \hat{\sigma}_{Z,j}}{2} \]  

(3.31)

where $J_{ij}$ is the scalar coupling constant given in Hertz. With this definition, a computationally tractable description of the system Hamiltonian in the lab frame can be made. Thus, under
3.2. Model Development

the stated approximations, the general Hamiltonian governing the system assumes the form

\[
\hat{H}_L(t) = -\sum_{i=1}^{N} \left( \frac{\hbar \omega_{0,i}}{2} \hat{\sigma}_{Z,i} + \frac{\hbar \omega_{N_{ij}}}{2} \left( \cos(\omega_{ref}t + \phi_p)\hat{\sigma}_{X,i} + \sin(\omega_{ref}t + \phi_p)\hat{\sigma}_{Y,i} \right) \right) + \sum_{i,j=1,j>i}^{N} 2\pi \hbar J_{ij} \hat{\sigma}_{Z,i} \hat{\sigma}_{Z,j} (3.32)
\]

This Hamiltonian is now further simplified to model the experimentally used molecule, CHCl\textsubscript{3}. It is known that Chlorine nuclei have motionally-suppressed J-couplings, and, thus, their couplings to the Carbon and Hydrogen nuclei in the molecule are neglected here [38]. This allows the above equation to be reduced to

\[
\hat{H}_L(t) = \frac{1}{2} \hbar \left( \omega_{0,C} \hat{\sigma}_{Z,C} \otimes \hat{I}_{H} + \omega_{0,H} \hat{I}_{C} \otimes \hat{\sigma}_{Z,H} \right) + \hat{H}_{RF,L}(t) + \frac{\pi}{2} \hbar J_{H,C} \hat{\sigma}_{Z,C} \otimes \hat{\sigma}_{Z,H} (3.33)
\]

Now, to more easily analyze the dynamics of the system due to the pulsed RF field, a rotating reference frame is used so that the rapid oscillations due to the strong, static longitudinal field can be neglected. To do this, reference frames with angular velocities of \( \omega_{ref,C} = \omega_{0,C} \) and \( \omega_{ref,H} = \omega_{0,H} \) are chosen whose orientation’s are along the Z-axis. This allows the rotating frame Hamiltonian to be expressed as \( \hat{H}_R(t) = \hat{R}_{CH}(t)\hat{H}_L(t)\hat{R}^\dagger_{CH}(t) \), where \( \hat{R}_{CH}(t) \equiv \hat{R}_{Z,C}(-\phi_C(t)) \otimes \hat{R}_{Z,H}(-\phi_H(t)) \) or
Chapter 3. Modeling the Entropy Generation and the Effects of a Varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

\[ \hat{H}_R(t) = \frac{-1}{2} \hbar \hat{R}_{CH}(t) \left( \omega_{0,C} \hat{\sigma}_{Z,C} \otimes \hat{I}_H + \omega_{0,H} \hat{I}_C \otimes \hat{\sigma}_{Z,H} \right) \hat{R}_{CH}^\dagger(t) \]

\[ - \hat{R}_{CH}(t) \hat{H}_{RF,L}(t) \hat{R}_{CH}^\dagger(t) - \frac{\pi}{2} \hbar J_{H,C} \hat{R}_{CH}(t) \hat{\sigma}_{Z,C} \otimes \hat{\sigma}_{Z,H} \hat{R}_{CH}^\dagger(t) \] (3.34)

Noting that $\hat{\sigma}_Z$ commutes with the rotation operator, the above reduces to

\[ \hat{H}_R(t) = \frac{-1}{2} \hbar \left( \omega_{0,C} \hat{\sigma}_{Z,C} \otimes \hat{I}_H + \omega_{0,H} \hat{I}_C \otimes \hat{\sigma}_{Z,H} \right) - \hat{H}_{RF,R}(t) - \frac{\pi}{2} \hbar J_{H,C} \hat{\sigma}_{Z,C} \otimes \hat{\sigma}_{Z,H} \] (3.35)

where the definition $\hat{H}_{RF,R}(t) = \hat{R}_{CH}(t) \hat{H}_{RF,L}(t) \hat{R}_{CH}^\dagger(t) = \hat{H}_{RF,R,C}(t) \otimes \hat{I}_H + \hat{I}_C \otimes \hat{H}_{RF,R,H}(t)$ has been made. As given in [3], the rotating-frame, pulsed-RF Hamiltonian during the quenching process for the Carbon atom is given as

\[ \hat{H}_{RF,R,C}(t) = 2\pi \hbar \nu(t) \left( \cos(\phi(t)) \hat{\sigma}_{X,C} + \sin(\phi(t)) \hat{\sigma}_{Y,C} \right) \] (3.36)

where $\nu(t) = \nu_0 \left( 1 - \frac{t}{\tau} \right) + \nu_\tau \frac{t}{\tau}$ is the linear modulation of the RF field characterized by the parameters $\nu_0 = 1$ kHz and $\nu_\tau = 1.8$ kHz. $\phi(t) = \pi t / 2 \tau$ is the relative phase of the RF field to the rotating reference frame, and $\tau$ represents the quench time, which is varied from 20 $\mu$s to 800 $\mu$s. Inserting $\hat{H}_R(t)$ into the SEAQT equation of motion in the rotating reference frame yields

\[ \frac{d\hat{\rho}_R}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_{RF,R}(t) + \frac{\pi}{2} \hbar J_{H,C} \hat{\sigma}_{Z,C} \otimes \hat{\sigma}_{Z,H} , \hat{\rho}_R \right] + \frac{D(\hat{\rho}_R)}{Dt} \] (3.37)

As can be seen, in the rotating reference frame, only the pulsed RF field and the qubit interaction affects the unitary dynamics, whereas the entire rotating reference frame Hamiltonian is
used in evaluating the SEAQT dissipation operator. With this, the final step in implementing the SEAQT equation of motion is to choose a relaxation time $\tau_D$. Section 3.2.3 presents a method relating the analytical expression for the system transition probability to $\tau_D$.

### 3.2.3 Transition Probability Based Relaxation Time

To develop a fully ab initio model in SEAQT, it is necessary to relate $\tau_D$ to the fundamental dynamics occurring within the system. In quantum information and quantum computing systems, one such process that could be related to the dynamics of the system is the Rabi Cycle, and the associated transition probabilities, which give the probability that the system has transitioned from $|0\rangle$ to $|1\rangle$ at a given time $t$. For the system at hand, this expression taken from [5] is

$$P_{0\rightarrow1}(t) = \left( \frac{2\pi \nu(t)}{\sqrt{(\omega_{RF} - \omega_{0,C})^2 + (2\pi \nu(t))^2}} \right)^2 \sin^2 \left( \frac{\sqrt{(\omega_{RF} - \omega_{0,C})^2 + (2\pi \nu(t))^2} t}{2} \right)$$

(3.38)

where $\nu(t)$ is the linear modulation of the RF field frequency in time. Now, by choosing $\omega_{RF} = \omega_{0,C}$, the expression for the transition probability reduces to

$$P_{0\rightarrow1}(t) = \sin^2 \left( \frac{2\pi \nu(t)t}{2} \right)$$

(3.39)

The time derivative of this expression is then given by

$$\frac{dP_{0\rightarrow1}(t)}{dt} = 2\pi \sin \left( \frac{2\pi \nu(t)t}{2} \right) \cos \left( \frac{2\pi \nu(t)t}{2} \right) \left( \nu(t) + t \frac{d\nu(t)}{dt} \right)$$

(3.40)
Some work has been done to relate this time rate of change of the transition probability to $\tau_D$ to see if it is an appropriate mechanism on which the relaxation time could be based. However, preliminary results are incomplete, and further work is needed but is beyond the scope of the present research. It is, thus, left for future work.

3.3 Results

This section presents results for the time evolution of the Kullback-Leibler relative entropy, $S_{KL}$, and the so-called “mean entropy production”, $\langle \Sigma \rangle$, based on various choices of the SEAQT relaxation time, $\tau_D$. Also presented is $\langle \Sigma \rangle$ versus the quench time. For the Kullback-Leibler evolution, results for quench times of 100 $\mu$s, 500 $\mu$s, and 700 $\mu$s are generated. For the the so-called “mean entropy production”, $\langle \Sigma \rangle$, quench times ranging from 20 $\mu$s to 800 $\mu$s are used in increments of 20 $\mu$s. Results using the von Neumann equation are given in Section 3.3.2, while results using the SEAQT equation of motion are provided in Section 3.3.3 using constant, experimentally-derived values of $\tau_{Matthisien,H} \approx 2.89$ s and $\tau_{Matthisien,C} \approx 0.32$ s [3] for the relaxation times, $\tau_{D,H(C)}$. Next, to gain insight into how the $\tau_{D,H(C)}$ affect the dynamics of $S_{KL}$ and $\langle \Sigma \rangle$, Section 3.3.4 presents results using the same values of $\tau_{D,H(C)}$ as in Section 3.3.3 but scaled down by a factor of 100.

The experimental values for the evolution of $S_{KL}$ through time are found by tracking the state of the Carbon atom during the quench using quantum state tomography [47, 48], which involves making multiple measurements of a given qubit from which each of the elements of the density operator at a given time can be computed. $P(\Sigma)$, from which the so-called “mean entropy production”, $\langle \Sigma \rangle$, can be calculated, is evaluated using NMR spectroscopy on the ancillary qubit (i.e., the Hydrogen atom). These two measurement techniques provide independent ways of quantifying the relationship between $S_{KL}$ and $\langle \Sigma \rangle$, thus, permitting the
3.3. Results

authors to experimentally verify the relation $S_{KL} = \langle \Sigma \rangle$ at the final quench time [3].

3.3.1 Generation of the Initial State from a Set of Pseudo-Pure States

Batalhao et al. [3] analyze the evolution of the pseudo-pure state $\hat{\rho}_{eq,C} \otimes |0\rangle_H \langle 0|_H$ where $\hat{\rho}_{eq,C} = \exp\left( -\beta_{eff} \hat{H}_{RF,R,C}(0) \right) / Z$ and $\beta_{eff}$ corresponds to an effective temperature of $T_{eff} \approx 75$ nK. To form this pseudo-pure state from the initial equilibrium states, a method based on the presentation by [47, 48] is used here. First, consider a density operator $\hat{\rho}_1$, which could represent a thermal equilibrium density operator, and two operations $\hat{P}_1$ and $\hat{P}_2$, that manipulate the elements of the density operator as

$$\hat{\rho}_1 = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ 0 & 0 & 0 & d \end{bmatrix}$$ (3.41)

and

$$\hat{\rho}_2 = \hat{P}_1 \hat{\rho}_1 \hat{P}_1^\dagger = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & c & 0 & 0 \\ 0 & 0 & d & 0 \\ 0 & 0 & 0 & b \end{bmatrix}, \quad \hat{\rho}_3 = \hat{P}_2 \hat{\rho}_1 \hat{P}_2^\dagger = \begin{bmatrix} a & 0 & 0 & 0 \\ 0 & d & 0 & 0 \\ 0 & 0 & b & 0 \\ 0 & 0 & 0 & c \end{bmatrix}$$ (3.42)

$\hat{P}_1$ and $\hat{P}_2$ can be realized by sequences of controlled NOT operations, which are henceforth referred to as preparation sequences. The summation of the three density operators gives
Chapter 3. Modeling the Entropy Generation and the Effects of a varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

\[ \sum_{i=1}^{3} \hat{\rho}_i = \begin{bmatrix} 3a & 0 & 0 & 0 \\ 0 & b + c + d & 0 & 0 \\ 0 & 0 & b + c + d & 0 \\ 0 & 0 & 0 & b + c + d \end{bmatrix} = (4a - 1) |0_A0_B\rangle \langle 0_A0_B| + (1 - a) \hat{I} \] (3.43)

which can be written in terms of the state $|0_A0_B\rangle$ or $|0_C0_H\rangle$. Because all observables in NMR experiments are traceless [47], the term $(1 - a) \hat{I}$ does not affect any measurement results.

Next, to relate this psuedo-pure state to $\hat{\rho}_{eq,C} \otimes |0\rangle_H \langle 0|_H$, rotations of angles $\theta$ and $\pi - \theta$ about the Y-axis can be applied following each $\hat{P}_i$ where $\theta$ is computed based on $\langle 0 | \hat{\rho}_{eq,C} | 1 \rangle$, yielding

\[ \hat{R}_{Y,C}(\theta) \left( \sum_{i=1}^{3} \hat{\rho}_i \right) \hat{R}_{Y,C}^\dagger(\theta) + \hat{R}_{Y,C}(\pi - \theta) \left( \sum_{i=1}^{3} \hat{\rho}_i \right) \hat{R}_{Y,C}^\dagger(\pi - \theta) = (4a - 1) \hat{R}_{Y,C}(\theta) |0_C0_H\rangle \langle 0_C0_H| \hat{R}_{Y,C}^\dagger(\theta) \\
+ (4a - 1) \hat{R}_{Y,C}(\pi - \theta) |0_C0_H\rangle \langle 0_C0_H| \hat{R}_{Y,C}^\dagger(\pi - \theta) + 2(1 - a) \hat{I} \] (3.44)

or

\[ \hat{R}_{Y,C}(\theta) \left( \sum_{i=1}^{3} \hat{\rho}_i \right) \hat{R}_{Y,C}^\dagger(\theta) + \hat{R}_{Y,C}(\pi - \theta) \left( \sum_{i=1}^{3} \hat{\rho}_i \right) \hat{R}_{Y,C}^\dagger(\pi - \theta) = (4a - 1) \left( \hat{R}_{Y}(\theta) |0_C\rangle \langle 0_C| \hat{R}_{Y}^\dagger(\theta) + \hat{R}_{Y}(\pi - \theta) |0_C\rangle \langle 0_C| \hat{R}_{Y}^\dagger(\pi - \theta) \right) \otimes |0_H\rangle \langle 0_H| \\
+ 2(1 - a) \hat{I} \] (3.45)
3.3. Results

where \( \theta \) is chosen such that

\[
\dot{\rho}_{eq,C} = \hat{R}_Y(\theta) \, |0_C\rangle \langle 0_C| + \hat{R}_Y(\pi - \theta) \, |0_C\rangle \langle 0_C| \hat{R}_Y^\dagger(\pi - \theta)
\]  

(3.46)

Thus, the above reduces to

\[
\hat{R}_{Y,C}(\theta) \left( \sum_{i=1}^{3} \hat{\rho}_i \right) \hat{R}_{Y,C}^\dagger(\theta) + \hat{R}_{Y,C}(\pi - \theta) \left( \sum_{i=1}^{3} \hat{\rho}_i \right) \hat{R}_{Y,C}^\dagger(\pi - \theta)
\]

\[
= (4a - 1) \, \rho_{eq,C} \otimes |0_H\rangle \langle 0_H| + 2(1 - a) \hat{I}
\]

(3.47)

It is then possible to obtain the evolution of the system in a state \( \dot{\rho}_{eq,C} \) by

\[
\dot{\rho}_{eq,C} = \frac{1}{4a - 1} \, \text{Tr}_H \left( \hat{R}_{Y,C}(\theta) \left( \sum_{i=1}^{3} \hat{\rho}_i \right) \hat{R}_{Y,C}^\dagger(\theta) \right.
\]

\[
+ \hat{R}_{Y,C}(\pi - \theta) \left( \sum_{i=1}^{3} \hat{\rho}_i \right) \hat{R}_{Y,C}^\dagger(\pi - \theta) - 2(1 - a) \hat{I} \left. \right) \quad (3.48)
\]

where the quenching operation and any other subsequent operation can be appended via the \( \hat{R}_{Y,C} \) rotations.

3.3.2 von-Neumann-Experimental Data Comparison

This section presents results for the evolution of the Kullback-Leibler relative entropy, \( S_{KL} \), and the effect of the quench time on the so-called “mean entropy production”, \( \langle \Sigma \rangle \), through time based on the von-Neumann equation of motion. Figure 3.1 shows the evolution of \( S_{KL} \) for quench times of 100 \( \mu s \) and 500 \( \mu s \), while Figure 3.2 does so for a quench time of 700 \( \mu s \).
Chapter 3. Modeling the Entropy Generation and the Effects of a varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

The latter figure also provides a plot of the so-called “mean entropy production”, $\langle \Sigma \rangle$, for quench times ranging from 20 $\mu$s to 800 $\mu$s.

In Figure 3.1a, the evolution of $S_{KL}$ predicted by the von Neumann equation for a 100 $\mu$s quench time differs during the middle of the evolution from that of the experimental data. After a normalized time of about 0.2, values of $S_{KL}$ are consistently higher and in the middle of the evolution significantly higher than the experimental data although trends are somewhat similar. The so-called “mean entropy production”, $\langle \Sigma \rangle$, predicted by the Tasaki-Crooks equation (black dashed line) using experimental data is also plotted and is lower than the $S_{KL}$ mean of the experimental data (orange dashed line), but is near the final value of $S_{KL}$ (blue solid line) at the quench time. As argued by Batalhao et al. [3], the final value of $S_{KL}$ should be in agreement with $\langle \Sigma \rangle$.

Figure 3.1b shows the corresponding evolution for a quench time of 500 $\mu$s. In general, the evolution of $S_{KL}$ predicted by the von Neumann equation (blue solid line) is much closer to that of the experimental data than was the case for a quench time of 100 $\mu$s. It agrees much better with the experimental data during the first half of the evolution but nonetheless deviates during the second half. The mean experimental value (orange dashed line) and the so-called “mean entropy production”, $\langle \Sigma \rangle$, (black dashed line) predicted using the Tasaki-Crooks equation also are in closer agreement for the 500 $\mu$s case. However, the von Neumann equation under predicts the final value of $S_{KL}$, which Batalhao et al. [3] suggest should be equivalent to $\langle \Sigma \rangle$.

Figure 3.2a shows that the evolution of $S_{KL}$ (blue solid line) for the 700 $\mu$s quench time is, as for the 100 $\mu$s case, in less agreement with the experimental data though again the final value of $S_{KL}$ seems to be near the $\langle \Sigma \rangle$ (black dashed line) predicted by the Tasaki-Crooks equation. Though there is some overlap between the evolution predicted by the von Neumann equation and the experimental data, in general the trends do not match, which is evident from the
3.3. Results

Figure 3.1: Kullback-Leibler relative entropy evolution; evolutions for quench times of 100 µs and 500 µs using the von Neumann equation are shown in addition to experimental values; the so-called “mean entropy production”, ⟨Σ⟩, predicted using the Tasaki-Crooks equation is shown as well.

absence of peaks in the experimental data.

Figure 3.2b shows the value of ⟨Σ⟩ as computed by equation (3.1) at the end of the evolution under the von Neumann equation compared to the experimental data and the so-called “mean entropy production”, ⟨Σ⟩, as calculated using transition probabilities, i.e., the Tasaki-Crooks equation. The values predicted by equation (3.1) under reversible dynamics agree well with the experimental data but slightly under predict the values for quench times less than 300 µs and at 500 µs.
Chapter 3. Modeling the Entropy Generation and the Effects of a varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

3.3.3 SEAQT $\tau_{D,H}(C) = \tau_{Matthiessen,H}(C)$ - Experimental Data Comparison

This section presents results for the evolution of the Kullback-Leibler relative entropy and the effect of the quench time on the so-called “mean entropy production”, $\langle \Sigma \rangle$, as predicted by the SEAQT equation of motion where the relaxation times have fixed values of $\tau_{D,H} = \tau_{Matthiessen,H} \approx 2.89$ s and $\tau_{D,C} = \tau_{Matthiessen,C} \approx 0.32$ s for the Hydrogen and Carbon atoms, respectively, in all cases. Figure 3.3 presents the evolution of $S_{KL}$ for quench times of 100 $\mu$s and 500 $\mu$s and Figure 3.4 presents the evolution of $S_{KL}$ for a quench time of 700 $\mu$s and the final value of $\langle \Sigma \rangle$, as computed by equation (3.1), for quench times ranging from 20 $\mu$s to 800 $\mu$s.

Figure 3.3a shows the evolution of $S_{KL}$ predicted by the SEAQT equation of motion for a 100 $\mu$s quench time. During the first third of the evolution, the values of $S_{KL}$ match well with the experimental data. However a large increase in $S_{KL}$ is seen during the middle of the evolution that does not match the experimental data before the SEAQT results drop and
3.3. Results

again match the experimental data well at the end of the evolution.

Figure 3.3b shows the corresponding evolution for a quench time of 500 $\mu$s. In general, the evolution predicted by SEAQT lies on top of or near the experimental data for $S_{KL}$ for roughly the first half of the experiment, but oscillates and under predicts $S_{KL}$ during the second. One notable aspect is that the final prediction of $S_{KL}$ is closer to $\langle \Sigma \rangle$ than what is predicted by the von Neumann equation.

Figure 3.3: Kullback-Leibler relative entropy evolution; evolutions for quench times of 100 $\mu$s and 500 $\mu$s using the SEAQT equation of motion are shown in addition to experimental values; the so-called “mean entropy production”, $\langle \Sigma \rangle$, predicted using the Tasaki-Crooks equation is shown as well.

Figure 3.4a shows that though there is some overlap between the evolution predicted by SEAQT and the experimental data, in general the trends do not match, which is evident from the absence of peaks in the experimental data. Here, the final value predicted for $S_{KL}$ by SEAQT is very close to the experimentally measured value of $\langle \Sigma \rangle$.

Figure 3.4b shows the value of $\langle \Sigma \rangle$ as computed by equation (3.1) at the end of the evolution under SEAQT compared to the experimental data and the so-called “mean entropy production”, $\langle \Sigma \rangle$, as calculated using transition probabilities (i.e., the Tasaki-Crooks equation). The values predicted by the SEAQT equation, equation (3.1), for a relaxation time equal
to $\tau_{Matthiessen}$ for each qubit matches the experimental data as well as, if not better than, the von Neumann equation for all quench times. Again, the values of $\langle \Sigma \rangle$ at quench times smaller than 300 $\mu$s are slightly under predicted, indicating that a time-varying formulation of $\tau_D$ may be necessary. However, values of $\langle \Sigma \rangle$ above 300 $\mu$s match very well.

![Kullback-Leibler Relative Entropy Evolution](image)

![Mean Kullback-Leibler Entropy vs. Quench Time](image)

Figure 3.4: So-called “mean entropy production”, $\langle \Sigma \rangle$, vs. quench time; the evolution of $\langle \Sigma \rangle$ as predicted by the SEAQT equation of motion for quench times between 20 $\mu$s and 800 $\mu$s are shown in addition to the Tasaki-Crooks “mean entropy production” and experimental values.

### 3.3.4 SEAQT $\tau_D = \tau_{Matthiessen}/100$-Experimental Data Comparison

This section presents results for the evolution of the Kullback-Leibler relative entropy and the effect of the quench time on the so-called “mean entropy production”, $\langle \Sigma \rangle$, as predicted by the SEAQT equation of motion where the relaxation time, $\tau_D$, has fixed values of $\tau_{D,H} = \tau_{Matthiessen,H}/100 \approx 28.9$ ms and $\tau_{D,C} = \tau_{Matthiessen,C}/100 \approx 3.2$ ms for the Hydrogen and Carbon atoms, respectively, in all cases. Figure 3.5 presents the evolution of $S_{KL}$ for quench times of 100 $\mu$s and 500 $\mu$s and Figure 3.6 presents the evolution of $S_{KL}$ for a quench time of 700 $\mu$s and the so-called “mean entropy production”, $\langle \Sigma \rangle$, during an evolution for quench times ranging from 20 $\mu$s to 800 $\mu$s.
3.3. Results

Figure 3.5a shows that the evolution of $S_{KL}$ predicted by the SEAQT equation of motion for a 100 $\mu$s quench time overlaps the experimental data well for a majority of the evolution, but under predicts the initial and final values. Further, the entire evolution of $S_{KL}$ has smaller values as compared to Figure 3.3a.

Figure 3.5b shows the corresponding evolution for a quench time of 500 $\mu$s. The SEAQT equation of motion under predicts $S_{KL}$ during the first half of the evolution before approaching the experimental data near the second half of the evolution. This indicates that $\tau_D = \tau_{Matthiessen}/100$ is too small for this particular quench time.

Figure 3.6a shows that the general trend of $S_{KL}$ for the 700 $\mu$s quench time does not match the experimental data, again indicating that $\tau_D = \tau_{Matthiessen}/100$ is too small. Figure 3.6b shows that $\langle \Sigma \rangle$ as predicted by equation (3.1) at the end of the evolution now significantly disagrees with the observed experimental data. The underpredictions observed at low quench times are more prominent and there are significant over predictions made for quench times above $\approx 280 \mu$s.
Chapter 3. Modeling the Entropy Generation and the Effects of a varying Relaxation Time $\tau_D$ on the Evolution of a Two-Level System

Figure 3.6: So-called “mean entropy production”, $\langle \Sigma \rangle$, vs. quench time; the evolution of $\langle \Sigma \rangle$ as predicted by the SEAQT equation of motion for quench times between 20 $\mu$s and 800 $\mu$s are shown in addition to the Tasaki-Crooks “mean entropy production” and experimental values.

3.4 Discussion and Conclusion

This work presents the derivation of the SEAQT equation of motion for a general quantum system in a rotating reference frame. Also, the primary assumptions made in the development of the NMR Hamiltonian and how it used in the equation of motion are discussed. Specifically, it is shown that only the transverse component $\hat{H}_{RF}$ and interaction term $\hat{H}_J$ affect the unitary dynamics in the rotating frame but that the entire Hamiltonian, including the portion accounting for the static longitudinal component, $\hat{H}_0$, must be used in computing the dissipation operator in the rotating frame.

Results of this modelling show that while the the values of $\langle \Sigma \rangle$ as predicted using equation (3.1) at the end of the evolution agree well with the experimental values, the general trends exhibited during the evolution of $S_{KL}$ do not match exactly. This suggests that refining the value of $\tau_D$ further such that it is time dependent may be necessary to accurately replicate the evolution, since the evolution of $S_{KL}$ is shown to be highly dependent upon $\tau_D$. Furthermore,
additional details of the experimental procedure used to obtain the evolutions of $S_{KL}$ may be necessary so that their effects can be modeled. One key takeaway, however, is that regardless of the quench time, the results of the SEAQT equation of motion for a quench time based on $\tau_{Matthiesen}$ either predicts the experimental results as well as or better than the von Neumann equation, suggesting that the entropy production as predicted by the SEA principle is real and sufficiently large at higher quench times to explain the differences between the SEAQT predictions and those of the von Neumann equation.

Nonetheless, the real entropy production (as predicted by SEAQT for the net change in the von Neumann entropy during a given set of forward and backward processes) is quite small even at large quench times. The primary reasons are the initial state of the system and the strong, static portion of the Hamiltonian. In this NMR experiment, the initial system state is described by the canonical distribution at room temperature where the system Hamiltonian is closely approximated by the strong static portion of the Hamiltonian, $\hat{H}_0$. Because $\hat{H}_0$ is so much larger in magnitude than the transverse portion of the Hamiltonian $\hat{H}_{RF}$, the net change in the overall system Hamiltonian, which is used in computing the dissipation operator, is small. Therefore, because the system starts out at a stable equilibrium state, and during the quenching process the overall system Hamiltonian remains approximately equal to $\hat{H}_0$, the net effect is that the system state is always near stable equilibrium. This results in little entropy being produced since $dS/dt \to 0$ as a system state approaches stable equilibrium.

