



UNIVERSITY OF CRETE

MASTER THESIS

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**Quantum-State Transfer Protocols and Robustness of  
Quantum Networks, in the Presence of Noise and  
Imperfections**

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# Contents



# Abstract

The ability to faithfully transmit quantum states from one place to another over short or long distances, depending on the task, is fundamental for quantum computing. In this thesis we study the performance of a transition of a single excitation in the presence of disorder, both diagonal and off-diagonal with respect to the mean fidelity  $\bar{F}$  and the input state fidelity  $F_\psi$ . Specifically we use the two most promising quantum communication protocols, the spin coupling protocol  $J_n = J_0 \sqrt{n(N-n)}$  and the optimal protocol (i.e. boundary controlled)  $J_1 = J_N = \alpha J, J_i = J, i = 2, \dots, N-1$ . It is shown that the two models are approximately equivalent and that the mean fidelity, typically employed in literature, can considerably overestimate or underestimate the performance of the protocol.



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# Chapter 1

## Introduction

Quantum computation promises great advantages over classical computers in solving some problems, such as simulating quantum systems, factorizing large numbers, and searching unsorted databases. Moreover quantum computers introduce new tasks that have no classical counterparts like quantum cryptography. Also the theory of quantum networks has proved that single-qubit gates and two-qubit gates are universal for quantum computation. Over the last decade a new idea has emerged, the transfer of quantum states from one location to another as a fundamental part to the construction of a practical quantum computer. As it is obvious the computational strength of a quantum computer increases with the number of qubits interacting with each other, but many physical interactions between qubits are short range, and therefore only act on nearest-neighbours. The basic idea of state transfer is to construct communication protocols that will allow distant qubits to interact by transporting their states. Of course the transfer will occur in an environment with several physical and technical obstacles like decoherence, quantum fluctuations and manufactural errors.

The purpose of this thesis is to study the act of state transfer in the presence of such an environment with the assumption that the characteristic time scales of dissipation and decoherence are much larger than the time of state transfer. Indeed this is a necessary condition for any further developments in the framework of quantum information processing, as in the opposite case, quantum information would never survive. Many state transfer protocols have been presented over the last decade and here we focus on the two most

promising ones i.e. the spin coupling protocol [?, ?] and the optimal protocol [?]. Our task is to study the performance of the protocols in the presence of static disorder, which is inevitable in any physical realization. This thesis is motivated by the work of Zwick et al [?] and Nikolopoulos [?]. Zwick et al compared the two models in the presence of off-diagonal disorder only and in the basis of the mean fidelity. Later on Nikolopoulos showed that the mean fidelity tends to overestimate the performance protocols, leading to faulty conclusions. He thus suggested alternative, more reliable measures for the quantification of the state transfer. In this thesis we compare the performance of the two above mentioned.

In chapter 2 and in the first half of the chapter 3 we introduce the reader to the theoretical background. Specifically we begin with some quantum mechanics tools which could be useful for an undergraduate reader, we continue with the definition of qubits and the construction of logical gates, but we do not analyse quantum algorithms and other fields of quantum computation due to the fact that they are a special subject by themselves. Next we proceed with the definition of a tool called fidelity and with some properties of spin chains. Finally we close this chapter with some properties of entropy. Although some of the subjects we refer to are not directly related to the work of this thesis, they are a necessary part of the whole theoretical framework of quantum state transfer. In the second half of chapter 3 we recapitulate the existing results and in chapter 4 we present our new results that make the comparison of the two protocols conclusive. Finally we close with some physical implementations for quantum computing in chapter 5.

# Chapter 2

## Theoretical Background

### 2.1 Basics of Quantum Mechanics

#### 2.1.1 Vector Spaces

**Definition** : (Norms and Normed spaces) Let  $\mathcal{X}$  be a vector space over the field  $\mathbb{C}$  of complex scalars. Then  $\mathcal{X}$  is a normed linear space if for every  $f \in \mathcal{X}$  there is a real number  $\|f\|$ , called the norm of  $f$ , such that:

- a)  $\|f\| \geq 0$
- b)  $\|f\| = 0$  iff  $f = 0$
- c)  $\|cf\| = |c|\|f\|$
- d)  $\|f + g\| \leq \|f\| + \|g\|$

**Definition** : (Convergent and Cauchy sequences). Let  $\mathcal{X}$  be a normed space, and let  $\{f_n\}_{n \in \mathbb{N}}$  be a sequence of elements of  $\mathcal{X}$ .