Finally, $\tau_D$ in this work is currently based on known characteristic relaxation times associated with NMR experiments. To obtain a fully fundamental model, it is necessary to compute $\tau_D$ based on the various fundamental processes occurring in the NMR experiment. One such process is the Rabi cycle and the associated probability that the system transitions from one state to another at a given time $t$. Further work investigating this process as well as other
effects of the general Hamiltonian in an NMR system should be explored to perhaps gain insight into developing a fundamental model for $\tau_D$. 
Appendices
Appendix B

Rotating Reference Frame Derivation Details

This appendix presents a proof that the terms in the ratio of determinants in the SEAQT dissipation operator can be evaluated equivalently in the rotating reference frame to how they are evaluated in the lab frame for a simple quantum system. First, the ratio of determinants in the lab frame is given as

\[
\tilde{D} = \frac{\begin{vmatrix} \hat{B} \ln(\hat{\rho}_L) & \hat{I} & \hat{H}_L \\ (\hat{I}, \hat{B} \ln(\hat{\rho}_L)) & (\hat{I}, \hat{I}) & (\hat{I}, \hat{H}_L) \\ (\hat{H}_L, \hat{B} \ln(\hat{\rho}_L)) & (\hat{H}_L, \hat{I}) & (\hat{H}_L, \hat{H}_L) \end{vmatrix}}{\Gamma} \tag{B.1}
\]

Now defining \( B_1, B_2, \) and \( \Gamma \) as

\[
B_1 \equiv \begin{vmatrix} (\hat{I}, \hat{B} \ln(\hat{\rho}_L)) & (\hat{I}, \hat{H}_L) \\ (\hat{H}_L, \hat{B} \ln(\hat{\rho}_L)) & (\hat{H}_L, \hat{H}_L) \end{vmatrix} \tag{B.2}
\]

\[
B_2 \equiv \begin{vmatrix} (\hat{I}, \hat{B} \ln(\hat{\rho}_L)) & (\hat{I}, \hat{I}) \\ (\hat{H}_L, \hat{B} \ln(\hat{\rho}_L)) & (\hat{H}_L, \hat{I}) \end{vmatrix} \tag{B.3}
\]
\[ \Gamma \equiv \left| \begin{array}{cc} (\hat{I}, \hat{I}) & (\hat{I}, \hat{H}_L) \\ (\hat{H}_L, \hat{I}) & (\hat{H}_L, \hat{H}_L) \end{array} \right| \] 

\[ \tilde{D} \text{ can be written as} \]

\[ \tilde{D} = \hat{B} \ln(\hat{\rho}_L) - \frac{B_1}{\Gamma} \hat{I} + \frac{B_2}{\Gamma} \hat{H}_L \]  

(B.5)

Applying rotation operators allows the above to be rewritten as

\[ \tilde{D}_R = \hat{B} \ln(\hat{\rho}_R) - \frac{B_1}{\Gamma} \hat{I} + \frac{B_2}{\Gamma} \hat{H}_R \]  

(B.6)

Next, to develop an expression in the rotating reference frame for the inner products involved in the ratio of determinants, a general form in terms of the generators of the motion in the lab frame is first considered. Thus,

\[ \left( \hat{R}_{i,L}, \hat{R}_{j,L} \right) = \frac{1}{2} \text{Tr} \left( \hat{\rho}_L \left\{ \hat{R}_{i,L}, \hat{R}_{j,L} \right\} \right) = \frac{1}{2} \text{Tr} \left( \hat{\rho}_L \left( \hat{R}_{i,L} \hat{R}_{j,L} + \hat{R}_{i,L} \hat{R}_{j,L} \right) \right) \]  

(B.7)

and noting the general definition relating an operator \( \hat{F} \) between the two frames as

\[ \hat{F}_L = \hat{R}_Z(-\phi(t)) \hat{F}_R \hat{R}_Z(-\phi(t)) \]  

(B.8)

conversions from the lab frame operators to the rotating frame operators can be done giving
\[
\left( \hat{R}_{i,L}, \hat{R}_{j,L} \right) = \frac{1}{2} \text{Tr} \left( \hat{\rho}_L \left( \hat{R}_{Z}^\dagger(-\phi(t)) \hat{R}_{i,R} \hat{R}_{Z}(-\phi(t)) \hat{R}_{i,R}^\dagger \hat{R}_{Z}(-\phi(t)) \right. \right.
\]
\[
+ \left. \hat{R}_{Z}^\dagger(-\phi(t)) \hat{R}_{j,R} \hat{R}_{Z}(-\phi(t)) \hat{R}_{j,R}^\dagger \hat{R}_{Z}(-\phi(t)) \right) \right) \tag{B.9}
\]

or
\[
\left( \hat{R}_{i,L}, \hat{R}_{j,L} \right) = \frac{1}{2} \text{Tr} \left( \hat{\rho}_L \hat{R}_{Z}^\dagger(-\phi(t)) \left\{ \hat{R}_{i,R}, \hat{R}_{j,R} \right\} \hat{R}_{Z}(-\phi(t)) \right) \tag{B.10}
\]

or
\[
\left( \hat{R}_{i,L}, \hat{R}_{j,L} \right) = \frac{1}{2} \text{Tr} \left( \hat{R}_{Z}^\dagger(-\phi(t)) \hat{\rho}_R \hat{R}_{Z}(-\phi(t)) \hat{R}_{Z}^\dagger(-\phi(t)) \left\{ \hat{R}_{i,R}, \hat{R}_{j,R} \right\} \hat{R}_{Z}(-\phi(t)) \right) \tag{B.11}
\]

or
\[
\left( \hat{R}_{i,L}, \hat{R}_{j,L} \right) = \frac{1}{2} \text{Tr} \left( \hat{\rho}_R \left\{ \hat{R}_{i,R}, \hat{R}_{j,R} \right\} \hat{R}_{Z}(-\phi(t)) \hat{R}_{Z}^\dagger(-\phi(t)) \right) \tag{B.12}
\]

where it is noted that the order of operators inside the Trace can be re-arranged cyclically, leaving
\[
\left( \hat{R}_{i,L}, \hat{R}_{j,L} \right) = \frac{1}{2} \text{Tr} \left( \hat{\rho}_R \left\{ \hat{R}_{i,R}, \hat{R}_{j,R} \right\} \right) = \left( \hat{R}_{i,R}, \hat{R}_{j,R} \right) \tag{B.13}
\]

which concludes the proof that all of the inner products in the determinants of the SEAQT dissipation operator yield the same result regardless of whether they are in the lab or rotating reference frame so long as all operators involved are in the same reference frame.
Chapter 4

A Method for Generating Random Perturbed Density Operators Subject to an Arbitrary Set of Constraints

4.1 Introduction

Quantum information and computing systems rely on the phenomena of superposition and entanglement to efficiently perform certain tasks that are otherwise inefficient when performed on classical computers. While any quantum system may exhibit superposition, only composite quantum systems (i.e., those consisting of two or more subsystems) may exhibit entanglement. Two systems are said to be entangled when it is not possible to describe the state of the composite system solely in terms of the states of the individual systems composing it. Mathematically, for a density operator, $\hat{\rho}_{AB}$, representing two entangled subsystems A and B, this can be written as

$$\hat{\rho}_{AB} \neq \hat{\rho}_A \otimes \hat{\rho}_B \quad (4.1)$$

where $\hat{\rho}_{A(B)} = \text{Tr}_{B(A)}(\hat{\rho}_{AB})$ and $\text{Tr}_{B(A)}(\hat{\rho}_{AB})$ denotes the partial trace of $\hat{\rho}_{AB}$ (an operator on $\mathcal{H}_A \otimes \mathcal{H}_B$) over the Hilbert space $\mathcal{H}_{B(A)}$, returning an operator on $\mathcal{H}_{A(B)}$. While there is no
fundamental definition quantifying how entangled two systems are, numerous metrics exist that aim to capture system entanglement [30]. Examples include the mutual information, concurrence, and the CHSH operator expectation value, each of which provide useful insight into the states of composite quantum systems.

Because each of these metrics quantify entanglement in a different way, they exhibit different behavior as the physical properties of the composite system change. Thus, to gain insight into the effect of the physical state of the system on various entanglement measures, and in particular the sensitivity of these measures to perturbations of the system state, this chapter focuses on perturbations of an entangled state.

In particular, a numerical method is presented for randomly perturbing an arbitrary baseline density operator $\hat{\rho}_0$ by a given magnitude $\epsilon$, subject to an arbitrary set of constraints on the expectation values associated with the density operator. This method is illustrated by perturbing a bipartite system where each subsystem has only two levels but may be straightforwardly extended to composite systems of arbitrary numbers of subsystems. To understand the effect of perturbations on entanglement, the baseline density operator, $\hat{\rho}_0$, which represents the state of the composite system consisting of subsystems $A$ and $B$, is chosen to be a Bell diagonal state represented by [44]

$$\hat{\rho}_0 = \frac{1}{4} \left( \hat{I}_A \otimes \hat{I}_B + \sum_{i=1}^{3} c_i \hat{\sigma}_{iA} \otimes \hat{\sigma}_{iB} \right) \quad (4.2)$$

where $\hat{\sigma}_1 = \hat{\sigma}_X$, $\hat{\sigma}_2 = \hat{\sigma}_Y$, and $\hat{\sigma}_3 = \hat{\sigma}_Z$ are the Pauli matrices and for this work, the scalar coefficients are chosen as $c_1 = 0.996$, $c_2 = 0.4$, and $c_3 = -0.4$. A Bell diagonal state is chosen for this work because it is a state of non-zero entropy that can be written directly as a sum of Bell states (which are composite system pure states of maximal entanglement). Thus, after the general density operator perturbation method is presented in Section 4.2, perturbations
of the baseline state $\hat{\rho}_0$ are generated under 4 different sets of constraints. Properties of the resulting perturbed states are presented in Section 4.3. Finally, the main trends exhibited in these sets of perturbations are discussed in Section 4.4 along with possible follow-up work.

4.2 Model Development

4.2.1 General Perturbation Approach and “Closeness” of Quantum States

This section presents a method for generating a randomly perturbed density operator whose distance from the original density operator is $O(\epsilon)$ where the notion of distance between two states is discussed in Section 4.2.3 and $\epsilon$ is a specified parameter. This approach permits the enforcement of arbitrary sets of constraints on the expectation values of the resulting perturbed operator, while ensuring that the entire space of states in the neighborhood of the original state is uniformly sampled.

While this approach can be applied to composite systems consisting of any numbers of subsystems, it is illustrated here using a bipartite system of two-level subsystems. To begin with, the square root of the baseline density operator to be perturbed, $\hat{\rho}_0$, is calculated as

$$\hat{\gamma}_0 = \sqrt{\hat{\rho}_0}$$  \hspace{1cm} (4.3)

Perturbing the square-root of the density operator ensures that the resulting perturbed density operator is positive semi-definite (i.e., all of its eigenvalues are non-negative). Now assuming that all of the Hilbert spaces associated with the subsystems are two dimensional, any arbitrary Hermitian operator on the Hilbert space can be represented in terms of the
identity operator \( \hat{I} = \hat{\sigma}_0 \) and the three Pauli spin matrices \( \hat{\sigma}_1 = \hat{\sigma}_X \), \( \hat{\sigma}_2 = \hat{\sigma}_Y \), and \( \hat{\sigma}_3 = \hat{\sigma}_Z \). 

Thus, to perturb \( \hat{\gamma}_0 \) over all possible degrees of freedom, the following expression is used:

\[
\hat{\gamma}_\epsilon = \hat{\gamma}_0 + \epsilon \bigotimes_{i=1}^{M} \left( \sum_{j=0}^{3} \eta_{ij} \hat{\sigma}_{ij} \right)
\]  

(4.4)

where \( M \) is the number of subsystems forming the composite system and each \( \eta_{ij} \) is a randomly generated number. Now assuming that the composite system is bipartite with subsystems \( A \) and \( B \), the above expression can be rewritten as

\[
\hat{\gamma}_\epsilon = \hat{\gamma}_0 + \epsilon \sum_{i,j=0}^{3} \eta_{ij} \hat{\sigma}_{iA} \otimes \hat{\sigma}_{jB}
\]  

(4.5)

The resulting perturbed operator, \( \hat{\gamma}_\epsilon \), while Hermitian, is no longer the square root of a true density operator, since \( \text{Tr}(\hat{\gamma}_\epsilon \hat{\gamma}_\epsilon^\dagger) \neq 1 \). Furthermore, no constraints have yet been enforced on the expectation value of the resulting perturbed density operator. To account for these constraints, a set of operators, \( \hat{C}_i \), are introduced whose corresponding expectation values serve as the constraints on the perturbed density operator. To relate these constraining operators to the desired perturbed operator, the component of the gradient of \( \hat{\gamma}_\epsilon \) in the direction of \( \text{Tr}\left( \hat{C}_i \hat{\gamma}_\epsilon \hat{\gamma}_\epsilon^\dagger \right) \) is introduced and denoted as \( x_i \). This effectively serves to correct the randomly perturbed operator \( \hat{\gamma}_\epsilon \) such that all desired constraints are enforced by removing the component of \( \hat{\gamma}_\epsilon \) along the gradient of each constraint. With these, the square root of the desired perturbed density operator, \( \hat{\gamma}_r \), can be related to \( \hat{\gamma}_\epsilon \) and the desired constraints as

\[
\hat{\gamma}_r = \sum_{i=1}^{N} x_i \hat{C}_i \hat{\gamma}_\epsilon
\]  

(4.6)

where \( N \) is the number of constraints to be enforced. To ensure that \( \text{Tr}(\hat{\rho}_r) = 1 \), where it is noted that \( \hat{\rho}_r = \hat{\gamma}_r \hat{\gamma}_r^\dagger \), the first constraint is chosen to be the identity operator, i.e., \( \hat{C}_1 = \hat{I} \).
To enforce a constant energy perturbation, a second constraining operator could be taken as the Hamiltonian, i.e., $\hat{C}_2 = \hat{H}$. Finally, to enforce a constant entropy constraint, another constraining operator can be chosen as $\hat{C}_3 = -\hat{B} \ln(\hat{\gamma}_r \hat{\gamma}_r^\dagger)$ where it is noted that in this case $\hat{C}_3$ is a nonlinear function of $\hat{\gamma}_r$.

For cases where a constraint is a function of the system state, (i.e., $\hat{C}_i = \hat{C}_i(\gamma)$ such as, e.g., a constant entropy constraint $\hat{C}(\hat{\gamma}_r) = -\hat{B} \ln(\hat{\gamma}_r \hat{\gamma}_r^\dagger)$), it is first necessary to compute a self-consistent solution for $\hat{\gamma}_r$ for given values of $x_i$ in equation (4.6). While for some sets of constraints it may be possible to find an analytical solution for $\hat{\gamma}_r$, this is not possible for the constant entropy constraint; and, thus, equation (4.6) must be solved numerically. After a self-consistent solution is found, $\hat{\rho}_r$ can be expanded as

$$\hat{\rho}_r = \hat{\gamma}_r \hat{\gamma}_r^\dagger = \left( \sum_{j=1}^{N} x_j \hat{C}_j \hat{\gamma}_\ell \right) \left( \sum_{k=1}^{N} x_k \hat{C}_k \hat{\gamma}_\ell \right)^\dagger = \sum_{j=1}^{N} \sum_{k=1}^{N} x_j x_k \hat{C}_j \hat{\gamma}_\ell \hat{\gamma}_\ell^\dagger \hat{C}_k^\dagger$$  \hspace{1cm} (4.7)

To enforce the constraint on the expectation value of the $\hat{C}_i$ operator, the following equation relating the expectation value of the unperturbed and perturbed density operators is used:

$$\text{Tr}\left(\hat{\rho}_0 \hat{C}_i\right) = \text{Tr}\left(\hat{\rho}_r \hat{C}_i\right) = \text{Tr}\left( \left( \sum_{j=1}^{N} \sum_{k=1}^{N} x_j x_k \hat{C}_j \hat{\gamma}_\ell \hat{\gamma}_\ell^\dagger \hat{C}_k^\dagger \right) \hat{C}_i \right)$$  \hspace{1cm} (4.8)

which reduces to

$$\text{Tr}\left(\hat{\rho}_0 \hat{C}_i\right) = \sum_{j=1}^{N} \sum_{k=1}^{N} x_j x_k \text{Tr}\left( \hat{\gamma}_\ell \hat{\gamma}_\ell^\dagger \hat{C}_k^\dagger \hat{C}_j \right)$$  \hspace{1cm} (4.9)

The resulting system of $N$ equations can be solved numerically for the values of $x_i$ where it is noted that solutions near $x_1 = 1$ and $x_i \neq 1 = 0$ are sought.
4.2.2 Example Constant Energy and Entropy Perturbations

To illustrate this procedure with the use of multiple constraints where one is nonlinear, constant energy and entropy constraints are chosen, resulting in $\hat{C}_2 = \hat{H}$ and $\hat{C}_3 = -\hat{B} \ln(\hat{\rho})$ where again $\hat{C}_1 = \hat{I}$. Because one of the constraints is nonlinear, equation (4.6) must first be solved numerically for given values of $x_i$ to ensure that a self-consistent value for the operator $\hat{C}_3 = -\hat{B} \ln(\hat{\gamma}_r \hat{\gamma}_r^\dagger)$ is found. After this is done, the first constraining relationship in the system of $N = 3$ equations becomes

$$0 = \text{Tr}(\hat{\rho}_0 \hat{I}) - \text{Tr}(\hat{\rho}_r \hat{I}) = \text{Tr}(\hat{\rho}_0 \hat{I}) - \sum_{j=1}^{3} \sum_{k=1}^{3} x_j x_k \text{Tr}(\hat{\gamma}_c \hat{\gamma}_c^\dagger \hat{C}_k^\dagger \hat{I} \hat{C}_j)$$

(4.10)

while the second is

$$0 = \text{Tr}(\hat{\rho}_0 \hat{H}) - \text{Tr}(\hat{\rho}_r \hat{H}) = \text{Tr}(\hat{\rho}_0 \hat{H}) - \sum_{j=1}^{3} \sum_{k=1}^{3} x_j x_k \text{Tr}(\hat{\gamma}_c \hat{\gamma}_c^\dagger \hat{C}_k^\dagger \hat{H} \hat{C}_j)$$

(4.11)

and the third is

$$0 = \text{Tr}\left(-\hat{\rho}_0 \hat{B} \ln(\hat{\rho}_0)\right) - \text{Tr}\left(-\hat{\rho}_r \hat{B} \ln(\hat{\rho}_r)\right)$$

$$= \text{Tr}\left(-\hat{\rho}_0 \hat{B} \ln(\hat{\rho}_0)\right) - \sum_{j=1}^{3} \sum_{k=1}^{3} x_j x_k \text{Tr}(\hat{\gamma}_c \hat{\gamma}_c^\dagger \hat{C}_k^\dagger \left(-\hat{B} \ln(\hat{\gamma}_r \hat{\gamma}_r^\dagger)\right) \hat{C}_j)$$

(4.12)

This system of equations can be evaluated iteratively for the values of $x_i$ where for each iteration (corresponding to a unique set of values for $x_i$) a self-consistent value for the operator $\hat{C}_3 = -\hat{B} \ln(\hat{\gamma}_r \hat{\gamma}_r^\dagger)$ must also be iteratively found before the evaluation of equations (4.10) to (4.12).
4.2. Model Development

4.2.3 Review of State Distance and Entanglement Measures

To understand the effects of the perturbations, measures examining the “closeness” of the perturbed state to the baseline state are first examined, followed by measures quantifying the entanglement of the two subsystems. First, a common measure of the similarity between two quantum states $\hat{\rho}_1$ and $\hat{\rho}_2$ is known as the fidelity $F$, which can be computed as

$$F(\hat{\rho}_1, \hat{\rho}_2) = \text{Tr} \left( \sqrt{\sqrt{\hat{\rho}_1} \hat{\rho}_2 \sqrt{\hat{\rho}_1}} \right)$$

(4.13)

where it is noted that for two identical states, $F(\hat{\rho}_1, \hat{\rho}_1) = 1$. Another measure of the distance between two states, given by Beretta [14], is in terms of the square roots of each of the density operators, $\hat{\gamma}_1$ and $\hat{\gamma}_2$, and is given in terms of the angle $\theta_d$ (referred to as the distance measure $\theta_d$) computed as

$$\cos(\theta_d) = \frac{1}{2} \text{Tr} \left( \hat{\gamma}_1^\dagger \hat{\gamma}_2 + \hat{\gamma}_1^\dagger \hat{\gamma}_2 \right)$$

(4.14)

where for two identical states, $\theta_d = 0$. To examine the effects of perturbations on the entanglement of the baseline Bell diagonal state, the mutual information, concurrence, and CHSH operator maximum expectation value are used. The mutual information, $\sigma(\hat{\rho})$, which is related to the entropy of the system, is computed as [47]

$$\sigma(\hat{\rho}) = \text{Tr}_A(\hat{\rho}_A \ln(\hat{\rho}_A)) + \text{Tr}_B(\hat{\rho}_B \ln(\hat{\rho}_B)) - \text{Tr}(\hat{\rho} \ln(\hat{\rho}))$$

(4.15)

The mutual information is a non-negative quantity, equal to zero only when the states of subsystems $A$ and $B$ are completely separable/uncorrelated. The concurrence, $C(\hat{\rho})$, as given by [29, 60] is an entanglement monotone (meaning that it increases as entanglement increases) and is computed as
\[ C(\hat{\rho}) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4) \] (4.16)

where the \( \lambda_i \) are the eigenvalues of the operator \( \hat{R} \) in decreasing order, and \( \hat{R} \) is determined from

\[ R = \sqrt{\hat{\rho} \hat{\rho} \sqrt{\hat{\rho}}} \] (4.17)

and

\[ \hat{\rho} = (\hat{\sigma}_Y \otimes \hat{\sigma}_Y) \hat{\rho}^* (\hat{\sigma}_Y \otimes \hat{\sigma}_Y) \] (4.18)

The final entanglement measure examined here is the violation of the Clauser-Horne-Shimony-Holt (CHSH) inequality [18]. The CHSH inequality, which is closely related to Bell’s inequality [4], states that local hidden variable theories cannot predict correlations above a value of 2, and, thus, correlations above this value must be due to the quantum phenomenon of entanglement. Cirel’son [17] showed that when accounting for quantum mechanical effects, the maximum value of the correlations exhibited between the subsystems in a composite quantum system is \( 2\sqrt{2} \). In an experiment, it is possible to compute various expectation values for the CHSH operator, \( \hat{B}_{CHSH} \), depending on the relative orientation of the experimental measurement. However, an analytical form for the maximum possible expectation value for a given state of the system can be computed from [30]

\[ \left< \hat{B}_{CHSH}(\hat{\rho}) \right>_{\text{max}} = 2\sqrt{t_{11}^2 + t_{22}^2} \] (4.19)

where \( t_{11} \) and \( t_{22} \) are the two largest eigenvalues of the matrix \( T_{\hat{\rho}}^T T_{\hat{\rho}} \), with the elements of \( T_{\hat{\rho}} \) given by \( t_{ij} = \text{Tr}(\hat{\rho} (\hat{\sigma}_i \otimes \hat{\sigma}_j)) \). With these entanglement measures, results for various
perturbations under various sets of constraints are presented in Section 4.3.

4.3 Results

This section presents the results of four different perturbation cases. For all cases, a perturbation magnitude $\epsilon = 10^{-2}$ is used and $N = 1000$ perturbed states are presented. All random numbers are generated from a uniform distribution between $[-0.5, 0.5]$. While it is understood that this sample size is much too small to thoroughly sample the entire 15-dimensional space required to fully characterize a normalized density operator of a bipartite system of two-level subsystems, for simplicity it is assumed that the trends exhibited by the perturbed states here are representative of this neighborhood of the entire 15-dimensional space. The quantities plotted are the system energy, entropy, mutual information, concurrence, and the CHSH operator maximum expectation value. In addition, the fidelity and distance measure $\theta_d$ of the perturbed state relative to the baseline state $\hat{\rho}_0$ are also shown. In all cases, the constraint for a normalized density operator is enforced (i.e., $\text{Tr}(\hat{\rho}) = 1$).

Section 4.3.1 provides perturbation results for the case where no additional constraints are enforced, while Section 4.3.2 presents results incorporating a constant energy constraint. Section 4.3.3 provides results under a constant entropy constraint followed by Section 4.3.4 which presents results under both constant energy and entropy constraints. For all cases, plots of perturbation energy vs. entropy, Fidelity vs. distance measure $\theta_d$, mutual Information vs. entropy, concurrence vs. mutual information, CHSH operator maximum expectation value vs. mutual information, and concurrence vs. CHSH operator maximum expectation value are shown.
4.3.1 Perturbations with No Constraints

This section presents results for perturbations where no constraints other than $\text{Tr}(\hat{\rho}) = 1$ are enforced. Figure 4.1a shows the energy vs. entropy diagram and Figure 4.1b shows the perturbed state fidelity vs. the distance measure $\theta_d$. Figure 4.1a shows that the energy and entropy distributions are roughly centered about the values of the baseline state. In addition, it is seen that these values span up to $\mathcal{O}(\sqrt{\epsilon})$ away from the baseline value. Figure 4.1b shows that the distance measure $\theta_d$ is $\mathcal{O}(\epsilon)$ from the baseline state and that the fidelity varies as $\mathcal{O}(\epsilon^2)$. While the two metrics are clearly related, this suggests that the distance measure $\theta_d$ is a more conservative measure of the distance between two states since it is more sensitive to the magnitude of the perturbation $\epsilon$.

![Figure 4.1: Perturbed state energy-entropy diagram and distance measure $\theta_d$ vs fidelity.](image)

Figure 4.2a shows the entropy vs. the mutual information of the perturbed state, and Figure 4.2b provides the perturbed state concurrence vs. the mutual information. Figure 4.2a shows that the perturbed state mutual information decreases approximately linearly as the entropy increases. Furthermore, it experiences a change in value relative to the baseline state $\hat{\rho}_0$ of approximately the same value as the entropy but of opposite sign. Figure 4.2b shows that the mutual information and concurrence both vary of $\mathcal{O}(\epsilon)$ from the baseline value, and
that there is a clear trend between the value of the mutual information and the value of the concurrence of a given state, which is expected.

Figure 4.2: Perturbed state entropy vs. mutual information and mutual information vs. concurrence.

Figure 4.3a shows the maximum CHSH operator expectation value vs. the mutual information of the perturbed state, and Figure 4.3b shows the perturbed state maximum CHSH operator expectation value vs. the concurrence. Figure 4.3a shows that the perturbed state maximum CHSH operator expectation value increases nearly directly proportionally to the mutual information among the perturbed states, which is again expected since both aim to quantify the entanglement of a system.

Figure 4.3b shows that the concurrence and the maximum CHSH operator expectation value both vary of $O(\epsilon)$ from the baseline value, and that there is a clear trend between the value of the mutual information and the value of the concurrence of a given state. In both Figures 4.3b and 4.2b, the spread of the perturbed state distribution seems to be slightly larger than in Figure 4.3a, suggesting that the concurrence may be more sensitive to perturbations than the mutual information or the maximum CHSH operator expectation value.
Chapter 4. A Method for Generating Random Perturbed Density Operators Subject to an Arbitrary Set of Constraints

4.3.2 Perturbations under the Constant Energy Constraint

This section presents results for perturbations where a constant energy constraint is also enforced. Figure 4.4a shows the energy vs. entropy diagram and Figure 4.4b shows the perturbed state fidelity vs. the distance measure $\theta_d$. Figure 4.4a shows that the entropy is distributed roughly evenly about the value of the baseline state and all perturbations have the same energy as that of the baseline state, as expected. In addition, this constraint does not affect the magnitude of the spread ($O(\sqrt{\epsilon})$) of the values of system entropy about the baseline state as compared to Figure 4.1a. Figure 4.4b shows that the distance measure $\theta_d$ is again $O(\epsilon)$ from the baseline state and that the fidelity again varies as $O(\epsilon^2)$. The constant energy constraint appears to have had no qualitative effect on the distribution in Figure 4.4b as compared to Figure 4.1b.

Figure 4.5a shows the entropy vs. the mutual information of the perturbed state and Figure 4.5b presents the perturbed state concurrence vs. the mutual information. As seen in Figure 4.5a, the perturbed state mutual information decreases approximately linearly as the entropy increases. It also experiences a change in value relative to the baseline state $\hat{\rho}_0$ of

![Figure 4.3: Perturbed state mutual information vs. maximum CHSH operator expectation value and maximum CHSH operator expectation value vs. concurrence.](image)

![Figure 4.4a: Energy vs. entropy diagram.](image)

![Figure 4.4b: Perturbed state fidelity vs. distance measure $\theta_d$.](image)

![Figure 4.5a: Entropy vs. mutual information of the perturbed state.](image)

![Figure 4.5b: Perturbed state concurrence vs. mutual information.](image)
4.3. Results

Figure 4.4: Perturbed state energy-entropy diagram and distance measure $\theta_d$ vs fidelity. Approximately the same value as the entropy but of opposite sign. Figure 4.5b shows that the mutual information and concurrence vary of $\mathcal{O}(\epsilon)$ from the baseline value, and that the trend of higher values of mutual information corresponding to higher concurrence values persists here. Thus, the constant energy constraint seems to have little qualitative effect on the trends of these distributions.

Figure 4.5: Perturbed state entropy vs. mutual information and mutual information vs. concurrence.

Figure 4.6a shows the maximum CHSH operator expectation value vs. the mutual information.
of the perturbed state, and Figure 4.6b presents the perturbed state maximum CHSH operator expectation value vs. the concurrence. As seen in Figure 4.6a, the perturbed state maximum CHSH operator expectation value increases proportionally to the mutual information among the perturbed states, while Figure 4.6b shows that the concurrence and the maximum CHSH operator expectation value both vary of $O(\epsilon)$ from the baseline value. Compared to Figures 4.3a and 4.3b, the constant energy perturbation has had no qualitative effects on these distributions either.

Figure 4.6: Perturbed state mutual information vs. maximum CHSH operator expectation value and maximum CHSH operator expectation value vs. the concurrence.

4.3.3 Perturbations under Constant Entropy Constraint

This section presents results for perturbations where a constant entropy constraint is enforced instead of a constant energy constraint. Figure 4.7a shows the energy vs. entropy diagram and Figure 4.7b provides the perturbed state fidelity vs. the distance measure $\theta_d$. AS seen in Figure 4.7a, the energy is distributed roughly evenly about the value of the baseline state and all perturbations have the same entropy as that of the baseline state, as expected. Figure 4.7b shows that the distance measure $\theta_d$ is again of $O(\epsilon)$ from the baseline state and that
the fidelity again varies as \( \mathcal{O}(\epsilon^2) \). The constant entropy constraint also appears to have no qualitative effect on the distribution in Figure 4.7b as compared to Figure 4.1b.

![Perturbed State Energy-Entropy Diagram](image1)

**Figure 4.7:** Perturbed state energy-entropy diagram and distance measure \( \theta_d \) vs fidelity.

Figure 4.8a shows the entropy vs. the mutual information of the perturbed state, while Figure 4.8b provides the perturbed state concurrence vs. the mutual information. As seen in Figure 4.8a, the perturbed state mutual information is now nearly identical to that of the baseline case, which is to be expected since the change in mutual information from the baseline case tends to be directly proportional to the change in entropy from the baseline case, which here is zero. Figure 4.8b shows that while the mutual information varies little under the constant entropy constraint, that the concurrence still varies of \( \mathcal{O}(\epsilon) \) from the baseline state. This indicates that under perturbations that take the form of a unitary operation, the concurrence is much more likely to exhibit change than the mutual information.

Figure 4.9a provides the maximum CHSH operator expectation value vs. the mutual information of the perturbed state and Figure 4.9b shows the perturbed state maximum CHSH operator expectation value vs. the concurrence. As seen in Figure 4.9a, the perturbed state maximum CHSH operator expectation value now exhibits a much smaller spread as compared to Figure 4.3a, and subsequently there is a smaller spread of values in Figure 4.9b.
Chapter 4. A Method for Generating Random Perturbed Density Operators Subject to an Arbitrary Set of Constraints

Figure 4.8: Perturbed state entropy vs. mutual information and mutual information vs. concurrence.

for the maximum CHSH operator expectation value vs. the concurrence. Figure 4.9b now shows a more linear trend between an increase in the maximum CHSH operator expectation value and concurrence. However, the concurrence still has a larger distribution of values. This indicates that the maximum CHSH operator expectation value is more closely correlated to the system entropy than is the concurrence.

Figure 4.9: Perturbed state mutual information vs. maximum CHSH operator expectation value and maximum CHSH operator expectation value vs. concurrence.
4.3. Results

4.3.4 Perturbations under Constant Energy and Entropy Constraints

This section presents results for perturbations where constant energy and entropy constraints are both enforced. Figure 4.10a shows the energy vs. entropy diagram, while Figure 4.10b provides the perturbed state fidelity vs. distance measure $\theta_d$. As expected, Figure 4.10a shows that there is no spread of the perturbed values about the baseline value on the E-S diagram. These constraints also have no qualitative effect on the distribution of states in Figure 4.10b as compared to previous sets of constraints.

![Figure 4.10: Perturbed state energy-entropy diagram and distance measure $\theta_d$ vs fidelity.](image)

Figure 4.11a shows the entropy vs. the mutual information of the perturbed state, and Figure 4.11b provides the perturbed state concurrence vs. the mutual information. As seen in Figure 4.11a, the perturbed state mutual information is again nearly identical to that of the baseline case, while Figure 4.11b shows that the concurrence still varies of $O(\epsilon)$ from the baseline state as was seen in Figure 4.8b.

Figure 4.12a provides the maximum CHSH operator expectation value vs. the mutual information of the perturbed state, and Figure 4.12b shows the perturbed state maximum
Chapter 4. A Method for Generating Random Perturbed Density Operators Subject to an Arbitrary Set of Constraints

Figure 4.11: Perturbed state entropy vs. mutual information and mutual information vs. concurrence.

CHSH operator expectation value vs. the concurrence. As seen in Figure 4.12a, the perturbed state maximum CHSH operator expectation value again exhibits a much smaller spread as compared to Figure 4.3a, while Figure 4.12b again shows an approximately linear trend between an increase in the maximum CHSH operator expectation value and the concurrence.

Figure 4.12: Perturbed state mutual information vs. maximum CHSH operator expectation value and maximum CHSH operator expectation value vs. concurrence.
4.4 Conclusions

This chapter has presented a general numerical perturbation method for randomly creating perturbed states that are a specified magnitude away from the original baseline state. Furthermore, this method permits arbitrary sets of constraints to be applied to the expectation values of the perturbed states. This method is illustrated by using combinations of energy and entropy constraints to generate perturbations of a Bell diagonal state. By using a Bell diagonal state, the effects of the various types of perturbations on the entanglement characteristics of the resulting perturbed states can be studied.

The first takeaway from this study is that the constant energy constraint has little effect on the distribution of the perturbed state entanglement characteristics, while the constant entropy constraint has a major effect. This suggests that the entanglement of two systems is much more closely correlated to the composite system entropy than the energy and that as the system entropy increases, the entanglement decreases. Regarding the entanglement measures, the distribution of concurrence values is relatively unaffected by the energy or entropy constraints, but the CHSH operator maximum expectation value and mutual information both are significantly affected by the entropy constraint/perturbation. Specifically, the magnitude in change of the mutual information from the baseline state is nearly directly proportional to that of the change in entropy from the baseline state, and, thus, for constant entropy perturbations, all perturbations have nearly identical values to that of the baseline case.

This behavior is likely dependent on the choice of baseline state (a Bell diagonal state), and further work should be done to examine this trend for a broader class of baseline states. Another interesting feature of the constant entropy perturbations is that the distribution of the perturbed state CHSH operator maximum expectation values is significantly smaller than
that seen in the absence of this constraint. These behaviors suggest that for perturbations that occur under a unitary process (where no entropy changes), that the concurrence is much more likely to be affected than the mutual information or the CHSH operator maximum expectation value.

It is also noted that the values of the perturbed state energy and entropy spanned of $O(\sqrt{\epsilon})$ away from the corresponding baseline values, and that the fidelity only varied of $O(\epsilon^2)$ away from the baseline value. The distance measure $\theta_d$ and all of the entanglement measures varied of $O(\epsilon)$ from the baseline values. In addition to the development of the general perturbation method, a study has been performed characterizing the effects of perturbing the system energy and entropy of a Bell diagonal state. Future extensions of this work include the development of a broader set of constraints to apply in the perturbation procedure (e.g., a constant concurrence perturbation) as well as a more in-depth statistical analysis to better see how certain types of perturbations change various system properties and to see what correlations between variables are strongest.
Chapter 5

Modeling the Effects of Perturbations and Steepest-Entropy-Ascent on the Time Evolution of Entanglement

5.1 Introduction

Quantum information and computing systems rely on the quantum phenomena of superposition and entanglement to implement useful tasks. In general, two qubits may become entangled if they interact, and certain applications may require that this entanglement persist for some specified amount of time, even if the qubits are no longer interacting (such as in the case of quantum teleporting applications [8]). Thus, as dissipation occurs throughout a process, it is necessary to understand the effects it has on the entangled state of the system. While various dissipative models predict different effects on the evolution of system state [68], this work focuses on the dynamics of the system state under the principle of steepest entropy ascent (SEA), using the SEA quantum thermodynamics equation of motion.

Liu et al. [44] theoretically predict the loss of entanglement between two non-interacting qubits in a Bell diagonal state using the Kraus-Operator-Sum approach. This modeling approach does not assume a specific physical realization for the qubits but does assume that
both of the qubits are interacting with an external global dephasing (decoherence) field, which is the cause of the dissipation and loss of entanglement. They show that the concurrence (a measure of entanglement) of the system remains unaffected by the dissipation due to this interaction, resulting in what is referred to as time-invariant entanglement. However, they also show that the maximum expectation value of the Clauser-Horne-Shimony-Holt (CHSH) operator (another measure of entanglement), $\langle \hat{B}_{CHSH} \rangle_{\text{max}}$, exhibits decay due to this interaction. Bell and Clauser [4, 18] et al. demonstrate that Local-Hidden-Variable theories can only produce correlations of the $\langle \hat{B}_{CHSH} \rangle$ having a maximum value of 2. Cirel’son [17] later shows that when accounting for quantum phenomena, that values as high as $2\sqrt{2}$ can be obtained.

Thus, Liu et al. [44] show that some entangled quantum states having values $\langle \hat{B}_{CHSH} \rangle_{\text{max}} > 2$ undergo an evolution in this global dephasing (or decoherence) environment that results in $\langle \hat{B}_{CHSH} \rangle_{\text{max}} < 2$ whereas others exhibit a decay but maintain $\langle \hat{B}_{CHSH} \rangle_{\text{max}} > 2$ and, thus, alway produce non-local correlations. A drop in value of $\langle \hat{B}_{CHSH} \rangle_{\text{max}}$ below 2 implies that the correlations resulting from measurements of a quantum system can no longer be attributed with certainty to the entangled nature of the quantum system, as it is possible for unentangled systems to exhibit values of $\langle \hat{B}_{CHSH} \rangle_{\text{max}}$ as high as 2. This is what is referred to as the sudden death of non-locality.

This modeling is validated by Liu et al. [44] experimentally in a quantum optics experiment using pairs of entangled photons that demonstrate that certain Bell diagonal states exhibit sudden death of non-locality (i.e., $\langle \hat{B}_{CHSH} \rangle_{\text{max}}$ drops below 2), whereas other Bell diagonal states maintain non-local correlations. In all cases, however, the entanglement as measured by the concurrence remains constant.

The present work quantifies the effects of SEA on the dynamics of an entangled system and consequently how the entanglement as measured by the concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{max}}$
5.2 Model Development

changes with system state. In addition, it is demonstrated that under SEA, certain states may also exhibit decay in $\langle \hat{B}_{CHSH} \rangle_{max}$ but never drop below 2 whereas others undergo sudden-death of non-locality.

To accomplish this, Section 5.2 first presents the models used to quantify system entanglement, the SEAQT equation of motion and Hamiltonian to be modeled in this experiment, and the behavior of Bell diagonal states relative to the SEAQT equation of motion. Because Bell diagonal states are non-dissipative in SEAQT, perturbation methods are also presented in Section 5.2 that perturb the non-dissipative baseline Bell diagonal state to a dissipative one. Specifically, three types of perturbations are used, and the resulting dynamics under the SEAQT equation of motion are presented in Section 5.3. Finally, 5.4 provides the primary conclusions of this work and future steps to expand the current model.

5.2 Model Development

To model the evolution of entanglement due to the principle of steepest entropy ascent, three entanglement measures and the SEAQT equation of motion are first reviewed. The entanglement measures are reviewed in Section 5.2.1 and are use to examine how the entanglement changes throughout the system’s evolution. Next, Section 5.2.2 presents the SEAQT equation of motion for a general quantum system, and how it is used to predict the dissipation and associated change in entanglement characteristics. The class of states of interest in this work are known as Bell-diagonal states and turn out to be non-dissipative relative to the SEAQT equation of motion (a brief proof of which is also presented in Section 5.2.2). Thus, to examine the dynamics of dissipation associated with SEAQT, it is necessary to generate dissipative, perturbed states from a baseline Bell diagonal state. Methods for creating these perturbed states are presented in Section 5.2.3 and common features relating the
perturbed state to that of the baseline state are highlighted. The evolutions of these perturbed states under the SEAQT equation of motion and the associated changes in entanglement are then presented in Section 5.3.

5.2.1 Entanglement Measures

To analyze the evolution of the entanglement under SEAQT, three different metrics are used: 1) the mutual information, $\sigma(\hat{\rho})$, 2) the concurrence $C(\hat{\rho})$, and 3) the maximum expectation value of the CHSH operator $\langle \hat{B}_{\text{CHSH}} \rangle$, though many other exist (for a rather comprehensive review see [30]). Additionally, the operator $\hat{\xi}$, which is related to the difference between the entangled composite system state and the product of the locally observed states of each subsystem, is also explored. Furthermore, to quantify the effects of the perturbations on the system state, measures of the distance between the baseline state and the perturbed state are also discussed. First, the mutual information between two subsystems, $\sigma(\hat{\rho})$, is defined as [10, 47]

$$\sigma(\hat{\rho}) = \text{Tr}_A(\hat{\rho}_A \ln(\hat{\rho}_A)) + \text{Tr}_B(\hat{\rho}_B \ln(\hat{\rho}_B)) - \text{Tr}(\hat{\rho} \ln(\hat{\rho}))$$ (5.1)

The mutual information is non-negative and only equals zero when the composite system state is completely separable, i.e., $\hat{\rho} = \hat{\rho}_A \otimes \hat{\rho}_B$. The concurrence, $C(\hat{\rho})$, proposed by Hill and Wooters [29, 60] is computed as

$$C(\hat{\rho}) = \max(0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4)$$ (5.2)

where $\lambda_i$ are the eigenvalues of the operator $\hat{R}$ in decreasing order as $i$ increases, and $\hat{R}$ is determined using the relation
5.2. Model Development

\[
\hat{R} = \sqrt{\hat{\rho} \hat{\rho} \sqrt{\hat{\rho}}}
\]  
(5.3)

where the matrix \( \hat{\rho} \) is computed as

\[
\hat{\rho} = (\hat{\sigma}_Y \otimes \hat{\sigma}_Y) \hat{\rho}^* (\hat{\sigma}_Y \otimes \hat{\sigma}_Y)
\]  
(5.4)

where \( \hat{\rho}^* \) is the complex conjugate of \( \hat{\rho} \).

The third common entanglement measure used here is the maximum expectation value of the CHSH operator, \( \langle \hat{B}_{\text{CHSH}}(\hat{\rho}) \rangle_{max} \), which is expressed as

\[
\langle \hat{B}_{\text{CHSH}}(\hat{\rho}) \rangle_{max} = 2\sqrt{t_{11}^2 + t_{22}^2}
\]  
(5.5)

where \( t_{11} \) and \( t_{22} \) are the two largest eigenvalues of the matrix \( T^\top \hat{\rho} T \), and the elements of \( T \) are given by \( t_{ij} = \text{Tr}(\hat{\rho} (\hat{\sigma}_i \otimes \hat{\sigma}_j)) \).

The final aspect associated with the entanglement of the system is the operator \( \hat{\xi} \), which is related to the system density operator by [16]

\[
\hat{\rho} = \hat{\rho}_A \otimes \hat{\rho}_B + \hat{\xi}
\]  
(5.6)

For entangled subsystems, \( \hat{\xi} \) is non-zero, and it is seen that for non-interacting subsystems, \( \hat{\xi} \) in the SEAQT equation of motion is only affected by the reversible dynamics. Thus, switching to the Heisenberg picture (i.e., the rotating frame), where there reversible dynamics effectively “disappear”, \( \hat{\xi} \) remains invariant under the SEAQT equation of motion. Now, if it is assumed that each subsystem \( A \) and \( B \) evolves to the local equilibrium state \( \hat{\rho}_{eq,A(B)} = e^{-\beta_{A(B)} \hat{H}_{A(B)}/Z_{A(B)}} \), then the final stationary state to which the composite system evolves is
Chapter 5. Modeling the Effects of Perturbations and Steepest-Entropy-Ascent on the Time Evolution of Entanglement

\[ \hat{\rho}_{SS} = \hat{\rho}_{eq,A} \otimes \hat{\rho}_{eq,B} + \hat{\xi}. \]

Currently a formal mathematical proof that this is the state to which non-interacting, yet entangled systems evolve under SEAQT does not exist.

Finally, to analyze the effects of a perturbation on the system, two measures quantifying the distance between two states are used. The first is the Fidelity, \( F(\hat{\rho}_1, \hat{\rho}_2) \), given as \[ 47 \]

\[ F(\hat{\rho}_1, \hat{\rho}_2) = \text{Tr}\left( \sqrt{\sqrt{\hat{\rho}_1} \hat{\rho}_2 \sqrt{\hat{\rho}_1}} \right) \]  \hspace{1cm} (5.7)

where for two identical states \( F(\hat{\rho}_1, \hat{\rho}_1) = 1 \). The second measure, given by Beretta [14], is computed in terms of the angle \( \theta_d \) as

\[ \cos(\theta_d) = \frac{1}{2} \text{Tr}\left( \gamma_1 ^\dagger \gamma_2 + \gamma_2 ^\dagger \gamma_1 \right) \]  \hspace{1cm} (5.8)

where \( \gamma_1 \) and \( \gamma_2 \) are the square roots of the density operators of the two states. For this measure, two identical states yield \( \theta_d = 0 \).

5.2.2 SEAQT Equation of Motion for a General Quantum System and Stationary States

Because entanglement is inherently a feature of composite system states, analyzing the change in entanglement requires analyzing the dynamics of the entire composite system. The associated Hilbert space for these composite systems is \( \mathcal{H} = \bigotimes_{J=1}^{M} \mathcal{H}_J \) where \( M \) is the number of subsystems in the composite system. Thus, to understand the effects of the dissipation associated SEA on the time evolution of the entanglement, the SEAQT equation of motion for a general quantum system is required and is expressed as
5.2. Model Development

\[
\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} [\hat{H}, \hat{\rho}] - \frac{D(\hat{\rho})}{Dt}
\]  

(5.9)

where the dissipation operator \( D (\hat{\rho}) / Dt \) for a composite of \( M \) subsystems is

\[
\frac{D(\hat{\rho})}{Dt} = \sum_{J=1}^{M} \frac{1}{\tau_{J}} \hat{D}_{J} \otimes \hat{\rho}_{\bar{J}}
\]  

(5.10)

and the partial trace of the composite density operator onto the \( J^{th} \) subsystem is given as

\[
\hat{\rho}_{J} = \text{Tr}_{\bar{J}}(\hat{\rho}) \quad \text{where} \quad \bar{J} \text{ represents the composite of all subsystems} \neq J.
\]

Likewise the density operator for the composite of all subsystems except the \( J^{th} \) can be computed as \( \hat{\rho}_{\bar{J}} = \text{Tr}_{J}(\hat{\rho}) \).

The dissipation operator for the \( J^{th} \) subsystem, \( \hat{D}_{J} \), is

\[
\hat{D}_{J} = \frac{1}{2} \left( \hat{\rho}_{J} \hat{D}_{J} + \left( \hat{\rho}_{J} \hat{D}_{J} \right)^{\dagger} \right)
\]  

(5.11)

and \( \hat{D}_{J} \) represents a ratio of determinants for the \( J^{th} \) subsystem, which ensures that the expectation values associated with the generators of the motion, \( \hat{R}_{iJ} \), of the \( J^{th} \) subsystem remain constant. \( \hat{D}_{J} \) is computed as

\[
\hat{D}_{J} = \sqrt{\hat{\rho}_{J}}
\]

\[
\begin{pmatrix}
(\hat{B} \ln(\hat{\rho}))^{J} & (\hat{R}_{1J})^{J} & (\hat{R}_{2J})^{J} & \cdots & (\hat{R}_{N(J)J})^{J} \\
(\hat{R}_{1J}, \hat{B} \ln(\hat{\rho}))^{J} & (\hat{R}_{1J}, \hat{R}_{1J})^{J} & (\hat{R}_{1J}, \hat{R}_{2J})^{J} & \cdots & (\hat{R}_{1J}, \hat{R}_{N(J)J})^{J} \\
(\hat{R}_{2J}, \hat{B} \ln(\hat{\rho}))^{J} & (\hat{R}_{2J}, \hat{R}_{1J})^{J} & (\hat{R}_{2J}, \hat{R}_{2J})^{J} & \cdots & (\hat{R}_{2J}, \hat{R}_{N(J)J})^{J} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
(\hat{R}_{N(J)J}, \hat{B} \ln(\hat{\rho}))^{J} & (\hat{R}_{N(J)J}, \hat{R}_{1J})^{J} & (\hat{R}_{N(J)J}, \hat{R}_{2J})^{J} & \cdots & (\hat{R}_{N(J)J}, \hat{R}_{N(J)J})^{J}
\end{pmatrix}
\]

\[
\frac{1}{\Gamma^{J}}
\]

(5.12)
where $N(J)$ is the number of generators of the motion for subsystem $J$ and the Gram determinant $\Gamma^J$ is computed as

$$\Gamma^J = \begin{vmatrix} \left( \hat{R}_{1J}, \hat{R}_{1J} \right)^J & \left( \hat{R}_{1J}, \hat{R}_{2J} \right)^J & \cdots & \left( \hat{R}_{1J}, \hat{R}_{N(J)J} \right)^J \\ \left( \hat{R}_{2J}, \hat{R}_{1J} \right)^J & \left( \hat{R}_{2J}, \hat{R}_{2J} \right)^J & \cdots & \left( \hat{R}_{2J}, \hat{R}_{N(J)J} \right)^J \\ \vdots & \vdots & \ddots & \vdots \\ \left( \hat{R}_{N(J)J}, \hat{R}_{1J} \right)^J & \left( \hat{R}_{N(J)J}, \hat{R}_{2J} \right)^J & \cdots & \left( \hat{R}_{N(J)J}, \hat{R}_{N(J)J} \right)^J \end{vmatrix} \quad (5.13)$$

For the remainder of this work, all subsystems $J$ will have the same two (and only two) generators of the motion. The first, $\hat{R}_{1J} = \hat{I}$, ensures that $\text{Tr}(\hat{\rho}) = 1$, and the second, $\hat{R}_{1J} = \hat{H}$, ensures that the system evolution conserves energy. With this the above reduces to

$$\tilde{D}_J = \sqrt{\hat{\rho}_J} \frac{\begin{vmatrix} \left( \hat{B} \ln(\hat{\rho}) \right)^J & \left( \hat{I} \right)^J & \left( \hat{H} \right)^J \\ \left( \hat{I}, \hat{B} \ln(\hat{\rho}) \right)^J & \left( \hat{I}, \hat{I} \right)^J & \left( \hat{I}, \hat{H} \right)^J \\ \left( \hat{H}, \hat{B} \ln(\hat{\rho}) \right)^J & \left( \hat{H}, \hat{I} \right)^J & \left( \hat{H}, \hat{H} \right)^J \end{vmatrix}}{\begin{vmatrix} \left( \hat{I}, \hat{I} \right)^J & \left( \hat{I}, \hat{H} \right)^J \\ \left( \hat{H}, \hat{I} \right)^J & \left( \hat{H}, \hat{H} \right)^J \end{vmatrix}} \quad (5.14)$$

where the terms $(\hat{F}, \hat{G})^J$ are defined as

$$\left( \hat{F}, \hat{G} \right)^J = \frac{1}{2} \text{Tr}_J(\hat{\rho}_J) \left\{ \left( \hat{F} \right)^J, \left( \hat{G} \right)^J \right\} \quad (5.15)$$

with

$$\left\{ \sqrt{\rho}_J \left( \hat{F} \right)^J, \sqrt{\rho}_J \left( \hat{G} \right)^J \right\} = \frac{1}{2} \text{Tr}_J \left( \sqrt{\rho}_J \left( \hat{F} \right)^\dagger \sqrt{\rho}_J \hat{G} + \sqrt{\rho}_J \left( \hat{G} \right)^\dagger \sqrt{\rho}_J \hat{F} \right) \quad (5.16)$$
and a so-called locally perceived operator \( \hat{F}^J \) computed as

\[
\left( \hat{F}^J \right) = \text{Tr}_J \left( \left( \hat{I}_J \otimes \hat{\rho}_J \right) \hat{F} \right)
\] (5.17)

For a composite system whose subsystems \( A \) and \( B \) are said to be weakly interacting, the composite system Hamiltonian can be written as the sum of Hamiltonians for each subsystem \( A \) and \( B \), i.e., \( \hat{H}_A \) and \( \hat{H}_B \), and an interaction term \( \hat{V}_{AB} \)

\[
\hat{H} = \hat{H}_A \otimes \hat{I}_B + \hat{I}_A \otimes \hat{H}_B + \hat{V}_{AB}
\] (5.18)

where \( \hat{I}_{A(B)} \) are the identity operators in \( \mathcal{H}_{A(B)} \) and the composite system identity operator can be computed as \( \hat{I} = \hat{I}_A \otimes \hat{I}_B \). While it is well known that two systems must interact to become entangled, this work examines the evolution of two systems who have already interacted to become entangled and are no longer interacting, implying that \( \hat{V}_{AB} = 0 \). With this model, it is possible to attribute any change in the entanglement characteristics of the composite system solely to dissipation, since the subsystems no longer interact to change entanglement characteristics through the reversible dynamics. Next, the dynamics of the SEAQT equation of motion is examined for a specific class of entangled states, known as Bell diagonal states, to better understand how entanglement changes.

**Stationary States**

In the SEAQT framework, any state that is non-dissipative (i.e., \( dS/dt = 0 \)) is called a non-dissipative or stationary state. Considering the SEAQT equation of motion written as

\[
\frac{d\hat{\rho}}{dt} = -\frac{i}{\hbar} \left[ \hat{H}, \hat{\rho} \right] - \frac{D(\hat{\rho})}{Dt}
\] (5.19)
this corresponds to $D(\hat{\rho})/Dt = 0$. The well known stable thermodynamic equilibrium states of a system, defined by the canonical distribution $\hat{\rho}_{eq} = \exp\left(-\beta \hat{H}\right)/Z$, which commutes with the Hamiltonian $\hat{H}$, thus, resulting in no reversible dynamics, also yields $D(\hat{\rho})/Dt = 0$. Thus, there is no change in the density operator for these states. In addition to these states, for simple quantum systems, there also exist so-called partially canonical states [13], which are not-stable-thermodynamic-equilibrium states that also result in no dissipation, though the existence of these states requires the quantum system to have at least 3 distinct energy eigenvalues. Furthermore, for composite systems, which may also experience partially canonical states, there also exist stationary states, sometimes referred to as limit cycles, where the reversible dynamics of the system are still present but the dissipation is zero. As an example, first consider the spectral representation of the composite system density operator given by

$$\hat{\rho} = \sum_i \lambda_i \hat{P}_i$$

(5.20)

where the $\lambda_i$ are the density operator eigenvalues and the $\hat{P}_i$ are the associated projectors. Now, if the system is assumed to be bipartite where both subsystems $A$ and $B$ have two energy eigenlevels and the composite system state is assumed to be a Bell diagonal state, the four projectors can be written as

$$\hat{P}_{\Phi^\pm} = |\Phi^\pm\rangle \langle \Phi^\pm| = \frac{1}{2} \begin{bmatrix} 1 & 0 & 0 & \pm 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ \pm 1 & 0 & 0 & 1 \end{bmatrix}$$

(5.21)
\[ \hat{P}_{\Psi^\pm} = |\Psi^\pm\rangle \langle \Psi^\pm| = \frac{1}{2} \begin{bmatrix} 0 & 0 & 0 & 0 \\ 0 & 1 & \pm1 & 0 \\ 0 & \pm1 & 1 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix} \] (5.22)

Now, to obtain a representation of the state for each subsystem, the partial trace of the composite can be evaluated as

\[ \hat{\rho}_J = \text{Tr}_J(\hat{\rho}) = \sum_i \lambda_i \text{Tr}_J(\hat{P}_i) = \sum_i \lambda_i \hat{I}_J/2 = \hat{I}_J/2 \] (5.23)

where \( J = A, B \) and \( \bar{J} = B, A \). Thus for any Bell diagonal state, the resulting density operator for subsystem \( A \) or \( B \) is maximally mixed. Noting that any function of a density operator can be written as a function of its eigenvalues, i.e.,

\[ f(\hat{\rho}) = \sum_i f(\lambda_i) \hat{P}_i \] (5.24)

it follows that for any Bell diagonal state, the partial trace of any function of the density operator (e.g., \( \hat{B} \ln(\hat{\rho}) \)) will be proportional to the identity operator. Next, consider Theorem 7 of [10], which states that any density operator satisfying the following relationship for all \( J \) is a nondissipative state of the composite system:

\[ \hat{\rho}_J \left( \hat{B} \ln(\hat{\rho}) \right)^J = \hat{\rho}_J \left[ \lambda_{IJ} \hat{I}_J + \lambda_{HJ} \hat{H} \right] \] (5.25)

Evaluating \( \left( \hat{B} \ln(\hat{\rho}) \right)^J \) for a Bell diagonal results in

\[ \left( \hat{B} \ln(\hat{\rho}) \right)^J = \text{Tr}_J \left( \left( \hat{I}_J \otimes \hat{\rho}_J \right) \hat{B} \ln(\hat{\rho}) \right) = \text{Tr}_J \left( \hat{B} \ln(\hat{\rho}) \right) = \alpha \hat{I}_J \] (5.26)
where $\alpha$ is some scalar coefficient dependent upon the eigenvalues of the Bell diagonal state. Thus, all Bell states satisfy equation (5.25) for non-dissipative, yet not-stable-thermodynamic equilibrium states relative to the dynamics of the SEAQT equation of motion. Therefore, to analyze the change of entanglement using the SEAQT equation of motion of states related to Bell diagonal states in particular, it is necessary to develop perturbation methods to find dissipative states that have similar features to Bell diagonal states.

### 5.2.3 Perturbation Approaches

The baseline density operator $\hat{\rho}_0$ that is perturbed here is the one for the Bell diagonal state given by

$$\hat{\rho}_0 = \frac{1}{4} \left( \hat{I}_A \otimes \hat{I}_B + \sum_{i=1}^{3} c_i \hat{\sigma}_{iA} \otimes \hat{\sigma}_{iB} \right)$$

(5.27)

where the $\hat{\sigma}_{iA(B)}$ are the Pauli X, Y, and Z matrices, respectively, and the scalar coefficient defining the state are $c_1 = 0.996$, $c_2 = 0.4$, and $c_3 = -0.4$. This section will present 3 distinct approaches for generating perturbed states from $\hat{\rho}_0$ where each perturbation approach produces perturbed states that share some particular feature with $\hat{\rho}_0$.

#### Pure State Weighted-Average Approach

The first approach proposed is a simple weighted average of $\hat{\rho}_0$ with the density operator, $\hat{\rho}_{Pure}$, of a pure state of zero energy whose subsystems both also have zero energy. To generate a perturbed state $\hat{\rho}_0'$, the following expression is used:

$$\hat{\rho}_0' = \zeta \hat{\rho}_0 + (1 - \zeta) \hat{\rho}_{Pure}$$

(5.28)
where

$$\hat{\rho}_{\text{Pure}} \equiv \hat{\rho}_{A,\text{Pure},X} \otimes \hat{\rho}_{B,\text{Pure},X} = \frac{1}{2} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} \otimes \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix}$$ (5.29)

Here the subscript $X$ denotes that the polarization vector of $\hat{\rho}_{A(B),\text{Pure},X}$ points along the $X$-axis of the Bloch sphere. The weighting parameter $\zeta$ ranges from $0 \rightarrow 1$. This method is used because the resulting pure state density operator, $\hat{\rho}'_0$, has the same energy as $\hat{\rho}_0$ (though only 1 particular value of $\zeta$ ensures that $\hat{\rho}'_0$ has the same entropy as $\hat{\rho}_0$) and also because no new entanglement is introduced to the perturbed state. Thus, while $\hat{\rho}'_0$ is not a Bell diagonal state, this guarantees that the stationary state to which $\hat{\rho}'_0$ evolves is a Bell diagonal state although one different than the original Bell diagonal state.