*convergent sequences*:  $\{f_n\}_{n \in \mathbb{N}}$  converges to  $f \in \mathcal{X}$  if

$$\lim_{n \rightarrow \infty} \|f_n - f\| = 0, \quad (2.1.1)$$

i.e., if

$$\forall \epsilon > 0, \exists N > 0, \forall n \geq N \quad (2.1.2)$$

$$\|f_n - f\| < \epsilon.$$

*Cauchy sequences:*  $\{f_n\}_{n \in \mathbb{N}}$  is Cauchy if

$$\begin{aligned} \forall \epsilon > 0 \quad , \quad \exists N > 0 \quad , \quad \forall n, m \geq N \\ \|f_m - f_n\| < \epsilon. \end{aligned} \tag{2.1.3}$$

**Definition**(Banach Space): A normed linear space  $\mathcal{X}$  which does have the property that all Cauchy sequences are convergent is said to be complete. A complete normed linear space is called a *Banach space*.

**Definition** (*inner products*): Let  $\mathcal{H}$  be a vector space. Then  $\mathcal{H}$  is an inner product space if for every  $f, g \in \mathcal{X}$  there exists a complex number  $\langle f, g \rangle$  called the inner product of  $f$  and  $g$ , such that:

- a)  $\langle f, f \rangle \in \mathbb{R}$  and  $\langle f, f \rangle \geq 0$
- b)  $\langle f, f \rangle = 0$  iff  $f = 0$
- c)  $\langle f, g \rangle = \langle g, f \rangle^*$
- d)  $\langle af_1 + bf_2, g \rangle = a\langle f_1, g \rangle + b\langle f_2, g \rangle$

Each inner product determines a norm by the formula  $\|f\| = \langle f, f \rangle^{1/2}$ . Hence every inner product space is a normed linear space. The *Cauchy-Schwarz* inequality states that  $|\langle f, g \rangle| \leq \|f\| \|g\|$ .

If an inner product space  $\mathcal{H}$  is complete, then it is called a Hilbert space. In other words, a Hilbert space is a Banach space whose norm is determined by an inner product( a 2-norm).

## 2.1.2 Operators of Quantum Mechanics

Suppose that we have two vector spaces  $V$  and  $W$ . An operator  $\mathcal{A}$  is a function  $\mathcal{A} : V \rightarrow W$

$$\mathcal{A}|\psi\rangle = |\phi\rangle. \tag{2.1.4}$$

A linear operator satisfies the following relation

$$\mathcal{A}(c_1|\psi_1\rangle + c_2|\psi_2\rangle) = c_1\mathcal{A}|\psi_1\rangle + c_2\mathcal{A}|\psi_2\rangle. \quad (2.1.5)$$

For a linear operator  $\mathcal{A}$ , one can always find a matrix representation. Again assume that we have an operator  $\mathcal{A} \rightarrow W$  and  $\{|u_i\rangle\}, \{|w_i\rangle\}$  is a basis of  $V$  and  $W$  respectively. The matrix representation of  $\mathcal{A}$ ,  $\mathcal{A}_{ij}$  is defined through the following relation

$$\mathcal{A}|u_j\rangle = \sum_i \mathcal{A}_{ij}|w_i\rangle. \quad (2.1.6)$$

Another property of operators is that although for operators, additivity and associativity holds, in general they do not commute/anticommute

$$[\mathcal{A}, \mathcal{B}] = \mathcal{A}\mathcal{B} - \mathcal{B}\mathcal{A} \neq 0. \quad (2.1.7)$$

$$\{\mathcal{A}, \mathcal{B}\} = \mathcal{A}\mathcal{B} + \mathcal{B}\mathcal{A} \neq 0. \quad (2.1.8)$$

The principle of non-commutation is a fundamental property of quantum mechanics as stated in the uncertainty principle.

**Theorem**(Uncertainty Principle): Let  $\mathcal{A}, \mathcal{B}$  be two arbitrary operators with commutator  $[\mathcal{A}, \mathcal{B}]$  and standard deviations  $\sigma_{\mathcal{A}} = \sqrt{\langle \mathcal{A}^2 \rangle - \langle \mathcal{A} \rangle^2}$ ,  $\sigma_{\mathcal{B}} = \sqrt{\langle \mathcal{B}^2 \rangle - \langle \mathcal{B} \rangle^2}$ . It holds that

$$\sigma_{\mathcal{A}}\sigma_{\mathcal{B}} \geq \frac{1}{2}|\langle [\mathcal{A}, \mathcal{B}] \rangle|. \quad (2.1.9)$$