**General Bipartite System Approach**

The second approach used is the general bipartite perturbation scheme presented in Chapter 4, which perturbs $\hat{\gamma}_0 = \sqrt{\hat{\rho}_0}$ a given magnitude $\epsilon$ overall all possible degrees of freedom for a bipartite system, i.e.,

$$\hat{\gamma}_\epsilon = \hat{\gamma}_0 + \epsilon \sum_{i,j=0}^{3} \eta_{ij} \hat{\sigma}_{iA} \otimes \hat{\sigma}_{jB}$$ (5.30)

This approaches enforces a desired set of constraints corresponding to operators $\hat{C}_i$ so that

$$\hat{\gamma}_r = \sum_{i=1}^{N} x_i \hat{C}_i \hat{\gamma}_\epsilon$$ (5.31)
Chapter 5. Modeling the Effects of Perturbations and Steepest-Entropy-Ascent on the Time Evolution of Entanglement

where $N$ is the number of constraints to be enforced. By relating the expectation value of the $\hat{C}_i$ associated with $\gamma_r$ to the original expectation value via enforcing $\text{Tr}(\hat{C}_i \hat{\gamma}_0 \hat{\gamma}_0^\dagger) = \text{Tr}(\hat{C}_i \hat{\gamma}_r \hat{\gamma}_r^\dagger)$, a set of $N$ equations can be formed and solved numerically to obtain $\hat{\gamma}_r$, which is then used to obtain a dissipative state via $\hat{\rho}'_0 = \hat{\gamma}_r \hat{\gamma}_r^\dagger$. This approach is used with two sets of constraints, first with only a constant energy constraint and second with both energy and entropy constraints. This approach is useful because it ensures that the associated properties of the perturbed state are the same as those of the initial state, which permits clear trends between the system entanglement and physical properties to be developed.

Unitary Operations Approach

The final approach proposed here is one based on a sequence of unitary operations, whose time durations produce a randomly perturbed state. In addition to inherently producing constant entropy perturbed states, the sequence of unitary operations is constrained such that the perturbed state $\hat{\rho}'_0$ is of the same energy as the original state $\hat{\rho}_0$. The sequence of unitary operations is given by

$$\hat{U}_{Ptb} = \left(\hat{R}_{XA}(\theta_A) \otimes \hat{R}_{XB}(\theta_A)\right) \left(H_A \otimes \hat{I}_B\right) \left(\hat{R}_{ZA}(\pi/2) \otimes \hat{I}_B\right) \hat{C}_{XAB}(\theta_X) \quad (5.32)$$

where

$$\hat{R}_{X(A,B)}(\theta_{A(B)}) = \exp\left\{-i\frac{\theta_{A(B)}}{2} \hat{\sigma}_X\right\} \quad (5.33)$$

represents a rotation of $\theta_{A(B)}$ radians about the X-axis of the Bloch sphere. $H_A$ represents a Hadamard gate on subsystem $A$, $\hat{R}_{ZA}(\pi/2)$ represents a rotation of $\pi/2$ radians about the Z-axis of the Bloch sphere for subsystem $A$, and $\hat{C}_{XAB}(\theta_A)$ is a controlled-X rotation where subsystem $A$ serves as the control qubit and subsystem $B$ is the target qubit, which is given
in the computational basis by the matrix

$$\hat{C}_{XAB}(\theta_X) = \begin{bmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & \cos(\theta_X/2) & -i \sin(\theta_X/2) \\
0 & 0 & -i \sin(\theta_X/2) & \cos(\theta_X/2)
\end{bmatrix}$$ (5.34)

To ensure that the rotations yield no net change in energy, the following definition is first made

$$G \equiv -\frac{\lambda_1 - \lambda_2 + \lambda_3 - \lambda_4}{\lambda_1 + \lambda_2 - \lambda_3 - \lambda_4}$$ (5.35)

where $\lambda_i$ are the eigenvalues corresponding to the eigenprojectors $\hat{P}_{\phi+}, \hat{P}_{\psi+}, \hat{P}_{\phi-},$ and $\hat{P}_{\psi-}$ for $i = 1, ..., 4$, respectively, of the baseline Bell diagonal state $\hat{\rho}_0$. Now, if $|G| < 1$ the following relation is used to compute $\theta_A$ in terms of a random $\theta_B$ and $\theta_X$:

$$\theta_A = \cos^{-1}\left(\frac{-\lambda_1 - \lambda_2 + \lambda_3 - \lambda_4}{\lambda_1 + \lambda_2 - \lambda_3 - \lambda_4} \sin\left(\theta_B + \frac{\theta_X}{2}\right)\right)$$ (5.36)

and if $|G| > 1$, $\theta_B$ is instead computed in terms of a random $\theta_A$ and $\theta_X$ as

$$\theta_B = \sin^{-1}\left(\frac{-\lambda_1 + \lambda_2 - \lambda_3 - \lambda_4}{\lambda_1 - \lambda_2 + \lambda_3 - \lambda_4} \cos(\theta_A) - \frac{\theta_X}{2}\right)$$ (5.37)

where it is noted that both of the above relations are derived by enforcing the constant energy constraint. All randomly generated angles are computed using $\theta = \cos(2\eta - 1)$ where $\eta$ is a randomly generated number from a uniform distribution between zero and one. All of the above operations forming $\hat{U}_{ptb}$ can be related to unitary evolutions under a time-varying Hamiltonian and the perturbed density operator can be found using
Chapter 5. Modeling the Effects of Perturbations and Steepest-Entropy-Ascent on the Time Evolution of Entanglement

\[ \hat{\rho}'_0 = \hat{U}_{ptb} \hat{\rho}_0 \hat{U}_{ptb}^\dagger \] (5.38)

The primary advantage of this approach is that the mutual information of the perturbed state monotonically decreases with the angle \( \theta_X \) as it varies from \( 0 \rightarrow \pi \), and, thus, it is easier to control the entanglement of the resulting perturbed states. However, while this approach enforces constant energy and entropy constraints, the perturbed state is not necessarily in the neighborhood of the unperturbed state. Even though this approach can be further constrained to small rotation angles such that the perturbed states are in the neighborhood of \( \hat{\rho}_0 \), it does not necessarily sample the entire neighborhood of states near \( \hat{\rho}_0 \). Furthermore, it does not necessarily sample the states that is does in a uniform fashion. Furthermore, although this method could be modified to sample a wider range of states in the neighborhood of \( \hat{\rho}_0 \), it currently only produces states that are a subset of those produced by the general bipartite approach under constant energy and entropy constraints. Thus, to examine the evolutions associated with the widest possible range of states, evolutions using the bipartite approach with constant energy and entropy constraints is used since the perturbed states potentially span the entire neighborhood of states near \( \hat{\rho}_0 \).

5.3 Results

This section presents results for the evolution of system entanglement using the SEAQT equation of motion starting from perturbed states. Additionally, other correlations between the properties of the perturbed and stationary states are presented. First Section 5.3.1 shows entanglement evolutions using the weighted average perturbation approach to generate the initial states used by the SEAQT equation of motion. Next, Section 5.3.2 does likewise except that the initial states used are generated by the general bipartite perturbation approach with
a constant energy constraint using a perturbation magnitude of $\epsilon = 10^{-1}$. Sections 5.3.3 and 5.3.4 then repeat this but with initial state generated by the general bipartite perturbation approach with constant energy and entropy constraints for perturbation magnitudes of $\epsilon = 10^{-1}$ and $\epsilon = 10^{-2}$, respectively.

To gain a qualitative understanding of the effects of dissipation due to an external environment on the entanglement properties of the system, theoretical and experimental results developed by Liu et al. [44] for the evolution of a Bell diagonal state in a stochastic global dephasing (or decoherence) field are shown in Figure 5.1. The theoretical results are developed using the Kraus-Operator-Sum approach and predict that the concurrence remains constant, while $\langle \hat{B}_{CHSH} \rangle_{Max}$ decays. Thus, after a finite time (dimensionless time of $t \approx 0.58$) the theoretical results suggest that the system undergoes so-called sudden death of non-locality, i.e., $\langle \hat{B}_{CHSH} \rangle_{Max}$ goes below 2. The experimental results produced by Liu et al. qualitatively validate the theoretical results since the measured concurrence remains roughly constant, while $\langle \hat{B}_{CHSH} \rangle_{Max}$ decays through time although sudden death of non-locality occurs at a dimensionless time of $t \approx 0.41$. 
5.3.1 Entanglement Evolution using Weighted-Average Perturbations

This section presents evolutions for the system concurrence $E(\hat{\rho})$ and the maximum expectation value of the CHSH operator, $\langle \hat{B}_{CHSH} \rangle_{Max}$, correlations between the stationary state Bell diagonal parameters $c_1 \pm c_2$ and the weighting parameter $\zeta$, correlations between the perturbed state and stationary state entropy, correlations of the entanglement operator $\hat{\xi}$ and the stationary state entropy, and correlations between the total entropy generation and the entanglement operator $\hat{\xi}$.

Figure 5.2 shows the evolutions of the concurrence and $\langle \hat{B}_{CHSH} \rangle_{Max}$ for nine different values of the weighting parameter $\zeta$. For both properties, initial decays in their value occur as entropy is produced before becoming constant as the system reaches a stationary state. In addition to the initial value dropping as $\zeta$ increases, the overall decay in value of each property also increases with $\zeta$ the weighting parameter. Figure 5.2b also shows that for values...
of $\zeta \approx 0.76$ and below, that the composite system undergoes sudden death of non-locality in the way that the Bell diagonal state predicted by Liu et al. does. For values above $\zeta \approx 0.76$, the correlations due to entanglement remain as the system relaxes to a stationary state.

Figure 5.2: Concurrence and $\left\langle \hat{B}_{\text{CHSH}} \right\rangle_{\text{max}}$ evolutions for values of the weighting parameter $\zeta = 1, 0.96, 0.92, 0.88, 0.84, 0.8, 0.76, 0.72, \text{ and } 0.68$ where $\zeta = 1$ corresponds to the uppermost solid orange line and each lower solid line corresponds to the next lower value of $\zeta$.

Figure 5.3 shows the change in the Bell diagonal state parameters $c_1 \pm c_2$ vs. the weighting parameter $\zeta$ and the perturbed and stationary state entropy values for values of the weighting parameter $\zeta$ between zero and one in increments of $10^{-3}$. In Figure 5.3a, the Bell diagonal parameters $c_1$ and $c_2$ only represent Bell states at the baseline state and at the stationary state, since the perturbed states are not Bell diagonal states. These parameters are calculated using $c_{1(2)} = 2(\hat{\rho}_{23} \pm \hat{\rho}_{14})$ for arbitrary density operators. As the system approaches a stationary state, $c_1 \pm c_2$ both approach a constant value, which is in contrast to the global dephasing model using Kraus operators that predicts that the value $c_1 - c_2$ decays to zero. Figure 5.3a shows that as $\zeta$ decreases, the values of $c_1 \pm c_2$ deviate further from the baseline state, as expected, and also that $c_1 \pm c_2$ exhibits more decay, which corresponds to the total entropy production, which is illustrated in Figure 5.3b. In this figure, the light blue dot corresponds
to the baseline case, i.e., the original Bell diagonal state, and the difference for any point on the black curve between the final state entropy and the perturbed state entropy is the entropy production for that particular evolution of state. 5.3b also shows that the perturbed state exhibits a slight increase in entropy before decreasing to zero as $\zeta$ decreases. Also seen is that as $\zeta$ decreases, and the perturbed state becomes further from the baseline state, that the overall amount of entropy production increases. Furthermore, by comparing this figure with Figure 5.2, it can be seen that greater the decay in either entanglement measure, the greater the total amount of entropy production is.

Figure 5.3: Perturbed and stationary state Bell diagonal parameters $c_1 \pm c_2$ vs. the weighting parameter $\zeta$ and perturbed and stationary state entropy correlation.

Figure 5.4 shows correlations between the entanglement operator $\hat{\xi}$, the stationary state entropy, and the total entropy generation. In Figure 5.4a, it is seen that as the magnitude of the entanglement operator, $|\hat{\xi}|$, increases, the stationary state entropy monotonically decreases, meaning that the stationary state moves further away from the stable thermodynamic equilibrium state at that energy. Figure 5.4b shows for weighted average perturbations that the magnitude of the entanglement operator, $|\hat{\xi}|$, monotonically decreases as the total entropy production (or generation) increases.
5.3. Results

Figure 5.4: Correlations between the entanglement operator $\hat{\xi}$, the stationary state entropy, and the total entropy production (or generation).

### 5.3.2 Entanglement Evolution using the General Bipartite Constant Energy Constrained Perturbations with $\epsilon = 10^{-1}$

This section presents results using the general bipartite system perturbation approach with a constant energy constraint and a value of $\epsilon = 10^{-1}$. Specifically, results are presented for evolutions for the system concurrence, $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$, correlations between the perturbed and stationary state concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$, correlations between the total entropy generation and the total change in concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$, and correlations between the entanglement operator $|\hat{\xi}|$, the stationary state entropy, and the total entropy generation.

Figure 5.5 shows the evolutions of the concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$ for nine random perturbations. For these perturbations, both entanglement measures exhibit little decay before the system reaches a stationary state.

Seen in Figure 5.6 is the correlation between the perturbed state and stationary values of the concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$. Consistent with the Figure 5.5, all perturbations exhibit little decay in the concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$. Furthermore, none of the evolutions undergo...
Figure 5.5: Concurrence and $\langle \hat{B}_{CHSH} \rangle_{Max}$ evolutions for nine random perturbations.

sudden death of non-locality, as shown in Figure 5.6b. This indicates that for this particular baseline Bell diagonal state, that perturbations of $\mathcal{O}(\epsilon = 10^{-1})$ and the resulting dissipation is insufficient to cause sudden death of non-locality.

Figure 5.6: Perturbed and stationary state concurrence and $\langle \hat{B}_{CHSH} \rangle_{Max}$ values.

Figure 5.7 shows the correlation between the total entropy production (or generation) and the total change of concurrence and $\langle \hat{B}_{CHSH} \rangle_{Max}$ from the perturbed state to the stationary state. Both properties show clear trends of decrease with increasing entropy production.
5.3. Results

(or generation). One interesting aspect to note is that while the concurrence is seen to only decrease, the evolution resulting from the SEAQT dynamics causes an increase in $\langle \hat{B}_{CHSH} \rangle_{Max}$ for a few of the perturbed states, i.e., points above the red line. This highlights a difference in the monotonic nature of the two measures. Since the SEAQT equation of motion and the resulting dissipation cannot increase the entanglement for two non-interacting subsystems, a monotonic measure of the entanglement, like the concurrence, must always decrease. However, for non-monotonic measures, like $\langle \hat{B}_{CHSH} \rangle_{Max}$, it is possible for a less entangled state to have a higher value of $\langle \hat{B}_{CHSH} \rangle_{Max}$ than a more entangled state (e.g., a completely unentangled state can have a value as high as 2 whereas entangled states can have values less than 2). Values of $\langle \hat{B}_{CHSH} \rangle_{Max}$ above 2 (i.e., in violation of the CHSH inequality) simply guarantee that measured correlations between subsystems $A$ and $B$ are due to entanglement.

![Figure 5.7: Correlations of change in concurrence and $\langle \hat{B}_{CHSH} \rangle_{Max}$ vs. the total entropy production (or generation).](image)

Seen in Figure 5.8 are the correlations between the magnitude of the entanglement operator $|\xi|$, the stationary state entropy, and the total entropy production (or generation). Figure 5.8a shows that there is again a clear trend between the total stationary entropy and $|\xi|$. 
This is in contrast to the correlation between the total entropy production (or generation) and $|\xi|$. Figure 5.4b shows a clear trend between these whereas Figure 5.8b does not.

![Figure 5.8: Correlations between $|\xi|$, the stationary state entropy, and the total entropy production (or generation).](image)

5.3.3 Entanglement Evolution using the General Bipartite Constant Energy and Entropy Constrained Perturbations with $\epsilon = 10^{-1}$

This section presents results using the general bipartite system perturbation approach with constant energy and entropy constraints for a perturbation magnitude of $\epsilon = 10^{-1}$. Evolutions and correlations between the perturbed and stationary state concurrence and $\left< \hat{B}_{CHSH} \right>_{Max}$ are shown in addition to correlations between the total entropy production (or generation) and the total change in concurrence and $\left< \hat{B}_{CHSH} \right>_{Max}$ and correlations between the entanglement operator $|\xi|$, the stationary state entropy, and the total entropy production (or generation). In addition, correlations between the state distance measure, $\theta_d$, and the total entropy production (or generation) are shown, as well as the correlation between the initial entropy
5.3. Results

production (or generation) rate and the maximum entropy production (or generation) rate. Figure 5.9 shows the evolutions of the concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$ for nine random perturbations. Again for these perturbations, both entanglement measures exhibit little decay before the system reaches a stationary state.

![Graphs showing concurrence and CHSH operator max expectation value evolutions](image)

**Figure 5.9:** Concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$ evolutions for nine random perturbations.

Figure 5.10 shows the correlation between the perturbed state and stationary values of the concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$. Figure 5.5, showing the initial and stationary state entanglement measures, shows that all perturbations exhibit little decay. However, now there is a significantly smaller spread in the initial and, thus, final values of each entanglement measure as compared to Figure 5.6. This indicates that the values of these measures are correlated to the value of the system entropy and that higher entropy systems tend to have less entanglement.

Seen in Figure 5.11 are the correlations between the total entropy production (or generation) and the total change of concurrence and $\langle \hat{B}_{CHSH} \rangle_{\text{Max}}$ from the perturbed state to the stationary state. Both properties show clear trends of decrease with increasing entropy production (or generation). As is seen in Figure 5.7, all changes in concurrence are negative.
Figure 5.10: Perturbed and stationary state concurrence and \( \langle \hat{B}_{CHSH} \rangle_{\text{Max}} \) values.

whereas a few perturbations exhibit a rise in \( \langle \hat{B}_{CHSH} \rangle_{\text{Max}} \), though again most changes are negative. This is again due to the fact that \( \langle \hat{B}_{CHSH} \rangle_{\text{Max}} \) is not a monotone of entanglement.

Figure 5.11: Correlations of change in concurrence and \( \langle \hat{B}_{CHSH} \rangle_{\text{Max}} \) vs. the total entropy production (or generation).

Figure 5.12 shows the correlations between the magnitude of the entanglement operator, \(|\hat{\xi}|\), the stationary state entropy, and the total entropy production (or generation). Figure 5.12a shows that there seems to be a trend of decreasing stationary state entropy as \(|\hat{\xi}|\) increases though more trials are necessary to illuminate this further. Figure 5.12b also suggests that
larger amounts of entropy generation correspond to smaller values of $|\dot{\xi}|$, though again more trials are needed to verify this.

![Figure 5.12: Correlations between $|\dot{\xi}|$, the stationary state entropy, and the total entropy production (or generation).](image)

Figure 5.12: Correlations between $|\dot{\xi}|$, the stationary state entropy, and the total entropy production (or generation).

In Figure 5.13a, the correlation between the total entropy generation and the state distance measure $\theta_d$ is displayed. As clearly seen, larger values of $\theta_d$ encompass a wider range of states, some of which lead to much higher amounts of entropy production (or generation). Figure 5.13b shows that the maximum entropy production (or generation) rate seen during an evolution from a dissipative perturbed state to a stationary state is always at the beginning of the evolution. This behavior is different from the entropy production (or generation) rate near so-called partially canonical states, which initially is very small and grows to some maximum value as the system evolves away from the partially canonical state before decreasing again [13]. This suggests that no other non-dissipative states lie in the neighborhood of any state along the the system’s evolution, and thus that there are no other local minimum entropy production (or generation) rates other than that at the stationary state to which the system evolves.
Chapter 5. Modeling the Effects of Perturbations and Steepest-Entropy-Ascent on the Time Evolution of Entanglement

5.3.4 Entanglement Evolution using the General Bipartite Constant Energy and Entropy Constrained Perturbations with \( \epsilon = 10^{-2} \)

This section presents results using the general bipartite system perturbation approach with constant energy and entropy constraints with a perturbation magnitude of \( \epsilon = 10^{-2} \). All of the same type of figures as in Section 5.3.3 are presented here. Figure 5.14 again shows evolutions of the concurrence and \( \langle \hat{B}_{CHSH} \rangle_{Max} \) for nine random perturbations. Compared to Figure 5.9, both entanglement measures now exhibit much less decay and have a much smaller spread (of \( \mathcal{O}(\epsilon) \)) about the corresponding baseline value.

Figure 5.15 shows the correlation between the perturbed state and stationary values of the concurrence and \( \langle \hat{B}_{CHSH} \rangle_{Max} \) using the same scale as Figure 5.10. As is consistent with Figure 5.14, there is very little spread and decrease of these entanglement measures, which are of \( \mathcal{O}(\epsilon = 10^{-2}) \)) whereas in Figure 5.10 they are of \( \mathcal{O}(\epsilon = 10^{-1}) \).
5.3. Results

Figure 5.14: Concurrence and $\left< B_{CHSH} \right>_{Max}$ evolutions for nine random perturbations.

Seen in Figure 5.16 are the correlations between the total entropy production (or generation) and the total change of concurrence and $\left< B_{CHSH} \right>_{Max}$ from the perturbed state to the stationary state. The same trends are observed as in Figure 5.12, though now the total change in both entanglement measures is of $O(10^{-4})$ whereas Figure 5.12 shows that the total change in both entanglement measures is $O(10^{-3})$.

Figure 5.17 shows that there are now no clear correlations between the magnitude of the entanglement operator $|\xi|$, the stationary state entropy, and the total entropy production (or generation). This is likely due to the small overall amount of entropy production (or generation) for the states in the neighborhood of the non-dissipative baseline state $\hat{\rho}_0$. Thus, more trials are necessary to see if any trends such as those exhibited in Figure 5.12 exist.

Finally, Figure 5.18a displays the correlation between the total entropy production (or generation) and the state distance measure $\theta_d$. Consistent with Figure 5.13a, larger values of $\theta_d$ again encompass a wider range of states that permit larger amounts of entropy production (or generation). Figure 5.18b again shows that the maximum entropy production (or generation) rate seen during an evolution from a dissipative perturbed state to a stationary state is
Figure 5.15: Perturbed and stationary state concurrence and $\langle \hat{B}_{\text{CHSH}} \rangle_{\text{Max}}$ values, always at the beginning of the evolution.
5.3. Results

Figure 5.16: Correlations of change in concurrence and $\langle \hat{B}_{\text{CHSH}} \rangle_{\text{Max}}$ vs. the total entropy production (or generation).

Figure 5.17: Correlations between $|\xi|$, the stationary state entropy, and the total entropy production (or generation).
Chapter 5. Modeling the Effects of Perturbations and Steepest-Entropy-Ascent on the Time Evolution of Entanglement

Figure 5.18: Correlation between the total entropy generation and the state distance measure $\theta_d$ and the initial entropy production (or generation) rate vs. the maximum entropy production (or generation) rate.
5.4 Conclusions

This chapter has presented the evolution of a bipartite system in an entangled state using the dynamics of the SEAQT equation of motion. Results for these evolutions are indirectly compared to evolutions predicted by the Kraus-Operator-Sum approach as well as to data obtained from a quantum optics experiment. While the dynamics predicted by SEAQT differ from those predicted by the Kraus-Operator-Sum approach, both predict the possibility of constant concurrence and frozen entanglement (via the CHSH operator maximum expectation value being above two) for stationary states. In addition, SEAQT also predicts the sudden death of non-locality via a drop below 2 of the maximum CHSH operator expectation value. While general trends of the experimental data can be matched for states generated using the weighted-average perturbation method, further refinement of the Hamiltonian representing the experimental system is needed to be able to directly match the experimental dynamics. In other words, since this experiment is a global relaxation process due to an interaction with an external environment, the SEAQT model needs to be generalized to account for this interaction. This could possibly be done by introducing a third subsystem in the composite that has a global interaction with the composite of subsystems $A$ and $B$. The interaction could be modeled with creation/annihilation operators or perhaps a spin $3/2$ operator on the composite Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. Further exploration on how Lindblad equation effects the system dynamics could also be useful in modifying the SEAQT model.

This work has also provided insight into entanglement dynamics within the SEAQT framework for non-interacting subsystems. It has shown that the entanglement operator $\hat{\xi} = \hat{\rho} - \hat{\rho}_A \otimes \hat{\rho}_B$ remains constant throughout the evolution in the rotating frame, though this has yet to be proven mathematically. Furthermore, for all of the thousands of evolutions generated, the maximum error between the entropy of the stationary state and the entropy of the state predicted by $\hat{\rho}' = \hat{\rho}_{eq, A} \otimes \hat{\rho}_{eq, B} + \xi$ is only 0.25%. This warrants further exploration to see if
this error is numerical in nature and $\hat{\rho}'$ the true stationary state or if there is some deviation between the true stationary state and $\hat{\rho}'$. Regardless, this work has shown that $\hat{\rho}'$ is at least a good estimate of the stationary state to which the system evolves.
Chapter 6

Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

6.1 Introduction

Quantum Information and Quantum Computing Systems (QIQCs) have the potential to greatly improve the speed in which certain calculations are performed. One specific application of this is in the factoring of large integers, which has application in common cryptographic methods. The time it takes for classical computing systems to factor large numbers scales exponentially with the size of the integer, and, thus, factoring times quickly become infeasible. For example, Kleinjung et al. [24] factored a 232 decimal-digit number in roughly two years using a supercomputer consisting of “many hundreds” of cores, and estimates that a 309 decimal-digit number would take approximately a thousand times longer (using the same computing power). Shor’s algorithm [51] for factoring integers on a quantum computer, however, scales polynomially in run time with the number of digits in the integer to be factored. Thus, for large integers, Shor’s algorithm on a quantum computer would be able to complete factorization in times many orders of magnitude faster than a classical computer could.
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

Therefore, the focus of this chapter is to model the effects of dissipation as Shor’s factoring algorithm is run on a Nuclear Magnetic Resonance (NMR) quantum computer (QC). This work is based on the work of Vandersypen et al. [58] and applies steepest-entropy-ascent quantum thermodynamics (SEAQT) to model the dissipation occurring as well as develop a decoherence (dephasing) control methodology.

First, in Section 6.2, the relevant aspects of modeling the Hamiltonian of a NMR QC are discussed along with how Shor’s algorithm is implemented. Additionally, the SEAQT equation of motion (also referred to as the Beretta equation), is presented since it provides the dynamics with which the dissipation is predicted. Following this, a novel derivation of an extension of the Beretta equation is presented to account for reservoir interactions, which is referred to as the Beretta+Reservoir equation. With this development, a methodology to use reservoir interactions to reduce the decoherence occurring during any quantum computing algorithm is introduced.

Next, Section 6.3 presents the results of the above irreversible modeling approaches as well as those produced by standard unitary dynamics applied to predicting the time evolution of the NMR QC system as it computes Shor’s algorithm. These results are then compared to the experimental results of [58] in addition to theoretical results obtained from using the Kraus-Operator-Sum approach to model the time evolution of the system.

Finally, Section 6.4 discusses the primary conclusions to be drawn from these results as well as where further modeling work can be done to improve the result presented here.
6.2 Model Development

This section presents the model development for the NMR quantum computing algorithm. First, Section 6.2.1 presents the NMR Hamiltonian, the implementation of Shor’s algorithm, and the development of so-called pseudo-pure states. Next, Section 6.2.2 presents the SEAQT equation of motion for a general quantum system, which is then used as a starting point for Section 6.2.3 where a derivation of the Beretta+Reservoir equation of motion is presented for a general quantum system where each subsystem locally experiences a heat interaction with a reservoir. Finally, Section 6.2.4 demonstrates the use of this Beretta+Reservoir in the development of a control scheme to mitigate decoherence (dephasing).

6.2.1 NMR Hamiltonian and Shor Algorithm Development

NMR Hamiltonian

As is presented in Chapter 3, the Hamiltonian primarily used in NMR quantum computing applications takes the form

\[
\hat{H}_L(t) = \hat{H}_{0,L} + \hat{H}_{RF,L}(t) + \hat{H}_{J,L}
\]  

(6.1)

where \(\hat{H}_{0,L}\) corresponds to the strong, static, longitudinal portion of the externally applied magnetic field, \(\hat{H}_{RF,L}(t)\) corresponds to the transverse time-varying radio-frequency portion of the Hamiltonian primarily used in implementing the gates associated with quantum algorithms, and \(\hat{H}_{J,L}\) corresponds to the through-bond or J-coupling interaction between the qubits. The portion of the Hamiltonian due to the static longitudinal field, \(\hat{H}_{0,L}\), is given as
\[ \hat{H}_{0,L} = \frac{\hbar}{2} \left( \omega_{0,1} \hat{\sigma}_{Z,1} \otimes \hat{I}_2 + \omega_{0,2} \hat{\sigma}_{Z,2} \right) \otimes \hat{I}_3 + \hat{I}_1 \otimes \hat{I}_2 \otimes \omega_{0,3} \hat{\sigma}_{Z,3} \right) \otimes \hat{I}_4 \ldots \]

(6.2)

where \( \omega_{0,i} \) is the Larmor frequency of the \( i \)th qubit due to the static longitudinal field, \( \hat{\sigma}_{Z,i} \) is the Pauli-Z matrix of the \( i \)th qubit related to its angular momentum by a factor of 1/2, and \( \hat{I}_i \) is the identity operator of the \( i \)th qubit. Next, the J-coupling interaction term takes the form

\[ \hat{H}_{0,L} = \sum_{i=1}^{M} \sum_{j>i}^{M} \hbar 2\pi J_{ij} \hat{\sigma}_{Z,i} \otimes \hat{\sigma}_{Z,j} \otimes \hat{I}_{ij} \]  

(6.3)

where \( \hat{I}_{ij} \) is the identity operator corresponding to all qubits \( \neq i,j \).

To implement an algorithm, it is useful to switch to a rotating reference frame (about the Z-axis) where the angular velocity of the reference frame for each qubit is \( \omega_{0,i} \). This effectively serves to hide the rapid oscillations associated with the static, longitudinal field. The corresponding composite system rotating reference frame operator is then formed as

\[ \hat{R}_{ref}(t) = \bigotimes_{i=1}^{M} \hat{R}_Z(-\phi_i(t)) = \bigotimes_{i=1}^{M} \exp \left\{ -i \frac{\phi_i(t)}{2} \hat{\sigma}_{Z,i} \right\} \]  

(6.4)

where \( M \) is the number of qubits and \( \phi_i \) is the relative angle between the rotating reference frame and the lab frame given as \( \phi_i(t) = \omega_i t + \phi_{0,i} \). Noting that the rotation operator commutes with the static and interaction portions of the Hamiltonian, the rotating frame Hamiltonian can be written as

\[ \hat{H}_{L}(t) = \hat{H}_{0,R} + \hat{H}_{RF,R}(t) + \hat{H}_{J,R} \]

(6.5)

where it is noted that \( \hat{H}_{0,R} = \hat{H}_{0,L} \) and \( \hat{H}_{J,R} = \hat{H}_{J,L} \) and the definition has been made
that \( \hat{H}_{RF,R}(t) = \hat{R}_{ref}(t)\hat{H}_{RF,L}(t)\hat{R}_{ref}^\dagger(t) \). To implement \( \hat{H}_{RF,R}(t) \), qubit selective pulses are implemented by changing the frequency of the RF pulse. The portion of the external RF field acting on qubit \( i \) is given as

\[
\hat{H}_{RF,i}(t) = P_{X,i}(t)\hat{\sigma}_X + P_{Y,i}(t)\hat{\sigma}_Y \tag{6.6}
\]

where the \( P_{X(Y)i}(t) \) take the same form as the pulse implementation described in Chapter 2. For simplicity, it is assumed in this work that the \( P_{X(Y)i}(t) \) can be realized by appropriately changing the amplitude, frequency, and phase of the applied RF field. With this, the total Hamiltonian representing the RF field for the system in the rotating reference frame can be represented as

\[
\hat{H}_{RF,R}(t) = \sum_{i=1}^{M} \hat{H}_{RF,i}(t) = \left( \left( \hat{H}_{RF,1}(t) \otimes \hat{I}_2 + \hat{I}_1 \hat{H}_{RF,2}(t) \right) \otimes \hat{I}_3 + \hat{I}_1 \otimes \hat{I}_2 \otimes \hat{H}_{RF,3}(t) \right) \otimes \hat{I}_4 \ldots \tag{6.7}
\]

This portion of the Hamiltonian is what will be used to implement qubit specific operations (i.e., rotations) in Shor’s factoring algorithm, discussed next.

### Algorithm and Gate Implementation

All known classical algorithms for factoring an \( l \) digit integer have running times that scale exponentially with the number of digits in \( l \) [34], which is considered inefficient. Thus, as the number of digits in \( l \) increases, factoring \( l \) into its primes quickly becomes intractable. This is due to the inability of classical algorithms to efficiently find the period of the function \( f(x) = a^x \mod(N) \) [58]. However, Shor’s algorithm, which utilizes a quantum computer to compute the period, has a running time that scales polynomially with the number of digits
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

in $l$ [51] (considered efficient), and, thus, for large $l$, Shor’s algorithm can be computed very quickly compared to a classical algorithm.

The goal of this algorithm is to find the order, $r$, of $a^x \mod (N)$, which is defined as $a^r = 1 \mod (N)$. For this work, which follows that presented in [58], a value $N = 15$ is chosen since it is the smallest odd composite number of two distinct numbers. In general cryptological applications, $N$ is the large $l$-digit number that needs to be factored.

To obtain $r$, generally it is necessary to evaluate the quantity $2^k c/r$, where $c$ is some unknown integer, and $k$ is the number of bits used to store $x$ in binary form on the quantum computer. Regardless of the value of $c$, this can be accomplished using a method known as continued fraction expansion. In general, $a$ is a randomly chosen number smaller than $N$ that has no common factors with $N$. Thus, for this example, $a = 2, 4, 7, 8, 11, 13, \text{or } 14$. For $a = 2, 7, 8, \text{or } 13$, the period is $r = 4$ and for the remaining possible values of $a$, the period is $r = 2$ (in practical applications the period is not known). Therefore, to represent $r$ on the quantum computer requires at most $k = 2$ qubits (corresponding to $r = 4$). However, for this work, $k = 3$ qubits will be used to represent $r$ and a total of 7 qubits will be used on the quantum computer.

For the simple case of $N = 15$, a continued fraction expansion does not need to be used and $r$ can be estimated from $2^k c/r$. This is done by directly analyzing the resulting spectra of the NMR experiment, which have some periodicity $P$ by which $r$ can be obtained as $r = 2^3/P$. For the two classes of numbers for $a$ here (corresponding to $r = 4$ and $r = 2$), the choice of $a = 11$ is made, and, thus, the goal is to obtain $r = 2$ from the periodicity of the spectra of the quantum computer (Vandersypen et al. [58] also analyze a more complex case of $a = 7$).

To obtain a factor of $N$, the greatest common denominator is found between $N$ and $a^{r/2} \pm 1$. For this example, the factors will turn out to be 3 and 5.
To compute the order of a function on a quantum computer, Shor’s algorithm utilizes a method known as modular exponentiation in addition to computing the inverse quantum Fourier transform. As the size of the problem \(N\) grows, the associated sequence of gates needed to perform these algorithms also becomes more complex (though running time for both still scales polynomially (efficiently) with the number of digits in \(N\)). Here, however, for the choice of \(N = 15\) and \(a = 11\), this algorithm can be reduced to a relatively simple gate sequence to implement on the quantum computer, the illustration of which is given in Figure 6.1.

![Quantum computing algorithm to compute the modular exponentiation with a base \(a = 11\) and the associated system state through the algorithm (adapted from [58]).](image)

Because NMR systems start in a thermal equilibrium state, temporal averaging is used to obtain a so-called pseudo-pure state, the details of which are discussed shortly. Next, a NOT
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

Gate is applied to qubit 7 such that the system is in the desired starting state for modular exponentiation, $|0000001\rangle$. So that $2^{k=3}$ values of $x$ can be computed in parallel, ranging from $x = 2^0 \rightarrow x = 2^{k=3}$, Hadamard gates are now simultaneously applied to qubits 1, 2, and 3. Because a Hadamard gate cannot be implemented directly on a NMR QC, in this work they are realized by a rotation about the Z-axis of $\pi/2$ radians (done by simply shifting the phase of the rotating reference frame relative to the qubit’s state) followed by a rotation about the Y-axis of positive $\pi/2$ radians.

Following this, modular exponentiation is realized in this case by the application of two controlled-NOT gates $C_{ij}$ where $i$ is the index of the control qubit and $j$ is the index of the target. The first controlled-NOT gate involves qubit 3 as the control and qubit 6 as the target, while the second controlled-NOT gate again uses qubit 3 as the control but then uses qubit 4 as the target. The specific implementation of these controlled-NOT gates depends on the sign of $J_{ij}$ between the control and target qubit. For $J_{ij} > 0$, the controlled-NOT gate is implemented as [57].

\[
\left( \hat{R}_{Z,i}(\pi/2) \otimes \hat{R}_{Y,j}(-\pi/2) \right) \hat{U}_J(1/2 J_{ij}) \left( \hat{I}_i \otimes \hat{R}_{X,j}(\pi/2) \right) \left( \hat{I}_i \otimes \hat{R}_{Z,j}(-\pi/2) \right)
\]

and for $J_{ij} < 0$ the controlled-NOT gate is realized by

\[
\left( \hat{R}_{Z,i}(\pi/2) \otimes \hat{R}_{Y,j}(-\pi/2) \right) \hat{U}_J(7/2 |J_{ij}|) \left( \hat{I}_i \otimes \hat{R}_{X,j}(\pi/2) \right) \left( \hat{I}_i \otimes \hat{R}_{Z,j}(-\pi/2) \right)
\]

where time proceeds from right to left in both cases and $\hat{U}_J(t)$ corresponds to the operator

\[
\hat{U}_J(t) = \exp\left\{ -i \pi J_{ij} t \hat{\sigma}_i Z \otimes \hat{\sigma}_j Z \right\}
\]

To realize this operator, it is necessary to implement a refocusing scheme, one of which is
described in [54]. This results in no net evolution for any of the other qubits (i.e., those \( \neq i, j \)) due to their J-coupling interactions, and, thus, the only qubits that undergo any net change of state are qubits \( i \) and \( j \).

Following the modular exponentiation, the inverse quantum Fourier transform is applied to qubits 1, 2, and 3, and their NMR spectra are subsequently obtained after applying a so-called measurement rotation (the measurement rotation is not illustrated in Figure 6.1). For the case of \( a = 11 \), because qubits 1 and 2 are in state \( |0\rangle \), it is not necessary to implement the controlled rotations in the inverse quantum Fourier transform because there is no net effect on the target qubit, and, thus, those operations are omitted.

**Pseudo-Pure State Development and Measurement**

NMR systems typically operate at room temperature and involve large numbers of molecules in a liquid solution. In the presence of strong magnetic fields, \( \approx 10 \) Tesla, the thermal equilibrium state of the system is given by the canonical distribution and can be approximated as

\[
\hat{\rho}_{eq} = \frac{e^{-\beta \hat{H}}}{\text{Tr}(e^{-\beta \hat{H}})} \approx \frac{1}{2^N} (\hat{I} - \beta \hat{H})
\]

where the approximation is made assuming the above conditions of magnetic field strength and room temperature. The problem with this, however, is that the thermal equilibrium state is not a useful initial state for the modular exponentiation portion of Shor’s algorithm. Thus, to obtain a state that is useful for this portion of the algorithm, a so-called pseudo-pure state is developed by a technique called temporal averaging. Temporal averaging consists of running multiple experiments where each experiment is prepared in a different initial state, and the summation of the signals obtained from each experiment interfere such that the net signal obtained is the same as would be obtained from an actual pure state. To illustrate the
development of a pseudo-pure state and the associated measurement, an example based on that given by Nielsen and Chuang [47] is presented here. Consider the density operator of a bipartite system given as

\[
\hat{\rho}_1 = \begin{bmatrix}
  a & 0 & 0 & 0 \\
  0 & b & 0 & 0 \\
  0 & 0 & c & 0 \\
  0 & 0 & 0 & d \\
\end{bmatrix}
\] (6.12)

which could correspond to the equilibrium density operator. To obtain a voltage signal as a function of time for a particular qubit, the operation \( \hat{R}_{X,J}(\pi/2) \otimes \hat{I}_J \) is applied to the system. After this operation is applied, the measured voltage signal of qubit \( J \) as a function of time is related to the system state as

\[
V_{J,1}(t) = V_0 \text{Tr} \left( \hat{\rho}_1(t) \left( \hat{M}_J \otimes \hat{I}_J \right) \right)
\] (6.13)

where \( V_0 \) is a scalar parameter associated with the physical properties (e.g., geometry) of the experimental set-up and \( \hat{M}_J = -i\hat{\sigma}_X - \hat{\sigma}_Y \) is the so-called measurement operator. The Fourier transform of \( V_{J,1}(t) \) can be taken to obtain the frequency spectra associated with qubit \( J \). Next, prior to applying the measurement rotation operation \( \hat{R}_{X,J}(\pi/2) \otimes \hat{I}_J \), the operations \( \hat{P}_1 \) and \( \hat{P}_2 \) are applied, which have the effect

\[
\hat{\rho}_2 = \hat{P}_1 \hat{\rho}_1 \hat{P}_1^\dagger = \begin{bmatrix}
  a & 0 & 0 & 0 \\
  0 & c & 0 & 0 \\
  0 & 0 & d & 0 \\
  0 & 0 & 0 & b \\
\end{bmatrix}, \quad \hat{\rho}_3 = \hat{P}_2 \hat{\rho}_1 \hat{P}_2^\dagger = \begin{bmatrix}
  a & 0 & 0 & 0 \\
  0 & d & 0 & 0 \\
  0 & 0 & b & 0 \\
  0 & 0 & 0 & c \\
\end{bmatrix}
\] (6.14)
where $\hat{P}_1$ and $\hat{P}_2$ can be realized by sequences of controlled NOT operations, which are henceforth be referred to as preparation sequences. Voltage signals $V_{J,2}(t)$ and $V_{J,3}(t)$ can also be obtained for these states. The sum of the 3 voltage signals, after applying the measurement rotation operation in each case, is then

$$
\sum_{i=1}^{3} V_{Ji}(t) = V_0 \left( \text{Tr} \left( \hat{\rho}_1(t) \left( \hat{M}_J \otimes \hat{I}_J \right) \right) + \text{Tr} \left( \hat{\rho}_2(t) \left( \hat{M}_J \otimes \hat{I}_J \right) \right) + \text{Tr} \left( \hat{\rho}_3(t) \left( \hat{M}_J \otimes \hat{I}_J \right) \right) \right)
$$

(6.15)

or

$$
\sum_{i=1}^{3} V_{Ji}(t) = V_0 \text{Tr} \left( \sum_{i=1}^{3} \hat{\rho}_i(t) \left( \hat{M}_J \otimes \hat{I}_J \right) \right)
$$

(6.16)

Now, evaluating the summation inside the trace yields

$$
\sum_{i=1}^{3} \hat{\rho}_i(t) = \begin{bmatrix}
3a & 0 & 0 & 0 \\
0 & b + c + d & 0 & 0 \\
0 & 0 & b + c + d & 0 \\
0 & 0 & 0 & b + c + d
\end{bmatrix}
= \begin{bmatrix}
4a & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & 1
\end{bmatrix} - \hat{I}a
$$

(6.17)

or finally

$$
\sum_{i=1}^{3} \hat{\rho}_i(t) = \begin{bmatrix}
4a - 1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0
\end{bmatrix} + \hat{I} - \hat{I}a = (4a - 1) |0_A0_B\rangle \langle 0_A0_B| + (1 - a) \hat{I}
$$

(6.18)
Inserting this expression back into equation (6.16) and including the measurement rotation operation gives

$$\sum_{i=1}^{3} V_{JI}(t) = V_0 \text{Tr} \left( \hat{R}_{X,J}(\pi/2) \left( (4a - 1) |0_A0_B\rangle \langle 0_A0_B| + (1 - a)\hat{I} \right) \hat{R}_{X,J}^\dagger(\pi/2) \left( \hat{M}_J \otimes \hat{I}_J \right) \right)$$  

(6.19)

Noting that the trace of the measurement operator $\hat{M}_J$ is zero, which is true for any NMR observable, the above reduces to

$$\sum_{i=1}^{3} V_{JI}(t) = V_0 (4a - 1) \text{Tr} \left( \hat{R}_{X,J}(\pi/2) \left( |0_A0_B\rangle \langle 0_A0_B| \right) \hat{R}_{X,J}^\dagger(\pi/2) \left( \hat{M}_J \otimes \hat{I}_J \right) \right)$$  

(6.20)

which corresponds to the voltage signal that would be obtained from the pure state $|0_A0_B\rangle \langle 0_A0_B|$, (which happens to be the ground state) and is, thus, called a pseudo-pure state. While this example corresponds to creating a pseudo-pure state for a bipartite system, the same idea can be applied to larger systems.

This method works well for small to moderately sized systems, but it has been shown that the signal to noise ratio of the voltage signal associated with the pseudo-pure state decays exponentially with the number of qubits involved in the process [54]; and, thus, as the NMR quantum computer becomes larger, the associated pseudo-pure state voltage signal eventually become too small to measure. For this work however, a scheme developed by Steffen [54], consisting of 36 preparation sequences, listed in Table 6.1, are used to create the pseudo-pure state.

In all of the pseudo-pure state preparation sequences, the controlled NOT gates are realized by the pulse sequence for $J_{ij} > 0$, 

\[\text{controlled NOT: } \hat{R}_{X,J}(\pi/2) \hat{R}_{X,J}^\dagger(\pi/2) \]
### Table 6.1: Pseudo-pure ground state preparation scheme taken from [54]; note that time proceeds from left to right and $N_j$ denotes a NOT gate on qubit $j$ and $C_{ij}$ denotes a controlled-NOT gate where qubit $i$ is the control qubit and qubit $j$ is the target - * A correction from the original document reading $S_{14} = S_5N_6N_7C_{61}$ was made here.

<table>
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<th>Set 1</th>
<th>Set 2</th>
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<tr>
<td>$S_1 = C_{32}C_{13}C_{51}C_{41}$</td>
<td>$S_{10} = S_1N_6N_7C_{61}$</td>
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<tr>
<td>$S_2 = C_{54}C_{25}C_{12}N_3$</td>
<td>$S_{11} = S_2N_6N_7C_{61}$</td>
</tr>
<tr>
<td>$S_3 = C_{25}C_{12}C_{31}N_4$</td>
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<td>$S_4 = C_{23}C_{12}C_{41}C_{31}N_4N_1$</td>
<td>$S_{13} = S_4N_6N_7C_{15}C_{61}C_{15}$</td>
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<td>$S_5 = C_{54}C_{25}C_{32}C_{54}$</td>
<td>$S_{14} = S_5N_6N_7C_{62}$</td>
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<td>$S_{18} = S_9N_6N_7C_{61}C_{62}$</td>
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<td>Set 4</td>
</tr>
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<tr>
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<td>$S_{35} = S_8C_{74}C_{67}$</td>
</tr>
<tr>
<td>$S_{27} = S_9C_{71}C_{72}$</td>
<td>$S_{36} = S_9C_{71}C_{72}C_{67}$</td>
</tr>
</tbody>
</table>
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

\[(\hat{I} \otimes \hat{R}_{X,j}(\pi/2)) \hat{U}_J \left( \frac{1}{4|J_{ij}|} \right) \left( \hat{R}_{X,i}(\pi) \otimes \hat{R}_{X,j}(\pi) \right) \hat{U}_J \left( \frac{1}{4|J_{ij}|} \right) \]

\[\left( \hat{R}_{X,i}(\pi) \otimes \hat{R}_{X,j}(\pi) \right) \left( \hat{I}_i \otimes \hat{R}_{Y,j}(\pi/2) \right) \] \hspace{1cm} (6.21)

and for \(J_{ij} < 0\)

\[(\hat{I} \otimes \hat{R}_{X,j}(\pi/2)) \hat{U}_J \left( \frac{1}{4|J_{ij}|} \right) \left( \hat{R}_{X,i}(\pi) \otimes \hat{R}_{X,j}(\pi) \right) \hat{U}_J \left( \frac{1}{4|J_{ij}|} \right) \]

\[\left( \hat{R}_{X,i}(\pi) \otimes \hat{R}_{X,j}(\pi) \right) \left( \hat{I}_i \otimes \hat{R}_{Y,j}(\pi/2) \right) \] \hspace{1cm} (6.22)

where now time proceeds from left to right and \(\hat{U}_J(t)\) again corresponds to equation (6.10). It is also noted that while this sequence of operations does not implement a true controlled-NOT gate, because the state of the equilibrium density operator is diagonal, the net result is the same as though an actual controlled-NOT gate were implemented.

This development is based on the approximation of the thermal equilibrium density matrix at room temperature and under a strong magnetic field, given by equation (6.11), that \(\hat{H} \approx \hat{H}_0\) and \(\omega_{0,1} \approx \omega_{0,2} \approx \omega_{0,3} \approx \omega_{0,4} \approx \omega_{0,5} \approx 4\omega_{0,6} \approx 4\omega_{0,7}\). The physical properties for the experimental NMR molecule are taken from [58] and given in Table 6.2.
6.2. Model Development

<table>
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<th>Qubit</th>
<th>$\omega_{0,i}/2\pi$</th>
<th>$T_{1,i}$</th>
<th>$T_{2,i}$</th>
<th>$J_{i,7}$</th>
<th>$J_{i,6}$</th>
<th>$J_{i,5}$</th>
<th>$J_{i,4}$</th>
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Table 6.2: Physical properties of the NMR quantum computer adapted from [58]; the values given for $\omega_{0,i}/2\pi$ are in Hz and relative to 470 MHz for qubits 1-5 and 125 MHz for qubits 6 and 7; the spin-lattice, or longitudinal, relaxation time and the spin-spin, or transverse, relaxation time are given by $T_1$ and $T_2$, respectively, in units of seconds, while $J_{i,j}$ is the J-coupling coefficient between qubits $i$ and $j$ given in units of Hz.

### 6.2.2 SEAQT Equation of Motion for a General Quantum System

To simulate the dynamics of a quantum computer, which inherently consists of multiple distinguishable particles (qubits), the SEAQT equation of motion for a general quantum system is used. This equation of motion requires that the system has the underlying Hilbert space $\mathcal{H} = \bigotimes_{J=1}^{M} \mathcal{H}_J$ where $M$ is the number of subsystems in the composite system and is given in the lab frame as

$$\frac{d\hat{\rho}_L}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_L(t), \hat{\rho}_L \right] - \frac{D(\hat{\rho}_L)}{Dt} \quad (6.23)$$

Noting that the rotating reference operator is separable into portions that act solely on the Hilbert spaces of each individual qubit $i$, the composite system equation of motion can be rewritten in the rotating reference frame. Assuming that the reference frame angular velocity is equal to the larmor frequency of the each qubit under the strong, static portion of the Hamiltonian, the composite system equation of motion in the rotating frame can be written as
\[ \frac{d\hat{\rho}_R}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_{RF,R}(t) + \hat{H}_{J,R}, \hat{\rho}_R \right] - \frac{D(\hat{\rho}_R)}{Dt} \]  

(6.24)

where the same derivation procedure applied in Chapter 3 for a simple system can be applied here. This shows that the reversible dynamics (in the rotating frame) are only affected by the RF field and the interaction portion of the Hamiltonian. For brevity, from here on it is assumed that all relevant operators are in the rotating frame unless otherwise stated. Thus, by appropriate timing of RF pulses, quantum algorithms can be implemented. The dissipation operator \( D(\hat{\rho})/Dt \) for a composite of \( M \) subsystems is written as

\[ \frac{D(\hat{\rho})}{Dt} = \sum_{J=1}^{M} \frac{1}{\tau_J} \hat{D}_J \otimes \hat{\rho}_J \]  

(6.25)

and the partial trace of the composite density operator onto the \( J \)th subsystem is given as \( \hat{\rho}_J = Tr_J(\hat{\rho}) \) where \( J \) represents the composite of all subsystems \( \neq J \). Likewise the density operator for the composite of all subsystems except the \( J \)th can be computed as \( \hat{\rho}_J = Tr_J(\hat{\rho}) \).

The dissipation operator for the \( J \)th subsystem, \( \hat{D}_J \), is

\[ \hat{D}_J = \frac{1}{2} \left( \hat{\rho}_J \hat{D}_J + \left( \hat{\rho}_J \hat{D}_J \right)^\dagger \right) \]  

(6.26)

where \( \hat{D}_J \) represents a ratio of gram determinants for the \( J \)th subsystem, which ensures that the expectation values associated with the generators of the motion, \( \hat{R}_{iJ} \), of the \( J \)th subsystem remain constant. For the remainder of this work, all subsystems \( J \) have two generators of the motion. The first, \( \hat{R}_{1J} = \hat{I} \), ensures that \( Tr(\hat{\rho}) = 1 \), and the second, \( \hat{R}_{1J} = \hat{H} \), ensures that the system evolution conserves the energy. With this definition, \( \hat{D}_J \) is computed as
6.2. Model Development

\[ D_J = \sqrt{\rho_J} \begin{pmatrix} \left( \hat{B} \ln(\hat{\rho}) \right)_J^J & \left( \hat{I} \right)_J^J & \left( \hat{H} \right)_J^J \\ \left( \hat{I}, \hat{B} \ln(\hat{\rho}) \right)_J^J & \left( \hat{I}, \hat{I} \right)_J^J & \left( \hat{I}, \hat{H} \right)_J^J \\ \left( \hat{H}, \hat{B} \ln(\hat{\rho}) \right)_J^J & \left( \hat{H}, \hat{I} \right)_J^J & \left( \hat{H}, \hat{H} \right)_J^J \end{pmatrix} \] (6.27)

where the terms \( (\hat{F}, \hat{G})_J^J \) are computed as

\[ (\hat{F}, \hat{G})_J^J = \frac{1}{2} \text{Tr}_J \left( |\hat{\rho}_J| \left\{ (\hat{F})_J^J, (\hat{G})_J^J \right\} \right) \] (6.28)

with

\[ \left\{ \sqrt{\rho_J} (\hat{F})_J^J, \sqrt{\rho_J} (\hat{G})_J^J \right\} = \frac{1}{2} \text{Tr}_J \left( \sqrt{\rho_J} (\hat{F})_J^J + \sqrt{\rho_J} (\hat{G})_J^J \right) \] (6.29)

and a so-called locally perceived operator \( (\hat{F})_J^J \) is computed as

\[ (\hat{F})_J^J = \text{Tr}_J \left( \left( \hat{I}_J \otimes \hat{\rho}_J \right) \hat{F} \right) \] (6.30)

With this definition, the SEAQT equation of motion for a composite system can be computed for an arbitrary number of subsystems.

Next, to extend this model further, Section 6.2.3 extends this equation by allowing each of the qubits to individually undergo a heat interaction with a reservoir.
6.2.3 SEAQT Equation of Motion for a General Quantum System Interacting with One or More Reservoirs

This section presents the derivation of a model within the SEAQT framework for a general quantum system where each subsystem may locally experience a heat interaction with a reservoir. The derivation is for a composite system of two subsystems $A$ and $B$, though the same concepts and assumptions can be extended to composite systems of arbitrary numbers of subsystems. First, the Hilbert space of the composite system is defined as

$$\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$$

where $A$ and $B$ denote the two subsystems of the overall composite system. Further, it is noted that $A$ and $B$ are themselves composite systems, i.e. $\mathcal{H}_A = \mathcal{H}_{A_S} \otimes \mathcal{H}_{A_R}$, and likewise for $B$, where $\mathcal{H}_{A_S}$ represents the Hilbert space of the system $A_S$ that will encapsulate the qubit for subsystem $S$, and $\mathcal{H}_{A_R}$ represents the Hilbert space of the reservoir with which $A_S$ interacts. In this work, it is assumed that for subsystem $J$, where $J = A, B$, that $J_S$ is a two-level system, implying that $\dim(\mathcal{H}_{J_S}) = 2$.

To derive an equation of motion under the principle of SEA for a composite quantum system where each subsystem locally interacts with a reservoir, it is necessary for each subsystem in $\mathcal{H}$, (i.e., $A$ and $B$ for this example) to reduce the Hilbert space of the subsystem $\mathcal{H}_J = \mathcal{H}_{J_S} \otimes \mathcal{H}_{J_R}$, which is of dimension $\dim(J_S) \cdot \dim(J_R)$, to a simpler form having dimension $\dim(J_S) + \dim(J_R)$.

It is furthermore assumed that the degrees of freedom representing the reservoir, $J_R$, with which $J_S$ interacts, are orthogonal and independent to the degrees of freedom of $J_S$. This allows for the two sets of energy levels (i.e., those of $J_S$ and $J_R$) to be broken into two
independent, unentanglable subsystems of energy levels. In an NMR system, this may potentially be realized by an interaction with a externally applied RF field of fixed frequency and amplitude, such that the RF field is in resonance with the transition frequency of the qubit embodied by \( J_S \). It is noted that the feasibility of implementing such a reservoir interaction may vary depending on the specific realization of the system and that other realizations of a QC may better facilitate the orthogonality between the degrees of freedom of \( J_S \) and \( J_R \). These assumptions on Hilbert space \( \mathcal{H}_J \) allow it to be simplified to

\[
\mathcal{H}_J = \mathcal{H}_{J_S} \oplus \mathcal{H}_{J_R}
\]  

(6.32)

where \( \oplus \) represents the direct sum of the two subspaces, \( \mathcal{H}_{J_S} \) represents the subspace corresponding to subsystem \( J_S \), encapsulating qubit \( J \), and likewise \( \mathcal{H}_{J_R} \) represents the subspace of the reservoir \( J_R \) with which \( J_S \) interacts. It is also noted that now \( \text{dim}(\mathcal{H}_J) = \text{dim}(\mathcal{H}_{J_S}) + \text{dim}(\mathcal{H}_{J_R}) \), as desired. Repeating these assumptions for both subsystems \( J = A, B \) in the overall composite system allows the overall composite system Hilbert space, \( \mathcal{H} \), to be rewritten as

\[
\mathcal{H} = (\mathcal{H}_{A_a} \otimes \mathcal{H}_{B_a}) \oplus (\mathcal{H}_{A_a} \otimes \mathcal{H}_{B_b}) \oplus (\mathcal{H}_{A_b} \otimes \mathcal{H}_{B_a}) \oplus (\mathcal{H}_{A_b} \otimes \mathcal{H}_{B_b})
\]  

(6.33)

where again \( \oplus \) represents the direct sum of subspaces, and the change of notation is made that \( S \to a \) and \( R \to b \). For brevity, the notation \( \mathcal{H}_{aa} \equiv \mathcal{H}_{A_a} \otimes \mathcal{H}_{B_a} \), and \( \mathcal{H}_{ab} \equiv \mathcal{H}_{A_a} \otimes \mathcal{H}_{B_b} \) is used, which allows the overall composite Hilbert space to be written as \( \mathcal{H} = \mathcal{H}_{aa} \oplus \mathcal{H}_{ab} \oplus \mathcal{H}_{ba} \oplus \mathcal{H}_{bb} \). To form an equation of motion on the Hilbert space \( \mathcal{H}_{aa} \), corresponding to the composite system of the qubits, the assumptions are made that the density operator, \( \hat{\rho} \), and the Hamiltonian, \( \hat{H} \) can both be written as block-diagonal matrices over all of the subspaces, i.e.,
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

\[
\dot{\rho} = \dot{\rho}_{aa} \oplus \dot{\rho}_{ab} \oplus \dot{\rho}_{ba} \oplus \dot{\rho}_{bb} \quad (6.34)
\]

and

\[
\dot{H} = \dot{H}_{aa} \oplus \dot{H}_{ab} \oplus \dot{H}_{ba} \oplus \dot{H}_{bb} \quad (6.35)
\]

where \(\oplus\) represents the so-called matrix direct sum. This implies that all of the projectors in a given subspace are orthogonal to the projectors in all of the other subspaces for both the density operator and the Hamiltonian. Thus, the eigenvalues of each operator in a given subspace can be computed solely by the components of the operator of that subspace. This results in the ability to write any function of these operators such as, for example, the square root, exponential, or logarithm as a block-diagonal matrix as well. Further, standard matrix multiplication of block-diagonal matrices whose “blocks” are the same size (like \(\dot{H}\) and \(\dot{\rho}\) above) can be written in terms of standard matrix multiplication of each of the individual blocks. This allows the general equation of motion on the overall composite system Hilbert space to be expanded as

\[
\frac{d}{dt} (\dot{\rho}_{aa} \oplus \dot{\rho}_{ab} \oplus \dot{\rho}_{ba} \oplus \dot{\rho}_{bb}) = -\frac{i}{\hbar} \left[ \dot{H}_{aa} \oplus \dot{H}_{ab} \oplus \dot{H}_{ba} \oplus \dot{H}_{bb}, \dot{\rho}_{aa} \oplus \dot{\rho}_{ab} \oplus \dot{\rho}_{ba} \oplus \dot{\rho}_{bb} \right] - \frac{D(\dot{\rho})}{Dt} \quad (6.36)
\]

or
\[ \frac{d\hat{\rho}_{aa}}{dt} \oplus \frac{d\hat{\rho}_{ab}}{dt} \oplus \frac{d\hat{\rho}_{ba}}{dt} \oplus \frac{d\hat{\rho}_{bb}}{dt} = \left( -i \frac{\hbar}{\hat{H}_{aa}, \hat{\rho}_{aa}} \right) \oplus \left( -i \frac{\hbar}{\hat{H}_{ab}, \hat{\rho}_{ab}} \right) \]
\[ \oplus \left( -i \frac{\hbar}{\hat{H}_{ba}, \hat{\rho}_{ba}} \right) \oplus \left( -i \frac{\hbar}{\hat{H}_{bb}, \hat{\rho}_{bb}} \right) - D(\hat{\rho})_D \tag{6.37} \]

Next, the composite system dissipation operator is decomposed into portions that act on a specific subspace (a proof of this is given in Appendix C.1). Thus,

\[ \frac{D(\hat{\rho})}{Dt} = \left( \frac{D(\hat{\rho})}{Dt} \right)_{aa} \oplus \left( \frac{D(\hat{\rho})}{Dt} \right)_{ab} \oplus \left( \frac{D(\hat{\rho})}{Dt} \right)_{ba} \oplus \left( \frac{D(\hat{\rho})}{Dt} \right)_{bb} \tag{6.38} \]

allowing the full equation of motion to be rewritten as

\[ \frac{d\hat{\rho}_{aa}}{dt} \oplus \frac{d\hat{\rho}_{ab}}{dt} \oplus \frac{d\hat{\rho}_{ba}}{dt} \oplus \frac{d\hat{\rho}_{bb}}{dt} = \left( -i \frac{\hbar}{\hat{H}_{aa}, \hat{\rho}_{aa}} \right) \oplus \left( -i \frac{\hbar}{\hat{H}_{ab}, \hat{\rho}_{ab}} \right) \]
\[ \oplus \left( -i \frac{\hbar}{\hat{H}_{ba}, \hat{\rho}_{ba}} \right) \oplus \left( -i \frac{\hbar}{\hat{H}_{bb}, \hat{\rho}_{bb}} \right) - \left( \frac{D(\hat{\rho})}{Dt} \right)_{aa} \oplus \left( \frac{D(\hat{\rho})}{Dt} \right)_{ab} \oplus \left( \frac{D(\hat{\rho})}{Dt} \right)_{ba} \oplus \left( \frac{D(\hat{\rho})}{Dt} \right)_{bb} \tag{6.39} \]

which can then be decomposed into four separate equations

\[ \frac{d\hat{\rho}_{ij}}{dt} = -i \frac{\hbar}{\hat{H}_{ij}, \hat{\rho}_{ij}} - \left( \frac{D(\hat{\rho})}{Dt} \right)_{ij} \tag{6.40} \]

where \( i, j = a, b \). Thus the system state in one subspace effects the dynamics of the other subspaces through the dissipation operator.

With a simplified form for the dissipation operator on the subspace of interest (i.e., \( H_{aa} \)), Eqs. (41a) and (41b) of [10] are used to derive the normalized equation of motion for a
composite system where each subsystem is locally experiencing a heat interaction with a reservoir. These equations are valid for a composite system of non-interacting, but possibly correlated, subsystems. Later, the assumption that the systems are non-interacting is relaxed. However, this does not affect the end result for the new form of the dissipation operator that is derived.

The Hamiltonian on $H_{aa}$ for a composite system of non-interacting subsystems can be written as

$$\hat{H}_{aa} = \hat{H}_A a \otimes \hat{I}_B a + \hat{I}_A a \otimes \hat{H}_B a$$

(6.41)

and Eqs. (41a) and (41b) of [10] are given as

$$\frac{d\hat{\rho}_A}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_A a, \hat{\rho}_A a \right] - \sum_{J=1}^{M} \frac{1}{\tau_J} \hat{D}_J a \otimes \hat{\rho}_J a$$

(6.42)

where $J \in A$, and likewise

$$\frac{d\hat{\rho}_B}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_B a, \hat{\rho}_B a \right] - \sum_{J=1}^{M} \frac{1}{\tau_J} \hat{D}_J a \otimes \hat{\rho}_J a$$

(6.43)

where $J \in B$. Now because in this case subsystems $A$ and $B$ cannot be reduced further into smaller subsystems (i.e., $A$ and $B$ are not composite systems themselves), the above reduces to

$$\frac{d\hat{\rho}_A}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_A a, \hat{\rho}_A a \right] - \frac{1}{\tau_A} \hat{D}_A a$$

(6.44)

and
\[
\frac{d\hat{\rho}_{Ba}}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_{Ba}, \hat{\rho}_{Ba} \right] - \frac{1}{\tau_B} \hat{D}_{Ba}
\] (6.45)

Now taking the tensor product of equation (6.44) with \( \hat{\rho}_{Ba} \) and the tensor product of equation (6.45) with \( \hat{\rho}_{Aa} \) gives

\[
\frac{d\hat{\rho}_{Aa}}{dt} \otimes \hat{\rho}_{Ba} = -\frac{i}{\hbar} \left[ \hat{H}_{Aa}, \hat{\rho}_{Aa} \right] \otimes \hat{\rho}_{Ba} - \frac{1}{\tau_A} \hat{D}_{Aa} \otimes \hat{\rho}_{Ba}
\] (6.46)

and

\[
\hat{\rho}_{Aa} \otimes \frac{d\hat{\rho}_{Ba}}{dt} = -\frac{i}{\hbar} \hat{\rho}_{Aa} \otimes \left[ \hat{H}_{Ba}, \hat{\rho}_{Ba} \right] - \frac{1}{\tau_B} \hat{\rho}_{Aa} \otimes \hat{D}_{Ba}
\] (6.47)

which, when added together, allows composite system dynamics to be written in a more succinct form as

\[
\sum_{J} \frac{d\hat{\rho}_{Ia}}{dt} \otimes \hat{\rho}_{Ja} = \sum_{J} \left[ -\frac{i}{\hbar} \left[ \hat{H}_{Ja}, \hat{\rho}_{Ja} \right] \otimes \hat{\rho}_{Ja} - \sum_{J} \frac{1}{\tau_J} \hat{D}_{Ja} \otimes \hat{\rho}_{Ja} \right]
\] (6.48)

Now using the definition \( \hat{\rho}_{Ja} = P_{Ja} \hat{\rho}_{Ja} \) where \( P_{Ja} = \text{Tr}(\hat{\rho}_{Ja}) \) and noting that \( P_{Ja} = P_{Ja} = P_{aa} \) for all \( J \) and \( \bar{J} \), the above can be rewritten as

\[
\sum_{J} \left( \frac{d}{dt} \left( P_{Ja} \hat{\rho}_{Ja} \right) \otimes \hat{\rho}_{Ja} \right) = \sum_{J} \left[ -\frac{i}{\hbar} \left[ \hat{H}_{Ja}, P_{Ja} \hat{\rho}_{Ja} \right] \otimes \hat{\rho}_{Ja} - \sum_{J} \frac{1}{\tau_J} \hat{D}_{Ja} \otimes \hat{\rho}_{Ja} \right]
\] (6.49)

Next applying the chain rule for derivatives gives

\[
\sum_{J} \left( \left( P_{Ja} \frac{d\hat{\rho}_{Ja}}{dt} + \hat{\rho}_{Ja} \frac{dP_{Ja}}{dt} \right) \otimes \hat{\rho}_{Ja} \right) = \sum_{J} \left[ -\frac{i}{\hbar} \left[ \hat{H}_{Ja}, P_{Ja} \hat{\rho}_{Ja} \right] \otimes \hat{\rho}_{Ja} - \sum_{J} \frac{1}{\tau_J} \hat{D}_{Ja} \otimes \hat{\rho}_{Ja} \right]
\] (6.50)
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

Distributing the tensor product with \( \hat{\rho}_J \), dividing through by \( P_{aa} \), and again factoring out \( P_{aa} \) to normalize \( \hat{\rho}_J \) yields

\[
\sum_J \frac{d\tilde{\rho}_J}{dt} \otimes \tilde{\rho}_J = \sum_J -i\frac{\hbar}{\hbar} \left[ H_J, \tilde{\rho}_J \right] \otimes \tilde{\rho}_J - \frac{1}{P_{aa}} \sum_J \left( \frac{\tilde{D}_J}{\tau_J} + \tilde{\rho}_J \frac{dP_J}{dt} \right) \otimes \tilde{\rho}_J \tag{6.51}
\]

Now if the assumption that the systems are non-interacting is relaxed, which requires the reversible dynamics to be rewritten, but leaves unchanged the irreversible dynamics (as is consistent with [10] in the paragraph following Eq. (41b)), the following equation is found

\[
\frac{d\tilde{\rho}_{aa}}{dt} = -i\frac{\hbar}{\hbar} \left[ H_{aa}, \tilde{\rho}_{aa} \right] - \frac{1}{P_{aa}} \sum_J \left( \frac{\tilde{D}_J}{\tau_J} + \tilde{\rho}_J \frac{dP_J}{dt} \right) \otimes \tilde{\rho}_J \tag{6.52}
\]

Next, rewriting \( \tilde{D}_J \) in normalized form as

\[
\tilde{D}_J = P_{aa} \frac{1}{2} \left( \tilde{\rho}_J \tilde{D}_J + \left( \tilde{\rho}_J \tilde{D}_J \right)^\dagger \right) = P_{aa} \tilde{D}'_J \tag{6.53}
\]

where the definition has been made that \( \tilde{D}'_J \equiv \frac{1}{2} \left( \tilde{\rho}_J \tilde{D}_J + \left( \tilde{\rho}_J \tilde{D}_J \right)^\dagger \right) \), allows the equation of motion to be expressed as

\[
\frac{d\tilde{\rho}_{aa}}{dt} = -i\frac{\hbar}{\hbar} \left[ H_{aa}, \tilde{\rho}_{aa} \right] - \sum_J \frac{1}{\tau_J} \left( \tilde{D}'_J + \tilde{\rho}_J \frac{dP_J}{dt} \right) \otimes \tilde{\rho}_J \tag{6.54}
\]

All that remains is to evaluate \( dP_{Ja}/dt \). To do so, the assumption of non-interacting subsytems is made (which again turns out to be arbitrary, it just provides for a convenient derivation), allowing the equation of motion for the \( J^{th} \) subsystem to be written as
6.2. Model Development

\[
\frac{d\hat{\rho}_{Ja}}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_{Ja}, \hat{\rho}_{Ja} \right] - \frac{1}{\tau_J} \hat{D}_{Ja} \tag{6.55}
\]

Evaluating the trace over \( \mathcal{H}_{Ja} \) gives

\[
\text{Tr}_{Ja} \left[ \frac{d\hat{\rho}_{Ja}}{dt} \right] = \frac{d}{dt} (\text{Tr}_{Ja} [\hat{\rho}_{Ja}]) = \text{Tr}_{Ja} \left[ -\frac{i}{\hbar} \left[ \hat{H}_{Ja}, \hat{\rho}_{Ja} \right] - \frac{1}{\tau_J} \hat{D}_{Ja} \right] \tag{6.56}
\]

or

\[
\frac{dP_{Ja}}{dt} = -\frac{P_{Ja}}{\tau_J} \left( \text{Tr}_{Ja} \left[ \tilde{\hat{\rho}}_{Ja} (\hat{B} \ln(\hat{\rho}))^{Ja} \right] - \text{Tr}_{Ja} \left[ \tilde{\hat{\rho}}_{Ja} \frac{B^1_J}{\Gamma_J} J_a \right] - \text{Tr}_{Ja} \left[ \tilde{\hat{\rho}}_{Ja} \frac{B^3_J}{\Gamma_J} (\hat{H})^{Ja} \right] \right) \tag{6.57}
\]

or finally

\[
\frac{d\tilde{\hat{\rho}}_{aa}}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_{aa}, \tilde{\hat{\rho}}_{aa} \right] - \sum_J \frac{1}{\tau_J} \left( \hat{D}'_{Ja} - \tilde{\hat{\rho}}_{Ja} \left( \langle \tilde{s} \rangle^{Ja} - \frac{B^1_J}{\Gamma_J \langle \tilde{\epsilon} \rangle^{Ja}} \right) \right) \otimes \tilde{\hat{\rho}}_{Ja} \tag{6.59}
\]

Next defining

\[
\hat{D}'_{Ja} \equiv \hat{D}_{Ja} - \tilde{\hat{\rho}}_{Ja} \left( \langle \tilde{s} \rangle^{Ja} - \frac{B^1_J}{\Gamma_J \langle \tilde{\epsilon} \rangle^{Ja}} \right) \tag{6.60}
\]

the above can be rewritten as
\[
\frac{d\tilde{\rho}_{aa}}{dt} = -\frac{i}{\hbar} \left[ \hat{H}_{aa}, \tilde{\rho}_{aa} \right] - \sum_j \frac{1}{\tau_j} \hat{D}''_J \otimes \tilde{\rho}_J \tag{6.61}
\]

which represents the equation of motion for a composite system where each subsystem is locally interacting with a reservoir. \( \hat{D}''_J \) can be simplified to

\[
\hat{D}''_J = \hat{D}'_J - \tilde{\rho}_J \left( \langle \tilde{s} \rangle^J - \frac{B_1^J}{\Gamma J} - \frac{B_3^J}{\Gamma J} \langle \tilde{e} \rangle^J \right) \tag{6.62}
\]

or

\[
\hat{D}''_J = \frac{1}{2} \left( \tilde{\rho}_J \left( \hat{D}_J - \hat{I}_J \left( \langle \tilde{s} \rangle^J - \frac{B_1^J}{\Gamma J} - \frac{B_3^J}{\Gamma J} \langle \tilde{e} \rangle^J \right) \right) + \left[ \tilde{\rho}_J \left( \hat{D}_J - \hat{I}_J \left( \langle \tilde{s} \rangle^J - \frac{B_1^J}{\Gamma J} - \frac{B_3^J}{\Gamma J} \langle \tilde{e} \rangle^J \right) \right] \right] \right) \tag{6.63}
\]

Now defining

\[
\tilde{D}_J \equiv \hat{D}_J - \hat{I}_J \left( \langle \tilde{s} \rangle^J - \frac{B_1^J}{\Gamma J} - \frac{B_3^J}{\Gamma J} \langle \tilde{e} \rangle^J \right) \tag{6.64}
\]

the above can be rewritten as

\[
\hat{D}''_J = \frac{1}{2} \left( \tilde{\rho}_J \tilde{D}_J + \tilde{\rho}_J \left( \tilde{D}_J \right) \right) \tag{6.65}
\]

where \( \tilde{D}_J \) can be simplified to

\[
\tilde{D}_J = \left( \hat{B} \ln(\hat{\rho}) \right)^J \hat{I} - \langle \tilde{s} \rangle^J \hat{I} \tag{6.66}
\]

\[
\hat{D}''_J = \left( \hat{H}^J \hat{I} - \langle \tilde{e} \rangle^J \hat{I} \right) \tag{6.66}
\]
It can be shown that when $\tilde{\rho}_{J_b}$ follows a canonical distribution characterized by $\beta_{J_b}$, that, regardless of the form of the Hamiltonian in subspace $J_b$, $B^J_3 / \Gamma^J = -\beta_{J_b}$ [40] and, thus,

$$\tilde{D}_{J_a} = \left( (\tilde{\mathcal{B}} \ln(\tilde{\rho}))^{J_a \tilde{J}_a} - \langle \tilde{s} \rangle^{J_a \tilde{I}_a} \right) + \beta_{J_b} \left( (\tilde{\mathcal{H}})^{J_a \tilde{J}_a} - \langle \tilde{e} \rangle^{J_a \tilde{I}_a} \right)$$  (6.67)

which accounts for the reservoir temperature $\beta_{J_b}$, is the final equation necessary for computing the equation of motion (equation (6.61) of a composite system where each subsystem is experiencing a local heat interaction with a reservoir.

### 6.2.4 Reservoir Heat Interaction Based Decoherence Control Scheme

With the development of a model to account for each qubit experiencing a reservoir heat interaction completed, a method to utilize this model to control decoherence is developed. This method is based on the unitary evolution that the system would undergo in the absence of dissipation. The state describing this ideal evolution, $\hat{\rho}_{\text{ideal}}(t)$, can be computed as

$$\hat{\rho}_{\text{ideal}}(t) = \hat{U}(t, t_0) \hat{\rho}_0 \hat{U}^\dagger(t, t_0)$$  (6.68)

where $\hat{U}(t, t_0)$ is the unitary time evolution operator, which can be computed with the time-varying Hamiltonian, $\hat{H}_{\text{RF}}(t)$, in addition to the interaction operator, $\hat{H}_I$, used to implement the algorithm. With this, the locally observed state of the ideal system for each qubit $J$, $\hat{\rho}_{\text{ideal}, J}(t)$, can be determined simply as

$$\hat{\rho}_{\text{ideal}, J}(t) = \text{Tr}_J(\hat{\rho}_{\text{ideal}}(t))$$  (6.69)

In the present experiment, the Hamiltonian for a given qubit $J$ is well approximated by $\hat{H}_{0,J}$,
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

(i.e., the magnitude $\omega_{0,J} >> 2\pi J_{i,J}$, where $J_{i,J}$ is the coupling strength between qubits $i$ and $J$), and, thus, the energy of qubit $J$ under the ideal evolution can be well approximated as $E_{\text{ideal},J} \approx \text{Tr} (\hat{\rho}_{\text{ideal},J} \hat{H}_{0,J})$. Next, equating this ideal energy, which is valid for any state, stable equilibrium or not, to the energy of the corresponding stable equilibrium state the following expression is found:

$$E_{\text{ideal},J}(t) = \text{Tr} (\hat{\rho}_{\text{eq},J}(t) \hat{H}_{0,J})$$ (6.70)

where again the overall Hamiltonian for qubit $J$ is approximated by $\hat{H}_{0,J}$. Substituting in $\hat{\rho}_{\text{eq},J} \approx \exp (\beta_{\text{ideal},J} \hat{H}_{0,J}) / Z_J$ and solving for $\beta_{\text{ideal},J}$, it is found that

$$\beta_{\text{ideal},J}(t) = \frac{1}{2 \hat{H}_{00,J}} \ln \left( \frac{\hat{H}_{00,J} - E_{\text{ideal},J}(t)}{\hat{H}_{00,J} + E_{\text{ideal},J}(t)} \right)$$ (6.71)

where it is noted that $\hat{H}_{00,J} = \langle 0 | \hat{H}_{0,J} | 0 \rangle$ (likewise for $\hat{H}_{11,J}$), and that $\hat{H}_{00,J} = -\hat{H}_{11,J}$, which is always true in the eigenbasis of two-level systems represented by Pauli spin matrices. Thus, to correct for differences in energy between the ideal state, which has an associated equilibrium temperature corresponding to $\beta_{\text{ideal},J}(t)$, and the state of the actual system at time $t$, the equality $\beta_{R,J}(t) = \beta_{\text{ideal},J}(t)$ is made between the reservoir (inverse) temperature at time $t$ and the (inverse) temperature of the ideal equilibrium state at constant energy.

Next, the effect of the dissipation operator (regardless of whether a reservoir interaction is taking place or not) is to draw the system state eigenvectors towards alignment with the eigenvectors of the Hamiltonian. Thus, because $\hat{H}_{0,J}$ is the dominant term in the Hamiltonian, the dissipation operator always has the effect of aligning the eigenvectors of $\hat{\rho}_J(t)$ with those of $\hat{H}_{0,J}$, which in the original formulation, are static. When pictured on the Bloch sphere, the eigenvectors of $\hat{H}_{0,J}$ lie along the Z-axis, and, thus, the dissipation operator moves the polarization vector associated with $\hat{\rho}_J(t)$ towards the Z-axis as well.
While this would work well if the system state during an algorithm always needs to be along the Z-axis, in general, qubits can spend significant portions of their evolution in states such that their polarization vector does not lie along the Z-axis of the Bloch sphere. An example of this would be qubit 1 after the first Hadamard gate is applied having a polarization vector that lies in the X-Y plane where it spends the majority of its evolution. Therefore, the dissipation operator (reservoir interaction present or not) causes decoherence of these states since they lose their X-Y polarization components. Thus, to account for this, $\hat{H}_{0,J}$ is changed such that its orientation is no longer static and the rotating reference frame orientation is changed accordingly. To properly orient $\hat{H}_{0,J}$, the polarization vector of the ideal state $\hat{\rho}_{\text{ideal},J}(t)$ is calculated as

$$
\begin{align*}
    r_{x,\text{ideal}}(t) &= \hat{\rho}_{01,\text{ideal}}(t) + \hat{\rho}_{10,\text{ideal}}(t) \\
    r_{y,\text{ideal}}(t) &= i(\hat{\rho}_{01,\text{ideal}}(t) - \hat{\rho}_{10,\text{ideal}}(t)) \\
    r_{z,\text{ideal}}(t) &= \hat{\rho}_{00,\text{ideal}}(t) - \hat{\rho}_{11,\text{ideal}}(t)
\end{align*}
$$

which is then related to the orientation of $\hat{H}_{0,J}$ as

$$
\hat{H}_{0,J}(t) = \frac{\hbar \omega_{0,J}}{2|\vec{r}_{\text{ideal}}(t)|} \left( r_{x,\text{ideal}}(t)\hat{\sigma}_X + r_{y,\text{ideal}}(t)\hat{\sigma}_Y + r_{z,\text{ideal}}(t)\hat{\sigma}_Z \right)
$$

Next, because $\hat{H}_{0,J}(t)$ is now a function of time (via its orientation), the orientation of the rotating reference for each qubit also needs to be adjusted as

$$
\hat{R}_{\text{ref}}(t) = \bigotimes_{i=1}^M \exp\left\{ -i \frac{\phi_i(t)}{2|\vec{r}_{\text{ideal},i}(t)|} \left( r_{x,\text{ideal},i}(t)\hat{\sigma}_{X,i} + r_{y,\text{ideal},i}(t)\hat{\sigma}_{Y,i} + r_{z,\text{ideal},i}(t)\hat{\sigma}_{Z,i} \right) \right\}
$$
and when deriving the SEAQT equation of motion in this rotating reference frame, it is noted that \((d\phi_i/dt)\vec{r}_{\text{ideal},i} >> \phi_i(t)d\vec{r}_{\text{ideal},i}/dt\), which says that the rotations about the Bloch sphere occur at an angular velocity that is significantly less than \(\omega_{0,i}\). This results in any rapid oscillations under the reversible dynamics due to a miss-alignment of the eigenvectors of \(\hat{r}_J(t)\) with those of \(\hat{H}_{0,J}(t)\) to be “hidden” during the course of the evolution. The result of this is that \(\hat{r}_J(t)\) is now properly oriented along the eigenvectors of \(\hat{H}_{0,J}(t)\) and experiences a reservoir heat interaction that maintains the ideal temperature of the system at time \(t\), thus, transferring energy and entropy out of the system to prevent decoherence as the algorithm is computed.

6.3 Results

This section presents the results of various spectra associated with the NMR experiment. First Section 6.3.1 presents the spectra associated with the thermal equilibrium state. Next, Section 6.3.2 shows the spectra associated with the ground state of the NMR molecule. Spectra generated using the theoretical ground state are shown along side those produced using the pseudo-pure ground state as well as the experimentally measured ground state in [58]. In addition, pseudo-pure state spectra predicted using the SEAQT equation of motion (i.e., the Beretta equation) as well as spectra produced using the SEAQT equation of motion including a reservoir interaction (i.e., the Beretta+Reservoir equation) are also presented for the ground state.

Section 6.3.3 shows spectra at the end of the algorithm for the experimental data, the ideal state, and the pseudo-pure state generated using reversible dynamics. Additionally, published theoretical spectra generated with the Kraus/Operator-Sum approach as well as the pseudo-pure state spectra predicted using the Beretta equation and the Beretta+Reservoir
6.3. Results

Equation are also presented. 6.3.4 shows the energy evolution and rate of entropy change of the system with and without reservoir interactions at every instant of time. In all cases involving the SEAQT equation of motion, the relaxation time for qubit $J$ is computed as

$$
\tau_{D,J} = \frac{T_{1J}T_{2J}}{100(T_{1J} + T_{2J})} = \frac{\tau_{Matthisien,J}}{100} \tag{6.77}
$$

where $\tau_{Matthisien,J}$ represents the relaxation time under both mechanisms (spin-lattice and spin-spin relaxation) occurring simultaneously for qubit $J$. The factor of $1/100$ is included to amplify the dissipation operator and the subsequent noise. In all cases involving a reservoir interaction, the reservoir interaction control scheme described in Section 6.2.4 is used to vary the reservoir temperature. All sections present the spectra for qubits 1, 2, and 3 only since these are the only spectra for which both theoretical and experimental published data exists. Also, for the spectra resulting from the Beretta equation, phase-correction techniques are applied such that the phase and sign of the resulting noise produced by the dissipation under the Beretta equation better align with that which is seen experimentally. This is done because it is well known that the phase at a given frequency of the spectra of the NMR experiment is highly dependent upon the pulse sequence used in the experiment [38]. Furthermore, the spectra presented in [58] are obtained utilizing phase-correction techniques [54, 57] in a post-processing step.

6.3.1 Thermal Equilibrium Spectra

This section presents the results of the spectra of the NMR QC system in a thermal equilibrium state. For this system of $N = 7$ qubits, it is expected that there are $2^{N-1} = 64$ peaks associated with the spectra of each qubit, where each peak corresponds to a unique combination of the other qubits being either spin up or spin down and the associated coupling strengths
When distinct combinations of the other qubits produce the same frequency shift, both peaks lie on top of one another and the resulting strength of the signal at that frequency is amplified. Figure 6.2a shows the spectra associated with qubit 1 where nearly all 64 peaks can clearly be distinguished. Figure 6.2b shows the thermal equilibrium spectra of qubit 2, where now there is overlap in some of the 64 frequency shifts, resulting in some peaks having magnitudes that are larger than others. Finally, Figure 6.2c shows the spectra of qubit 3 where again there is some overlap of the predicted spectra. However in all cases, the numerically generated spectra are in good agreement with that which is published.

Figure 6.2: Thermal equilibrium spectra of qubits 1, 2, and 3; all frequencies are relative to those given in Table 6.2.
6.3. Results

6.3.2 Ground State Spectra

This section presents the results of the spectra of the NMR QC system in the ground state. Because the ground state does not involve any superposition of states, only a single peak is expected, corresponding to all other qubits being spin down. Figure 6.3 shows the theoretical spectra of qubits 1, 2, and 3 along with those produced using the pseudo-pure state under the reversible von Neumann equation as well as the published experimental data of [58]. While there is some slight noise in the experimental data, the major peaks align well for all qubits. This result shows that the numerical implementation of Shor’s algorithm results in little error under the reversible dynamics.

Figure 6.4 shows the spectra of qubits 1, 2, and 3 of the pseudo-pure ground state predicted with the Beretta and the Beretta+Reservoir equations, and of the published experimental data of [58]. The noise generated due to the dissipation of the Beretta equation is slightly larger than what is observed experimentally for some frequencies, while in contrast and, as expected, this noise is canceled out with the Beretta+Reservoir equation, pointing to the usefulness of the reservoirs for controlling the dissipative effects present. As to the cause of the larger noise predictions with the Beretta equation, this is in part if not in whole due to the fact that the RF pulse sequence implemented here is not as refined as that implemented in [58]; and, thus, the quantum factoring algorithm takes longer to run, allowing more time for dissipation to occur and as a result increasing the noise present. This is confirmed by the fact that the same pulse sequence is used here as was used in the reversible dynamics of the von Neumann equation (which had no noise), suggesting that the numerical error associated with the numerical implementation of the pulse sequence is amplified by the dissipation operator.
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

Figure 6.3: Ground state spectra of qubits 1, 2, and 3; experimental results are shown in addition to the theoretical spectra and those obtained from the pseudo-pure state using the von Neumann equation; all frequencies are relative to those given in Table 6.2
6.3. Results

Figure 6.4: Ground state spectra of qubits 1, 2, and 3; experimental results are shown in addition to the pseudo-pure state spectra obtained from the Beretta and Beretta+Reservoir equations; all frequencies are relative to those given in Table 6.2 and \( \tau_{D,J} = \tau_{Matthisien,J}/100 \).
6.3.3 End State Spectra

This section presents the results of the spectra of the NMR QC system at the end of the algorithm. Here, it is known that the system should be in a superposition of 4 states, and, thus, 4 peaks are expected for each qubit. Figure 6.5 shows the theoretical spectra of qubits 1, 2, and 3 along with those produced using the pseudo-pure state under the reversible von Neumann equation as well as the published experimental data of [58]. In general, all major peaks predicted here are again in good agreement with the published results (the slight discrepancy in frequency for qubit 3 is due to the numerical extraction of the published data). To produce the spectra for qubit 3, an additional Hadamard gate must be applied before the measurement $\hat{R}_X(\pi/2)$ operation to produce the plotted peaks (this is done simply for plotting purposes to show two distinct peaks, one positive and the other negative, at differing frequencies). Here, only the net integral of the spectrum is of interest to obtain the orientation (spin up or down) of the qubit. Qubits 1 and 2 clearly have positive integrals and are, thus, spin up. Qubit 3 has a net integral of zero (which is unaffected by the extra Hadamard operation) and is, thus, in a superposition of $|0\rangle + |1\rangle$. The resulting state of the first three qubits is then $|100\rangle + |000\rangle = |4\rangle + |0\rangle$ which has a periodicity of $P = 4$ (note that the inverse quantum Fourier transform switches the order of qubits 1, 2, and 3 in the above ket state representation). Therefore, the order $r$ can be computed as $r = 2^3/P = 2$, as expected for the case of $a = 11$ and the subsequent factors of 15 being 3 and 5 can be computed.

Figure 6.6 shows the experimental spectra of qubits 1, 2, and 3 along with those produced using the pseudo-pure state with the Beretta equation of motion as well as published theoretical predictions by [58] under the evolution of the Kraus-Operator-Sum approach. For all qubits, the frequencies of the major peaks match. However, as before, the noise resulting from the decoherence due to the dissipation occurring with the Beretta equation is larger than the
6.3. Results

Figure 6.5: End state spectra of qubits 1, 2, and 3; experimental results are shown in addition to the theoretical spectra and those obtained from the pseudo-pure state using the von Neumann equation; all frequencies are relative to those given in Table 6.2.

Experimental noise. As indicated previously, this is in part if not in whole due to the fact that the RF pulse sequence implemented here is not as refined as that implemented in [58]; and, thus, the quantum numerical algorithm gate implementation takes longer to run, allowing more time for dissipation to occur and as a result increasing the noise present. An aspect that SEAQT does predict better than the Kraus/Operator-Sum approach is that the magnitude of the noise at various frequencies better matches the experimental data.

Figure 6.7 shows the experimental spectra of qubits 1, 2, and 3 along with that produced
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

(a) Qubit 1 End State Spectra
(b) Qubit 2 End State Spectra
(c) Qubit 3 End State Spectra

Figure 6.6: End state spectra of qubits 1, 2, and 3; experimental results are shown in addition to theoretical results predicted under the evolution of the Kraus/Operator-Sum approach [58] and the pseudo-pure state spectra obtained from the Beretta equation, all frequencies are relative to those given in Table 6.2.

using the pseudo-pure state under the Beretta+Reservoir equation of motion as well as published theoretical predictions by [58] using the Kraus-Operator-Sum approach. Here, the reservoir interaction control scheme described in Section 6.2.4 is used to minimize decoherence. Again for all qubits, the frequencies of the major peaks match, and as can be seen, the noise associated with the Beretta+Reservoir equation is much lower than that of the experimental or Kraus/Operator-Sum results. This indicates that the control scheme is working as intended and as entropy is generated during the algorithm, both energy and entropy are transferred to
6.3. Results

the reservoir. For the Beretta + Reservoir equation, the spectra are nearly identical to the reversible results, which, of course, is the desired effect.

Figure 6.7: End state spectra of qubits 1, 2, and 3; experimental results are shown in addition to the theoretical results predicted under the evolution of the Kraus/Operator-Sum approach [58] and the pseudo-pure state spectra obtained from the Beretta + Reservoir equation; all frequencies are relative to those given in Table 6.2.

6.3.4 Reservoir Energy and Entropy Transfer Analysis

Figure 6.8 shows the total rate of entropy change of the composite system of qubits for both the Beretta and Beretta + Reservoir equations. For the Beretta equation, the rate
of system entropy change is equivalent to the entropy generation rate, whereas for the Beretta+Reservoir equation, the rate of system entropy change is equivalent to the difference of the entropy generation rate of the qubits and the rate of entropy transferred from the qubits to the reservoir. This evolution begins after the first temporal averaging scheme has been implemented, and, thus, there exists entanglement between some of the qubits. Figure 6.8a shows that for predictions of the Beretta equation alone, spikes occur in the entropy generation rate or the rate of system entropy change during the pulses implementing the algorithm, but during free evolution, the entropy generation rate is relatively small. This is expected since during the times that pulses are not being applied, the system is very close to stable equilibrium where there is little entropy generation. Figure 6.8b shows that the rate of system entropy change predicted by the Beretta+Reservoir equation is of the same order of magnitude at the beginning of the algorithm as for the case of the Beretta equation alone, but, after an initial spike of entropy transfer to the reservoir (corresponding to $\dot{S} < 0$), it remains relatively close to zero. This is also expected since the effect of the reservoir interaction is to transfer entropy from the system to the reservoir as it is generated by the system during pulse implementation as well as free evolution. This results in the system remaining for the vast majority of the time very close to the initial stable equilibrium state where little entropy is generated even in the presence of the implemented pulses.
6.3. Results

Figure 6.8: Composite system entropy evolution; (a) shows the rate of entropy change for the composite system as predicted by the Beretta equation, which is equivalent to the entropy generation rate, while (b) shows the rate of entropy change for the composite system as predicted by the Beretta+Reservoir equation, which is equivalent to the difference of the entropy generation rate of the qubits and the rate of entropy transferred from the qubits to their respective reservoirs. The rate of entropy change predicted by the Beretta+Reservoir is significantly smaller than that predicted by the Beretta equation alone.

Figures 6.9 through 6.12 show the energy evolutions of each qubit throughout the algorithm for the Beretta and the Beretta+Reservoir equations. Again, this evolution begins after the first temporal averaging scheme has been implemented, and, thus, there is entanglement between some of the qubits. To obtain an estimate of the energy transfer between the qubit and reservoir, the qubit energy evolutions for both the Beretta and Beretta+Reservoir equations are compared. For instances when the qubit energy as predicted by the Beretta+Reservoir equation is higher than that predicted by the Beretta equation, energy transfer from the reservoir to the qubit occurs. Likewise, when the qubit energy predicted by the Beretta+Reservoir equation is lower than that predicted by the Beretta equation, energy is transferred from the qubit to the reservoir.

Figure 6.9 shows that during various portions of the algorithm, there is energy transfer either to or from qubit 1 to the reservoir, depending on the state of the qubit. Figure 6.9b shows...
that the rapid changes in energy are in fact continuous and due to the pulsed Hamiltonians that implement the qubit rotations.

Figure 6.9: Energy evolution of qubit 1 after the preparation sequence has taken place; (a) shows that as the state of qubit 1 is manipulated during the algorithm, energy is either transferred to or from the reservoir, while (b) shows that the sharp changes in energy are not discontinuous but happen relatively very rapidly in time compared to the length of the algorithm.

Figure 6.10a shows that the energy evolution of qubit 2 exhibits qualitatively similar features to that of qubit 1. In contrast, Figure 6.10b shows that throughout the algorithm for qubit 3, there is primarily energy transfer from the reservoir to the qubit, increasing the relative magnitude of the energy. This is opposite to the behavior seen for qubits 1 and 2 where the reservoir energy transfer serves to lower the relative magnitude of the energy.

Figures 6.11 and 6.12 show the energy evolutions of qubits 4, 5, 6, and 7. The energy evolution of qubit 6, shown in Figure 6.12a exhibits qualitatively similar behavior to that of qubits 1 and 2. The energy evolutions of qubits 4, 5, and 7, shown in Figures 6.11a, 6.11b, and 6.12b, respectively, show that there is relatively little energy transfer between these qubits and their respective reservoirs since the difference between the energies predicted by the Beretta equation and the Beretta+Reservoir equation are small compared to the magnitude of the energies.
6.3. Results

Figure 6.10: Energy evolution of qubits 2 and 3 after the preparation sequence has taken place; (a) shows that, like qubit 1, there is energy transfer both to and from the reservoir to qubit 2, while (b) shows that there is primarily energy transfer from the reservoir to qubit 3 throughout the algorithm.

Figure 6.11: Energy evolution of qubits 4 and 5 after the preparation sequence has taken place; (a) and (b) show that there is negligible energy transfer to/from qubits 4 and 5, respectively, and their respective reservoirs during the algorithm.
Chapter 6. Modeling the Effects of Dissipation in a Quantum Algorithm on an NMR Quantum Computer

Figure 6.12: Energy evolution of qubits 6 and 7 after the preparation sequence has taken place; (a) shows that, like qubit 1, there is energy transfer both to and from the reservoir to qubit 6, while (b) shows that there is negligible energy transfer to/from qubit 7 and its reservoir during the algorithm.
6.4 Conclusions

This chapter first reviews some preliminary concepts involved in the development of the NMR Hamiltonian and how it is used to realize Shor’s factoring algorithm, including the development of pseudo-pure states. The SEAQT equation of motion for a general, composite quantum system (the Beretta equation) is then introduced before providing a derivation for a model of a composite quantum system where each subsystem locally experiences a heat interaction with a reservoir (the Beretta+Reservoir). With this development, a control scheme is devised to limit the decoherence occurring during a quantum algorithm by transferring the entropy generated during the course of the algorithm to the reservoir.

After this development, the reversible dynamics of the von Neumann equation along with the irreversible dynamics of the Beretta and Beretta+Reservoir equations are used to predict the spectra of the NMR experiment as it executes Shor’s algorithm. It is seen in all cases that the major frequency peaks are in good agreement. However, for the Beretta equation, the noise is often predicted to be larger than what is observed experimentally. It is expected that this is due to the numerical implementation of the RF pulse sequence used to implement Shor’s algorithm, which is not optimized as the one is used in the experiment. Further, this is also because of the scaling of the SEAQT relaxation time, $\tau_D$, which for larger values (after scaling), would result in less dissipation and subsequent noise.

Thus, it is anticipated that with additional details regarding the full implementation of the experimental pulse sequence (which currently are not available) as well as the process of converting the system state to a voltage signal which is then evaluated using a Fourier transform, and a different value of $\tau_D$, the noise characteristics could also be more accurately be produced. Thus, future work should includes further refinement of the pulse sequence and better characterization of what affects the sign of the noise. A positive takeaway from this
work is that the Beretta equation better predicts at which frequencies noise occurs than does the Kraus/Operator-Sum approach.

The Beretta+Reservoir equation implementing the decoherence control scheme is successful in effectively removing all noise produced by the Beretta equation alone, showing that reservoir interactions can be an effective tool for minimizing decoherence. For NMR systems, a potential realization for qubit specific reservoir interactions may be a superposition of RF fields where the specific frequencies of the fields forming the superposition are each in resonance with a specific qubit. The specific reservoir temperatures may be realized by using the RF fields to maintain each qubit at an energy with a corresponding stable equilibrium temperature that is equivalent to the desired reservoir temperature. While the feasibility of such reservoir interactions may vary depending on the specific realization of the qubit (e.g., it may be difficult to realize some of the reservoir temperatures in an NMR QC using the above approach), the underlying mathematics of the reservoir heat interaction model are general, and, thus, can be applied to other QIQC systems that may better facilitate qubit specific reservoir interactions. Regardless, this work has shown that SEAQT can be used to predict dissipation and the subsequent decoherence occuring in NMR QC systems as well as the ability to limit this decoherence by transferring entropy from the system to a reservoir as it is produced during a quantum computing algorithm.
Appendices
Appendix C

Composite System Reservoir
Interaction Dissipation Operator Evaluation

C.1 Dissipation Operator

To form an equation of motion on the Hilbert space $H_{aa}$, corresponding to the composite system of interest, it is necessary to find the portion of the dissipation operator that acts on $H_{aa}$. First consider the general form of the density operator

$$\frac{D(\hat{\rho})}{Dt} = \sum_{J} \frac{1}{\tau_J} \hat{D}_J \otimes \hat{\rho}_J$$

(C.1)

where $\hat{\rho}_J$ and $\hat{\rho}_J$ are defined as

\[\hat{\rho}_J = \text{Tr}_J(\hat{\rho}) = \text{Tr}_J(\hat{\rho}_{aa} \oplus \hat{\rho}_{ab} \oplus \hat{\rho}_{bb}) = \text{Tr}_J(\hat{\rho}_{JaJa} \oplus \hat{\rho}_{JaJb} \oplus \hat{\rho}_{JbJa} \oplus \hat{\rho}_{JbJb}) \]

(C.2)

or

\[\hat{\rho}_J = \left(\text{Tr}_{Ja}(\hat{\rho}_{JaJa}) + \text{Tr}_{Jb}(\hat{\rho}_{JbJb})\right) \oplus \left(\text{Tr}_{Ja}(\hat{\rho}_{JaJb}) + \text{Tr}_{Jb}(\hat{\rho}_{JbJa})\right) \]

(C.3)

\[\hat{\rho}_{JaJa} \oplus \hat{\rho}_{JaJb} \oplus \hat{\rho}_{JbJa} \oplus \hat{\rho}_{JbJb} \]
C.1. Dissipation Operator

or

\[ \hat{\rho}_J = \hat{\rho}_J a \oplus \hat{\rho}_J b \]  \hspace{1cm} (C.4)

where

\[ \hat{\rho}_J a = \text{Tr}_{J a} (\hat{\rho}_{J a} J a) + \text{Tr}_{J b} (\hat{\rho}_{J a} J b) \]  \hspace{1cm} (C.5)

and

\[ \hat{\rho}_J b = \text{Tr}_{J a} (\hat{\rho}_{J b} J a) + \text{Tr}_{J b} (\hat{\rho}_{J b} J b) \]  \hspace{1cm} (C.6)

Now if it is assumed that there are no states in the Hilbert space \( H_{ab} = H_{Ja,Ja} \) or \( H_{ba} = H_{Jb,Ja} \), meaning that \( \hat{\rho}_{J a} J b = \hat{0}_{Ja,Jb} \) and \( \hat{\rho}_{J b} J a = \hat{0}_{Jb,Ja} \), then the above reduces to

\[ \hat{\rho}_J a = \text{Tr}_{Ja} (\hat{\rho}_{Ja} J a) \]  \hspace{1cm} (C.7)

and

\[ \hat{\rho}_J b = \text{Tr}_{Jb} (\hat{\rho}_{Jb} J b) \]  \hspace{1cm} (C.8)

A similar process can be done for \( \hat{\rho}_J \).

C.1.1 \( J^{th} \) Subsystem Dissipation Operator

Now, the dissipation operator for the \( J^{th} \) subsystem can be written as
\[ \hat{D}_J = \frac{1}{2} \left( \dot{\rho}_J \hat{D}_J + (\dot{\rho}_J \hat{D}_J)^\dagger \right) \]  

(C.9)

where \( \hat{D}_J \) can be written as

\[
\hat{D}_J = \frac{1}{\Gamma^J} \begin{vmatrix}
(\hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{0,J})^J & (\hat{R}_{1,J})^J & (\hat{R}_{2,J})^J \\
(\hat{R}_{0,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{0,J}, \hat{R}_{0,J})^J & (\hat{R}_{0,J}, \hat{R}_{1,J})^J & (\hat{R}_{0,J}, \hat{R}_{2,J})^J \\
(\hat{R}_{1,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{1,J}, \hat{R}_{0,J})^J & (\hat{R}_{1,J}, \hat{R}_{1,J})^J & (\hat{R}_{1,J}, \hat{R}_{2,J})^J \\
(\hat{R}_{2,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{2,J}, \hat{R}_{0,J})^J & (\hat{R}_{2,J}, \hat{R}_{1,J})^J & (\hat{R}_{2,J}, \hat{R}_{2,J})^J
\end{vmatrix}
\]

(C.10)

and where \( \Gamma^J \) is defined as

\[
\Gamma^J = \begin{vmatrix}
(\hat{R}_{0,J}, \hat{R}_{0,J})^J & (\hat{R}_{0,J}, \hat{R}_{1,J})^J & (\hat{R}_{0,J}, \hat{R}_{2,J})^J \\
(\hat{R}_{1,J}, \hat{R}_{0,J})^J & (\hat{R}_{1,J}, \hat{R}_{1,J})^J & (\hat{R}_{1,J}, \hat{R}_{2,J})^J \\
(\hat{R}_{2,J}, \hat{R}_{0,J})^J & (\hat{R}_{2,J}, \hat{R}_{1,J})^J & (\hat{R}_{2,J}, \hat{R}_{2,J})^J
\end{vmatrix}
\]

(C.11)

where \( \hat{R}_{0,J}, \hat{R}_{1,J}, \) and \( \hat{R}_{2,J} \) represent the generators of the motion for the \( J^{th} \) subsystem. For each subsystem \( J \), the first generator of the motion, \( \hat{R}_{0,J} \), is

\[
\hat{R}_{0,J} = \left( \hat{I}_{J_a} \otimes \hat{I}_{J_a} \right) \oplus (\hat{0}_{J_a} \otimes \hat{0}_{J_b}) \oplus (\hat{0}_{J_b} \otimes \hat{0}_{J_a}) \oplus (\hat{0}_{J_b} \otimes \hat{0}_{J_b})
\]

(C.12)

or

\[
\hat{R}_{0,J} = \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{ba} \oplus \hat{0}_{bb} = \left( \hat{I}_{aa} \otimes \hat{0}_{ab} \right) \oplus (\hat{0}_{ba} \otimes \hat{0}_{bb}) = \hat{R}_{0,J_a} \oplus \hat{R}_{0,J_b}
\]

(C.13)

Likewise, the second generator of the motion, \( \hat{R}_{1,J} \), is
\[ \hat{R}_{1J} = (\hat{0}_{Ja} \otimes \hat{0}_{Ja}) \oplus (\hat{0}_{Ja} \otimes \hat{0}_{Jb}) \oplus (\hat{0}_{Jb} \otimes \hat{0}_{Ja}) \oplus \left( \hat{I}_{Jb} \otimes \hat{I}_{Jb} \right) \] (C.14)

or

\[ \hat{R}_{1J} = \hat{0}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb} = (\hat{0}_{aa} \otimes \hat{0}_{ab}) \oplus (\hat{0}_{ba} \otimes \hat{I}_{bb}) = \hat{R}_{1Ja} \oplus \hat{R}_{1Jb} \] (C.15)

and finally the third generator of the motion, \( \hat{R}_{2J} = \hat{H} \), is

\[ \hat{R}_{2J} = \hat{H} = (\hat{H}_{aa} \oplus \hat{H}_{ab}) \oplus (\hat{H}_{ba} \oplus \hat{H}_{bb}) = \hat{R}_{2Ja} \oplus \hat{R}_{2Jb} \] (C.16)

To continue deriving an equation of motion on the Hilbert space \( \mathcal{H}_{aa} \), it is next necessary to examine the perceived operators. For brevity, this is done in Appendix D. Using the results for the perceived operators allows equation C.10 to be written as

\[
\tilde{D}_J = \begin{vmatrix}
(\hat{B} \ln(\hat{\rho}))^{Ja} \oplus (\hat{B} \ln(\hat{\rho}))^{Jb} & (\hat{R}_{0J})^{Ja} \oplus (\hat{R}_{0J})^{Jb} & (\hat{R}_{1J})^{Ja} \oplus (\hat{R}_{1J})^{Jb} & (\hat{R}_{2J})^{Ja} \oplus (\hat{R}_{2J})^{Jb} \\
(\hat{R}_{0J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{0J}, \hat{R}_{0J})^J & (\hat{R}_{0J}, \hat{R}_{1J})^J & (\hat{R}_{0J}, \hat{R}_{2J})^J \\
(\hat{R}_{1J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{1J}, \hat{R}_{0J})^J & (\hat{R}_{1J}, \hat{R}_{1J})^J & (\hat{R}_{1J}, \hat{R}_{2J})^J \\
(\hat{R}_{2J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{2J}, \hat{R}_{0J})^J & (\hat{R}_{2J}, \hat{R}_{1J})^J & (\hat{R}_{2J}, \hat{R}_{2J})^J
\end{vmatrix}
\]

\[ \Gamma^J \] (C.17)

which is equivalent to

\[ \tilde{D}_J = \tilde{D}_{Ja} \oplus \tilde{D}_{Jb} \] (C.18)

where
Chapter C. Composite System Reservoir Interaction Dissipation Operator Evaluation

\[ \tilde{D}_J = \frac{1}{2} \begin{pmatrix} (\hat{B} \ln(\hat{\rho}))^J_a & (\hat{R}_{0,J})^J_a & (\hat{R}_{1,J})^J_a & (\hat{R}_{2,J})^J_a \\ (\hat{R}_{0,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{0,J}, \hat{R}_{0,J})^J & (\hat{R}_{0,J}, \hat{R}_{1,J})^J & (\hat{R}_{0,J}, \hat{R}_{2,J})^J \\ (\hat{R}_{1,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{1,J}, \hat{R}_{0,J})^J & (\hat{R}_{1,J}, \hat{R}_{1,J})^J & (\hat{R}_{1,J}, \hat{R}_{2,J})^J \\ (\hat{R}_{2,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{2,J}, \hat{R}_{0,J})^J & (\hat{R}_{2,J}, \hat{R}_{1,J})^J & (\hat{R}_{2,J}, \hat{R}_{2,J})^J \end{pmatrix} \Gamma_J \]  

(C.19)

and similarly for \( \tilde{D}_b \). Therefore \( \hat{D}_J \) can be written as

\[ \hat{D}_J = \frac{1}{2} \left( \hat{\rho}_J \hat{D}_J + (\hat{\rho}_J \hat{D}_J)^\dagger \right) = \frac{1}{2} \left[ (\hat{\rho}_J \hat{D}_J + (\hat{\rho}_J \hat{D}_J)^\dagger) \oplus (\hat{\rho}_b \hat{D}_b + (\hat{\rho}_b \hat{D}_b)^\dagger) \right] \]  

(C.20)

or \( \hat{D}_J = \hat{D}_J_a \oplus \hat{D}_J_b \). This allows the composite system dissipation operator to be written as

\[ \frac{D(\hat{\rho})}{D_t} = \sum_j \frac{1}{\tau_j} \hat{D}_J \otimes \hat{\rho}_J = \sum_j \frac{1}{\tau_j} \left( \hat{D}_J_a \oplus \hat{D}_J_b \right) \otimes (\rho_J_a \oplus \rho_J_b) \]  

(C.21)

or

\[ \frac{D(\hat{\rho})}{D_t} = \left( \sum_j \frac{1}{\tau_j} \left( \hat{D}_J_a \otimes \rho_J_a \right) \right) \oplus \left( \sum_j \frac{1}{\tau_j} \left( \hat{D}_J_a \otimes \rho_J_b \right) \right) \oplus \left( \sum_j \frac{1}{\tau_j} \left( \hat{D}_J_b \otimes \rho_J_a \right) \right) \oplus \left( \sum_j \frac{1}{\tau_j} \left( \hat{D}_J_b \otimes \rho_J_b \right) \right) \]  

(C.22)

or finally

\[ \frac{D(\hat{\rho})}{D_t} = \left( \frac{D(\hat{\rho})}{D_t} \right)_{aa} \oplus \left( \frac{D(\hat{\rho})}{D_t} \right)_{ab} \oplus \left( \frac{D(\hat{\rho})}{D_t} \right)_{ba} \oplus \left( \frac{D(\hat{\rho})}{D_t} \right)_{bb} \]  

(C.23)

which shows that for the assumed form of the generators of the motion and density operator,
C.2 Dissipation Operator Simplification

The ratio of Gram determinants found in the dissipation operator can be written as

\[
\tilde{D}_J = \frac{\begin{vmatrix} (\hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{0,J})^J & (\hat{R}_{1,J})^J & (\hat{R}_{2,J})^J \\ (\hat{R}_{0,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{0,J}, \hat{R}_{0,J})^J & (\hat{R}_{0,J}, \hat{R}_{1,J})^J & (\hat{R}_{0,J}, \hat{R}_{2,J})^J \\ (\hat{R}_{1,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{1,J}, \hat{R}_{0,J})^J & (\hat{R}_{1,J}, \hat{R}_{1,J})^J & (\hat{R}_{1,J}, \hat{R}_{2,J})^J \\ (\hat{R}_{2,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{2,J}, \hat{R}_{0,J})^J & (\hat{R}_{2,J}, \hat{R}_{1,J})^J & (\hat{R}_{2,J}, \hat{R}_{2,J})^J \end{vmatrix}}{\Gamma^J} \quad (C.24)
\]

or

\[
\tilde{D}_J = (\hat{B} \ln(\hat{\rho}))^J - \frac{B_1^J}{\Gamma^J} (\hat{R}_{0,J})^J + \frac{B_2^J}{\Gamma^J} (\hat{R}_{1,J})^J - \frac{B_3^J}{\Gamma^J} (\hat{R}_{2,J})^J \quad (C.25)
\]

where \(\Gamma^J\) is defined by equation C.11, and \(B_1^J, B_2^J,\) and \(B_3^J\) are defined as

\[
B_1^J = \begin{vmatrix} (\hat{R}_{0,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{0,J}, \hat{R}_{1,J})^J & (\hat{R}_{0,J}, \hat{R}_{2,J})^J \\ (\hat{R}_{1,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{1,J}, \hat{R}_{1,J})^J & (\hat{R}_{1,J}, \hat{R}_{2,J})^J \\ (\hat{R}_{2,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{2,J}, \hat{R}_{1,J})^J & (\hat{R}_{2,J}, \hat{R}_{2,J})^J \end{vmatrix} \quad (C.26)
\]

\[
B_2^J = \begin{vmatrix} (\hat{R}_{0,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{0,J}, \hat{R}_{0,J})^J & (\hat{R}_{0,J}, \hat{R}_{2,J})^J \\ (\hat{R}_{1,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{1,J}, \hat{R}_{0,J})^J & (\hat{R}_{1,J}, \hat{R}_{2,J})^J \\ (\hat{R}_{2,J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{2,J}, \hat{R}_{0,J})^J & (\hat{R}_{2,J}, \hat{R}_{2,J})^J \end{vmatrix} \quad (C.27)
\]
Chapter C. Composite System Reservoir Interaction Dissipation Operator Evaluation

\[
B_3^J = \begin{vmatrix}
(\hat{R}_{0J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{0J}, \hat{R}_{1J})^J & (\hat{R}_{1J}, \hat{R}_{1J})^J \\
(\hat{R}_{1J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{1J}, \hat{R}_{1J})^J & (\hat{R}_{2J}, \hat{R}_{1J})^J \\
(\hat{R}_{2J}, \hat{B} \ln(\hat{\rho}))^J & (\hat{R}_{2J}, \hat{R}_{0J})^J & (\hat{R}_{2J}, \hat{R}_{1J})^J \\
\end{vmatrix}
\] (C.28)

To simplify \( \tilde{D}_J \) further, it is next necessary to evaluate all of the inner products of the perceived generators of the motion, which is done in Appendix E.

C.2.1 Evaluation of the Gram Determinant

Using the results found in Appendix E, the ratio of gram determinants can be rewritten as

\[
\tilde{D}_J = \frac{\begin{vmatrix}
P_{Ja} (\tilde{B} \ln(\tilde{\rho}))^{Ja} & P_{Ja} \hat{I}_a & \hat{o}_Ja & P_{Ja} (\tilde{H})^{Ja} \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
P_{Ja} (\tilde{e})^{Ja} & P_{Ja} (\tilde{e})^{Ja} & P_{Ja} (\tilde{e})^{Ja} & P_{Ja} (\tilde{e})^{Ja} \\
\end{vmatrix}}{\Gamma^J}
\] (C.29)

where

\[
\Gamma^J \equiv \begin{vmatrix}
P_{Ja}^3 & 0 & P_{Ja}^3 (\tilde{e})^{Ja} \\
0 & P_{Ja}^3 (\tilde{e})^{Ja} \\
P_{Ja}^3 (\tilde{e})^{Ja} & P_{Ja}^3 (\tilde{e})^{Ja} & P_{Ja}^3 (\tilde{e})^{Ja} + P_{Ja}^3 (\tilde{e})^{Ja} \\
\end{vmatrix}
\] (C.30)

C.2.2 Evaluation of \( \Gamma^J \)

Now expanding \( \Gamma^J \) gives
C.2. Dissipation Operator Simplification

\[ \Gamma^J = P^3_{J_a} P^3_{J_b} \left( P^3_{J_a} \left( \tilde{e}^2 J_a - (\bar{\epsilon}) J_a \right)^2 + P^3_{J_b} \left( \tilde{e}^2 J_b - (\bar{\epsilon}) J_b \right)^2 \right) \] (C.31)

C.2.3 Definitions of \( B_{J^1} \) and \( B_{J^2} \)

\[ B_{J^1} \equiv \begin{vmatrix} P^3_{J_a} (\tilde{s}) J_a & 0 & P^3_{J_a} (\bar{\epsilon}) J_a \\ P^3_{J_b} (\tilde{s}) J_b & P^3_{J_b} (\bar{\epsilon}) J_b & P^3_{J_b} (\tilde{e}) J_b \\ P^3_{J_a} (\tilde{e}s) J_a + P^3_{J_b} (\tilde{e}s) J_b & P^3_{J_b} (\bar{\epsilon}s) J_b & P^3_{J_a} (\tilde{e}^2) J_a + P^3_{J_b} (\bar{e}^2) J_b \end{vmatrix} \] (C.32)

\[ B_{J^2} \equiv \begin{vmatrix} P^3_{J_a} (\tilde{s}) J_a & P^3_{J_a} & P^3_{J_a} (\bar{\epsilon}) J_a \\ P^3_{J_b} (\tilde{s}) J_b & 0 & P^3_{J_b} (\bar{\epsilon}) J_b \\ P^3_{J_a} (\tilde{e}s) J_a + P^3_{J_b} (\tilde{e}s) J_b & P^3_{J_a} (\bar{\epsilon}s) J_a & P^3_{J_a} (\tilde{e}^2) J_a + P^3_{J_b} (\bar{e}^2) J_b \end{vmatrix} \] (C.33)

C.2.4 Evaluation of \( B_{J^3} \)

\[ B_{J^3} \equiv \begin{vmatrix} P^3_{J_a} (\tilde{s}) J_a & P^3_{J_a} & 0 \\ P^3_{J_b} (\tilde{s}) J_b & 0 & P^3_{J_b} \end{vmatrix} \] (C.34)

or

\[ B_{J^3} = P^3_{J_a} P^3_{J_b} \left( P^3_{J_a} \left( \tilde{e}s J_a - (\tilde{s}) J_a (\bar{\epsilon}) J_a \right) + P^3_{J_b} \left( \tilde{e}s J_b - (\tilde{s}) J_b (\bar{\epsilon}) J_b \right) \right) \] (C.35)

C.2.5 Evaluation of \( B_{J^3} / \Gamma^J \)

\[ \frac{B_{J^3}}{\Gamma^J} = \frac{P^3_{J_a} P^3_{J_b} \left( P^3_{J_a} \left( \tilde{e}s J_a - (\tilde{s}) J_a (\bar{\epsilon}) J_a \right) + P^3_{J_b} \left( \tilde{e}s J_b - (\tilde{s}) J_b (\bar{\epsilon}) J_b \right) \right)}{P^3_{J_a} P^3_{J_b} \left( P^3_{J_a} \left( \tilde{e}^2 J_a - (\tilde{\epsilon}) J_a \right)^2 + P^3_{J_b} \left( \tilde{e}^2 J_b - (\tilde{\epsilon}) J_b \right)^2 \right)} \] (C.36)
or

\[
\frac{B_3^J}{\Gamma^J} = \frac{P_{Ja}^3 \left( (\tilde{e}s)_a - (\tilde{s})_a (\tilde{e})_a \right) + P_{Jb}^3 \left( (\tilde{e}s)_b - (\tilde{s})_b (\tilde{e})_b \right)}{P_{Ja}^3 \left( (\tilde{e}^2)_a - ((\tilde{e})_a)^2 \right) + P_{Jb}^3 \left( (\tilde{e}^2)_b - ((\tilde{e})_b)^2 \right)}
\]  

(C.37)

or

\[
\frac{B_3^J}{\Gamma^J} \approx \frac{P_{Ja}^3 \left( (\tilde{e}s)_a - (\tilde{s})_a (\tilde{e})_a \right) + P_{Jb}^3 \left( (\tilde{e}s)_b - (\tilde{s})_b (\tilde{e})_b \right)}{P_{Ja}^3 \left( (\tilde{e}^2)_a - ((\tilde{e})_a)^2 \right) + P_{Jb}^3 \left( (\tilde{e}^2)_b - ((\tilde{e})_b)^2 \right)}
\]  

(C.38)

And in the limit that \( P_{Jb} \gg P_{Ja} \), the above reduces to

\[
\frac{B_3^J}{\Gamma^J} \approx \frac{(\tilde{e}s)_b - (\tilde{s})_b (\tilde{e})_b}{(\tilde{e}^2)_b - ((\tilde{e})_b)^2}
\]  

(C.39)
Appendix D

Evaluation of Perceived Quantities for the Generators of the Motion

D.0.1 General Operator \( \hat{F} \)

In the general equation of motion, a perceived operator \( \hat{F} \) is defined as

\[
(\hat{F})^J = \text{Tr}_J \left[ I_J \otimes \hat{\rho}_J \right] \hat{F} \tag{D.1}
\]

This operator will next be decomposed into a portion that acts on subspace \( J_a \) and a portion that acts on subspace \( J_b \)

\[
(\hat{F})^J = \text{Tr}_J \left[ (I_{J_a} \oplus I_{J_b}) \otimes \hat{\rho}_J \right] \hat{F} \tag{D.2}
\]

or

\[
(\hat{F})^J = \text{Tr}_J \left[ (I_{J_a} \otimes \hat{\rho}_J) \hat{F}_{J_a,j} \right] \oplus \text{Tr}_J \left[ (I_{J_b} \otimes \hat{\rho}_J) \hat{F}_{J_b,j} \right] = (\hat{F})^{J_a} \oplus (\hat{F})^{J_b} \tag{D.3}
\]

Now \( (\hat{F})^{J_a} \) can be broken down further as

\[
(\hat{F})^{J_a} = \text{Tr}_J \left[ (I_{J_a} \otimes \hat{\rho}_J) \hat{F}_{J_a,j} \right] = \text{Tr}_J \left[ (I_{J_a} \otimes (\hat{\rho}_{J_a} \oplus \hat{\rho}_{J_b})) \hat{F}_{J_a,j} \right] \tag{D.4}
\]
or

\[
\hat{F}^J_a = \text{Tr}_{\hat{J}_a} \left[ (\hat{I}_{\hat{J}_a} \otimes \hat{\rho}_{\hat{J}_a}) \hat{F}_{\hat{J}_a \hat{J}_a} \right] + \text{Tr}_{\hat{J}_b} \left[ (\hat{I}_{\hat{J}_a} \otimes \hat{\rho}_{\hat{J}_b}) \hat{F}_{\hat{J}_a \hat{J}_b} \right] \quad (D.5)
\]

and now using the definitions \( \hat{\rho}_{\hat{J}_a(b)} = P_{\hat{J}_a(b)} \hat{\rho}_{\hat{J}_a(b)} = P_{\hat{J}_b(b)} \hat{\rho}_{\hat{J}_b(b)} \)

\[
\hat{F}^J_a = \text{Tr}_{\hat{J}_a} \left[ (\hat{I}_{\hat{J}_a} \otimes (P_{\hat{J}_a} \hat{\rho}_{\hat{J}_a})) \hat{F}_{\hat{J}_a \hat{J}_a} \right] + \text{Tr}_{\hat{J}_b} \left[ (\hat{I}_{\hat{J}_a} \otimes (P_{\hat{J}_b} \hat{\rho}_{\hat{J}_b})) \hat{F}_{\hat{J}_a \hat{J}_b} \right] \quad (D.6)
\]

or

\[
\hat{F}^J_a = P_{\hat{J}_a} \text{Tr}_{\hat{J}_a} \left[ (\hat{I}_{\hat{J}_a} \otimes \hat{\rho}_{\hat{J}_a}) \hat{F}_{\hat{J}_a \hat{J}_a} \right] + P_{\hat{J}_b} \text{Tr}_{\hat{J}_b} \left[ (\hat{I}_{\hat{J}_a} \otimes \hat{\rho}_{\hat{J}_b}) \hat{F}_{\hat{J}_a \hat{J}_b} \right] \quad (D.7)
\]

or

\[
\hat{F}^J_a = P_{\hat{J}_a} (\hat{F}^J_a \hat{J}_a) + P_{\hat{J}_b} (\hat{F}^J_a \hat{J}_b) \quad (D.8)
\]

And an analogous procedure can be done for \( \hat{F}^J_b \) to find

\[
\hat{F}^J_b = P_{\hat{J}_a} (\hat{F}^J_b \hat{J}_a) + P_{\hat{J}_b} (\hat{F}^J_b \hat{J}_b) \quad (D.9)
\]

Therefore

\[
\hat{F}^J = \hat{F}^J_a \oplus \hat{F}^J_b \quad (D.10)
\]

can be reduced to

\[
\hat{F}^J = \left( P_{\hat{J}_a} (\hat{F}^J_a \hat{J}_a) + P_{\hat{J}_b} (\hat{F}^J_a \hat{J}_b) \right) \oplus \left( P_{\hat{J}_a} (\hat{F}^J_b \hat{J}_a) + P_{\hat{J}_b} (\hat{F}^J_b \hat{J}_b) \right) \quad (D.11)
\]
If we again use the assumption that $\hat{F}_{J_a J_b} = \hat{0}_{J_a J_b}$ and that $\hat{F}_{J_b J_a} = \hat{0}_{J_b J_a}$, then the above reduces to

\[
\left(\hat{F}\right)^J = P_{J_a} \left(\hat{F}\right)^{J_a J_a} \oplus P_{J_b} \left(\hat{F}\right)^{J_b J_b} = P_{J_a} \left(\hat{F}\right)^{J_a J_a} \oplus P_{J_b} \left(\hat{F}\right)^{J_b J_b} \tag{D.12}
\]

### D.0.2 Evaluation of $\left(\hat{B} \ln(\hat{\rho})\right)^J$

Following the above process, $\left(\hat{B} \ln(\hat{\rho})\right)^J$ can be evaluated as

\[
\left(\hat{B} \ln(\hat{\rho})\right)^J = P_{J_a} \left(\hat{B} \ln(\hat{\rho})\right)^{J_a J_a} \oplus P_{J_b} \left(\hat{B} \ln(\hat{\rho})\right)^{J_b J_b} \tag{D.13}
\]

where

\[
\left(\hat{B} \ln(\hat{\rho})\right)^{J_a J_a} = \text{Tr}_{J_a} \left[ \left(\hat{I}_{J_a} \otimes \tilde{\rho}_{J_a}\right) \hat{B}_{J_a J_a} \ln(\hat{\rho}_{J_a J_a}) \right] = \text{Tr}_{J_a} \left[ \left(\hat{I}_{J_a} \otimes \tilde{\rho}_{J_a}\right) \hat{B}_{aa} \ln(\hat{\rho}_{aa}) \right] \tag{D.14}
\]

and

\[
\left(\hat{B} \ln(\hat{\rho})\right)^{J_b J_b} = \text{Tr}_{J_b} \left[ \left(\hat{I}_{J_b} \otimes \tilde{\rho}_{J_b}\right) \hat{B}_{J_b J_b} \ln(\hat{\rho}_{J_b J_b}) \right] = \text{Tr}_{J_b} \left[ \left(\hat{I}_{J_b} \otimes \tilde{\rho}_{J_b}\right) \hat{B}_{bb} \ln(\hat{\rho}_{bb}) \right] \tag{D.15}
\]
Chapter D. Evaluation of Perceived Quantities for the Generators of the Motion

D.0.3 Evaluation of \( \left( \hat{I}_{Ja} \hat{J}_a \oplus \hat{0}_{Ja} \hat{J}_b \oplus \hat{0}_{Jb} \hat{J}_a \right)^J \)

\[
\left( \hat{I}_{Ja} \hat{J}_a \oplus \hat{0}_{Ja} \hat{J}_b \oplus \hat{0}_{Jb} \hat{J}_a \right)^J = \left( P_{Ja} \left( \hat{I}_{Ja} \hat{J}_a \oplus \hat{0}_{Ja} \hat{J}_b \oplus \hat{0}_{Jb} \hat{J}_a \right)^J \right) \oplus \left( P_{Ja} \left( \hat{I}_{Ja} \hat{J}_a \oplus \hat{0}_{Ja} \hat{J}_b \oplus \hat{0}_{Jb} \hat{J}_a \right)^J \right)
\]

simplifies to

\[
\left( \hat{I}_{Ja} \hat{J}_a \oplus \hat{0}_{Ja} \hat{J}_b \oplus \hat{0}_{Jb} \hat{J}_a \right)^J = \left( P_{Ja} \hat{I}_{Ja} \oplus P_{Ja} \hat{0}_{Ja} \right) \oplus \left( P_{Ja} \hat{0}_{Ja} + P_{Ja} \hat{0}_{Ja} \right) \quad (D.17)
\]

or

\[
\left( \hat{I}_{Ja} \hat{J}_a \oplus \hat{0}_{Ja} \hat{J}_b \oplus \hat{0}_{Jb} \hat{J}_a \right)^J = P_{Ja} \hat{I}_{Ja} \oplus \hat{0}_{Ja} = P_{Ja} \hat{I}_{Ja} \oplus \hat{0}_{Ja} \quad (D.18)
\]

D.0.4 Evaluation of \( \left( \hat{0}_{Ja} \hat{J}_a \oplus \hat{0}_{Ja} \hat{J}_a \oplus \hat{1}_{Ja} \hat{J}_b \right)^J \)

Following an analagous procedure to the above section, one can find

\[
\left( \hat{0}_{Ja} \hat{J}_a \oplus \hat{0}_{Ja} \hat{J}_a \oplus \hat{1}_{Ja} \hat{J}_b \right)^J = \hat{0}_{Ja} \oplus P_{Ja} \hat{1}_{Ja} = \hat{0}_{Ja} \oplus P_{Ja} \hat{1}_{Ja} \quad (D.19)
\]

D.0.5 Evaluation of \( (H)^J \)

\[
(\tilde{H})^J = \left( P_{Ja} (\tilde{H})^J_a \tilde{J}_a + P_{Ja} (\tilde{H})^J_a \tilde{J}_b \right) \oplus \left( P_{Ja} (\tilde{H})^J_a \tilde{J}_b + P_{Ja} (\tilde{H})^J_a \tilde{J}_b \right) \quad (D.20)
\]

where
\[
\left( \tilde{\hat{H}} \right)_{JaJ_a} = \text{Tr}_{J_a} \left[ (\hat{I}_{J_a} \otimes \tilde{\hat{\rho}}_{\bar{J}_a}) \hat{H}_{JaJ_a} \right] = \text{Tr}_{J_a} \left[ (\hat{I}_{J_a} \otimes \tilde{\hat{\rho}}_{\bar{J}_a}) \hat{H}_{aa} \right] \tag{D.21}
\]

\[
\left( \tilde{\hat{H}} \right)_{J_b\bar{J}_b} = \text{Tr}_{J_b} \left[ (\hat{I}_{J_b} \otimes \tilde{\hat{\rho}}_{\bar{J}_b}) \hat{H}_{J_b\bar{J}_b} \right] = \text{Tr}_{J_b} \left[ (\hat{I}_{J_b} \otimes \tilde{\hat{\rho}}_{\bar{J}_b}) \hat{H}_{ab} \right] \tag{D.22}
\]

\[
\left( \tilde{\hat{H}} \right)_{J_a\bar{J}_a} = \text{Tr}_{J_a} \left[ (\hat{I}_{J_a} \otimes \tilde{\hat{\rho}}_{\bar{J}_a}) \hat{H}_{J_a\bar{J}_a} \right] = \text{Tr}_{J_a} \left[ (\hat{I}_{J_a} \otimes \tilde{\hat{\rho}}_{\bar{J}_a}) \hat{H}_{ba} \right] \tag{D.23}
\]

\[
\left( \tilde{\hat{H}} \right)_{J_b\bar{J}_b} = \text{Tr}_{J_b} \left[ (\hat{I}_{J_b} \otimes \tilde{\hat{\rho}}_{\bar{J}_b}) \hat{H}_{J_b\bar{J}_b} \right] = \text{Tr}_{J_b} \left[ (\hat{I}_{J_b} \otimes \tilde{\hat{\rho}}_{\bar{J}_b}) \hat{H}_{bb} \right] \tag{D.24}
\]

Now if we assume that the Hamiltonian on $\mathcal{H}_{ab}$ is $\hat{H}_{ab} = \hat{0}_{ab}$ and likewise on $\mathcal{H}_{ba}$ that $\hat{H}_{ba} = \hat{0}_{ba}$, then the above reduces to

\[
\left( \hat{H} \right)^J = P_{J_a} \left( \tilde{\hat{H}} \right)_{JaJ_a} \oplus P_{J_b} \left( \tilde{\hat{H}} \right)_{J_b\bar{J}_b} = P_{J_a} \left( \tilde{\hat{H}} \right)_{JaJ_a} \oplus P_{J_b} \left( \tilde{\hat{H}} \right)_{J_b\bar{J}_b} \tag{D.25}
\]
Appendix E

Evaluation of Inner Products of the Perceived Quantities

E.0.1 General Definition of the Inner Product between Two Perceived Quantities

In general, the inner product of two perceived operators \((\hat{F})^J\) and \((\hat{G})^J\) is defined as

\[
(\hat{F}, \hat{G})^J = (\hat{G}, \hat{F})^J = \frac{1}{2} \text{Tr}_J \left| \hat{\rho}_J \right\{ (\hat{F})^J, (\hat{G})^J \} \right\}
\] (E.1)

or

\[
(\hat{F}, \hat{G})^J = \frac{1}{2} \text{Tr}_J \left( |\hat{\rho}_{Ja}| \oplus |\hat{\rho}_{Jb}| \left\{ (\hat{F})^{Ja} \oplus (\hat{F})^{Jb}, (\hat{G})^{Ja} \oplus (\hat{G})^{Jb} \right\} \right) \] (E.2)

or

\[
(\hat{F}, \hat{G})^J = \frac{1}{2} \text{Tr}_{Ja} \left( |\hat{\rho}_{Ja}| \left\{ (\hat{F})^{Ja}, (\hat{G})^{Ja} \right\} \right) + \frac{1}{2} \text{Tr}_{Jb} \left( |\hat{\rho}_{Jb}| \left\{ (\hat{F})^{Jb}, (\hat{G})^{Jb} \right\} \right) \] (E.3)

or
\[
(\hat{F}, \hat{G})^J = \frac{1}{2} \text{Tr}_{J_a} \left( P_{J_a} |\tilde{\rho}_{J_a} \rangle \langle \tilde{\rho}_{J_a} | \left\{ (\hat{F})^J_{J_a}, (\hat{G})^J_{J_a} \right\} \right) + \frac{1}{2} \text{Tr}_{J_b} \left( P_{J_b} |\tilde{\rho}_{J_b} \rangle \langle \tilde{\rho}_{J_b} | \left\{ (\hat{F})^J_{J_b}, (\hat{G})^J_{J_b} \right\} \right)
\]

(E.4)

or

\[
(\hat{F}, \hat{G})^J = \frac{P_{J_a}}{2} \text{Tr}_{J_a} \left( |\tilde{\rho}_{J_a} \rangle \langle \tilde{\rho}_{J_a} | \left\{ (\hat{F})^J_{J_a}, (\hat{G})^J_{J_a} \right\} \right) + \frac{P_{J_b}}{2} \text{Tr}_{J_b} \left( |\tilde{\rho}_{J_b} \rangle \langle \tilde{\rho}_{J_b} | \left\{ (\hat{F})^J_{J_b}, (\hat{G})^J_{J_b} \right\} \right)
\]

(E.5)

Now recalling that in general a perceived operator can be written as

\[
(\hat{F})^J = (\hat{F})^J_{J_a} \oplus (\hat{F})^J_{J_b} =
= \left( P_{J_a} (\hat{F})^J_{J_a} + P_{J_b} (\hat{F})^J_{J_b} \right) \oplus \left( P_{J_a} (\tilde{\rho})^J_{J_a} + P_{J_b} (\tilde{\rho})^J_{J_b} \right)
\]

(E.6)

If we again use the assumption that \( \hat{F}_{J_a J_b} = 0_{J_a J_b} \) and that \( \hat{F}_{J_b J_a} = 0_{J_b J_a} \), then the above reduces to

\[
(\hat{F})^J = P_{J_a} (\hat{F})^J_{J_a} \oplus P_{J_b} (\hat{F})^J_{J_b} = P_{J_a} (\tilde{\rho})^J_{J_a} \oplus P_{J_b} (\tilde{\rho})^J_{J_b}
\]

(E.7)

and the inner product of two perceived operators can be written as

\[
(\hat{F}, \hat{G})^J = \frac{P_{J_a}^3}{2} \text{Tr}_{J_a} \left( |\tilde{\rho}_{J_a} \rangle \langle \tilde{\rho}_{J_a} | \left\{ (\hat{F})^J_{J_a}, (\hat{G})^J_{J_a} \right\} \right) + \frac{P_{J_b}^3}{2} \text{Tr}_{J_b} \left( |\tilde{\rho}_{J_b} \rangle \langle \tilde{\rho}_{J_b} | \left\{ (\hat{F})^J_{J_b}, (\hat{G})^J_{J_b} \right\} \right)
\]

(E.8)
E.0.2 Evaluation of \( (\hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ}, \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ})^J \)

\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ}, \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J = \frac{P^3_{Ja}}{2} \text{Tr}_{Ja} \left( \left| \tilde{\rho}_{Ja} \right| \left\{ \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J, \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J \right\} \right) + \frac{P^3_{Jb}}{2} \text{Tr}_{Jb} \left( \left| \tilde{\rho}_{Jb} \right| \left\{ \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J, \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J \right\} \right) \quad (E.9)
\]

or

\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ}, \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J = \frac{P^3_{Ja}}{2} \text{Tr}_{Ja} \left( \left| \tilde{\rho}_{Ja} \right| \left\{ \hat{I}_{Ja}, \hat{I}_{Ja} \right\} \right) + \frac{P^3_{Jb}}{2} \text{Tr}_{Jb} \left( \left| \tilde{\rho}_{Jb} \right| \left\{ \hat{0}_{Ja}, \hat{0}_{Ja} \right\} \right) \quad (E.10)
\]

or

\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ}, \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J = P^3_{Ja} \quad (E.11)
\]

E.0.3 Evaluation of \( (\hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb}, \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb})^J \)

Following a procedure analagous to the above, we see that

\[
\left( \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb}, \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb} \right)^J = P^3_{Jb} \quad (E.12)
\]
E.0.4 Evaluation of \( \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} , \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb} \right)^J \) and
\[
\left( \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb} , \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J
\]
\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} , \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb} \right)^J = \left( \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb} , \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J = 0 \quad (E.13)
\]

E.0.5 Evaluation of \( \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} , \hat{H} \right)^J \)

\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} , \hat{H} \right)^J = \frac{P^3_{Ja}}{2} \text{Tr}_{Ja} \left( \left| \tilde{\rho}_{Ja} \right| \left\{ \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J_{Ja} , \left( \hat{H} \right)^J_{Ja} \right\} \right)
\]
\[
+ \frac{P^3_{Jb}}{2} \text{Tr}_{Jb} \left( \left| \tilde{\rho}_{Jb} \right| \left\{ \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^J_{Jb} , \left( \hat{H} \right)^J_{Jb} \right\} \right) \quad (E.14)
\]
or

\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} , \hat{H} \right)^J = \frac{P^3_{Ja}}{2} \text{Tr}_{Ja} \left( \left| \tilde{\rho}_{Ja} \right| \left\{ \left( \hat{I}_{aa} \right)^J_{Ja} , \left( \hat{H} \right)^J_{Ja} \right\} \right)
\]
\[
+ \frac{P^3_{Jb}}{2} \text{Tr}_{Jb} \left( \left| \tilde{\rho}_{Jb} \right| \left\{ \hat{0}_{Jb} , \left( \hat{H} \right)^J_{Jb} \right\} \right) \quad (E.15)
\]
or

\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} , \hat{H} \right)^J = P^3_{Ja} \text{Tr}_{Ja} \left( \left| \tilde{\rho}_{Ja} \right| \left( \hat{H} \right)^J_{Ja} \right) + 0 \quad (E.16)
\]
or

\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} , \hat{H} \right)^J = P^3_{Ja} \left( \hat{e} \right)^J_{Ja} \quad (E.17)
\]
where

\[
(\tilde{e})^J_a \equiv \text{Tr}_J \left( \left| \tilde{\rho}_J \right| (\tilde{H})^{J_a J_a} \right)
\]  
(E.18)

**E.0.6 Evaluation of** \( \left( \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb}, \hat{H} \right)^J \)

Following an analogous procedure to the above section, we can find that

\[
\left( \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{I}_{bb}, \hat{H} \right)^J = P_{J_b}^3 (\tilde{e})^J_b
\]  
(E.19)

where

\[
(\tilde{e})^J_b \equiv \text{Tr}_{J_b} \left( \left| \tilde{\rho}_{J_b} \right| (\tilde{H})^{J_b J_b} \right)
\]  
(E.20)

**E.0.7 Evaluation of** \( \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ}, \hat{B} \ln(\hat{\rho}) \right)^J \)

\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ}, \hat{B} \ln(\hat{\rho}) \right)^J = \frac{P_{J_a}^3}{2} \text{Tr}_{J_a} \left( \left| \tilde{\rho}_{J_a} \right| \left\{ \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^{J_a J_a}, \left( \hat{B} \ln(\hat{\rho}) \right)^{J_a J_a} \right\} \right)
\]  
\[+ \frac{P_{J_b}^3}{2} \text{Tr}_{J_b} \left( \left| \tilde{\rho}_{J_b} \right| \left\{ \left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ} \right)^{J_b J_b}, \left( \hat{B} \ln(\hat{\rho}) \right)^{J_b J_b} \right\} \right)
\]  
(E.21)

or

\[
\left( \hat{I}_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ}, \hat{B} \ln(\hat{\rho}) \right)^J = \frac{P_{J_a}^3}{2} \text{Tr}_{J_a} \left( \left| \tilde{\rho}_{J_a} \right| \left\{ \hat{I}_{J_a}, \left( \hat{B} \ln(\hat{\rho}) \right)^{J_a J_a} \right\} \right)
\]  
\[+ \frac{P_{J_b}^3}{2} \text{Tr}_{J_b} \left( \left| \tilde{\rho}_{J_b} \right| \left\{ \hat{0}_{J_b}, \left( \hat{B} \ln(\hat{\rho}) \right)^{J_b J_b} \right\} \right)
\]  
(E.22)
or

\[
\left( I_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ}, \hat{B} \ln(\hat{\rho}) \right)^J = P_{Ja}^3 \text{Tr}_{Ja} \left( \left| \tilde{\rho}_{Ja} \right| \left( \hat{B} \ln(\hat{\rho}) \right)^{JaJ_a} \right) + 0 \tag{E.23}
\]

or

\[
\left( I_{aa} \oplus \hat{0}_{ab} \oplus \hat{0}_{bJ}, \hat{B} \ln(\hat{\rho}) \right)^J = P_{Ja}^3 (\tilde{s})^{Ja} \tag{E.24}
\]

where

\[
(\tilde{s})^{Ja} \equiv \text{Tr}_{Ja} \left( \left| \tilde{\rho}_{Ja} \right| \left( \hat{B} \ln(\hat{\rho}) \right)^{JaJ_a} \right) \tag{E.25}
\]

E.0.8 Evaluation of \( \left( \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{1}_{bb}, \hat{B} \ln(\hat{\rho}) \right)^J \)

Following an analogous procedure to the above section, we can find that

\[
\left( \hat{0}_{aJ} \oplus \hat{0}_{ba} \oplus \hat{1}_{bb}, \hat{B} \ln(\hat{\rho}) \right)^J = P_{Ja}^3 (\tilde{s})^{Ja} \tag{E.26}
\]

where

\[
(\tilde{s})^{Ja} \equiv \text{Tr}_{Ja} \left( \left| \tilde{\rho}_{Ja} \right| \left( \hat{B} \ln(\hat{\rho}) \right)^{JaJ_a} \right) \tag{E.27}
\]

E.0.9 Evaluation of \( \left( \hat{H}, \hat{B} \ln(\hat{\rho}) \right)^J \)

\[
\left( \hat{H}, \hat{B} \ln(\hat{\rho}) \right)^J = \frac{P_{Ja}^3}{2} \text{Tr}_{Ja} \left( \left| \tilde{\rho}_{Ja} \right| \left\{ \left( \hat{H} \right)^{JaJ_a}, \left( \hat{B} \ln(\hat{\rho}) \right)^{JaJ_a} \right\} \right) \tag{E.28}
\]

or
\[ \left( \hat{H}, \hat{B} \ln(\hat{\rho}) \right)^J = P_{Ja}^3 (\tilde{e} s)^Ja + P_{Jb}^3 (\tilde{e} s)^Jb \] (E.29)

where

\[ (\tilde{e} s)^Ja = \frac{1}{2} \text{Tr} J_a \left( |\tilde{\rho}_{Ja}| \left\{ \left( \tilde{H} \right)^{Ja}, \left( \hat{B} \ln(\hat{\rho}) \right)^{JaJa} \right\} \right) \] (E.30)

and

\[ (\tilde{e} s)^Jb = \frac{1}{2} \text{Tr} J_b \left( |\tilde{\rho}_{Jb}| \left\{ \left( \tilde{H} \right)^{Jb}, \left( \hat{B} \ln(\hat{\rho}) \right)^{JbJb} \right\} \right) \] (E.31)

\textbf{E.0.10 Evaluation of} \( (\hat{H}, \tilde{H})^J \)

\[ (\hat{H}, \tilde{H})^J = \frac{P_{Ja}^3}{2} \text{Tr} J_a \left( |\tilde{\rho}_{Ja}| \left\{ \left( \tilde{H} \right)^{Ja}, \left( \tilde{H} \right)^{JaJa} \right\} \right) + \frac{P_{Jb}^3}{2} \text{Tr} J_b \left( |\tilde{\rho}_{Jb}| \left\{ \left( \tilde{H} \right)^{Jb}, \left( \tilde{H} \right)^{JbJb} \right\} \right) \] (E.32)

or

\[ (\hat{H}, \tilde{H})^J = P_{Ja}^3 (\tilde{e}^2)^Ja + P_{Jb}^3 (\tilde{e}^2)^Jb \] (E.33)

where

\[ (\tilde{e}^2)^Ja = \frac{1}{2} \text{Tr} J_a \left( |\tilde{\rho}_{Ja}| \left\{ \left( \tilde{H} \right)^{Ja}, \left( \tilde{H} \right)^{JaJa} \right\} \right) \] (E.34)

and
\[ (\tilde{e}^2)^{J_b} = \frac{1}{2} \text{Tr}_{J_b} \left( |\tilde{\rho}_{J_b}| \left\{ (\tilde{H})^{J_b J_b}, (\hat{H})^{J_b J_b} \right\} \right) \] (E.35)
Bibliography