An important class of operators are self-adjoint or Hermitian operators, as observables are described by them. The adjoint of an operator  $\mathcal{A}$  which acts on a vector space  $V$  is an operator denoted by  $\mathcal{A}^\dagger$  acting on the dual space  $V^*$  with the property

$$\langle (\mathcal{A}^\dagger\psi)|\phi\rangle = \langle \psi|(\mathcal{A}\phi)\rangle \quad , \quad \forall |\phi\rangle, |\psi\rangle. \quad (2.1.10)$$

A self-adjoint operator is an operator such that  $\mathcal{A}$  and  $\mathcal{A}^\dagger$  operate on the same domain and with the property

$$\langle \phi|\mathcal{A}|\psi\rangle = \langle \psi|\mathcal{A}|\phi\rangle^*. \quad (2.1.11)$$

From the characteristic polynomial  $\det(\mathcal{A} - I\lambda) = 0$  we can find the eigenvalues of an operator  $\mathcal{A}$  and from the equation  $\mathcal{A}|\psi_n\rangle = \lambda_n|\psi_n\rangle$  its corresponding eigenvectors. Specifically for a self-adjoint operator we have the following properties:

- 1) All eigenvalues of a hermitian operator  $\mathcal{A}$  are real
- 2) If  $|\psi_i\rangle$  and  $|\psi_j\rangle$  are eigenvectors of a hermitian operator  $\mathcal{A}$  with respective  $a_i$  and  $a_j$ , which are not equal, then the two eigenvectors are orthogonal to each other  $\langle\psi_i|\psi_j\rangle = 0$
- 3) The eigenvectors of a hermitian operator  $\mathcal{A}$  form a complete basis.
- 4) If two hermitian operators  $\mathcal{A}, \mathcal{B}$  are commutable, they can be diagonalized simultaneously and thus they share the same set of eigenvectors.

Apart from the hermitian operators another useful type of operators are the unitary operators  $\mathcal{U}$  which satisfy the identity

$$\mathcal{U}\mathcal{U}^\dagger = \mathcal{U}^\dagger\mathcal{U} = I \Rightarrow \mathcal{U}^\dagger = \mathcal{U}^{-1} \quad (2.1.12)$$

In general one can also define functions of operators  $f(\mathcal{A})$  defined through Taylor series. Hence assuming that the Taylor series exists for the function  $f$  we define  $f(\mathcal{A})$  as

$$f(\mathcal{A}) \equiv \sum_{n=0}^{\infty} \frac{f^{(n)}(0)}{n!} \mathcal{A}^n. \quad (2.1.13)$$

The exponential function of the operator  $\mathcal{A} + \mathcal{B}$  leads us to the Baker-Hausdorff relation

$$e^{\mathcal{A}+\mathcal{B}} = e^{\mathcal{A}}e^{\mathcal{B}}e^{-\frac{1}{2}[\mathcal{A},\mathcal{B}]}, \quad (2.1.14)$$

which holds if  $[\mathcal{A}, [\mathcal{A}, \mathcal{B}]] = [\mathcal{B}, [\mathcal{A}, \mathcal{B}]] = 0$ .

Operators can be expanded in their eigenvectors basis. For example assume that a linear operator  $\mathcal{A}$  has a discrete spectrum of eigenvalues  $a_n, n = 0, 1, 2, \dots$  and a continuous part of  $a \in [a_{min}, a_{max}]$ . Hence  $\mathcal{A}$  is written as

$$\mathcal{A} = \sum_n a_n |a_n\rangle\langle a_n| + \int_{a_{min}}^{a_{max}} a |a\rangle\langle a| \quad (2.1.15)$$

and any vector  $|\phi\rangle$  can be decomposed as

$$|\phi\rangle = \sum_n |a_n\rangle \langle a_n | \phi \rangle + \int_{a_{min}}^{a_{max}} |a\rangle \langle a | \phi \rangle. \quad (2.1.16)$$

The spectrum of an operator  $\mathcal{A}$  is the set of all  $\zeta \in \mathbb{C}$  for which the resolvent operator  $R(\zeta, \mathcal{A}) = (\zeta I - \mathcal{A})^{-1}$  does not exist and is denoted as  $\sigma(\mathcal{A})$ . The complementary space is called the resolvent set and is denoted by  $\rho(\mathcal{A}) = \mathbb{C} \setminus \sigma(\mathcal{A})$ .

### 2.1.3 Tensor Products

The tensor product is a way of putting vector spaces together to form larger vector spaces. This construction is crucial to understanding the quantum mechanics of multiparticle systems. Assume that we have two vector spaces  $V$  and  $W$  of dimension  $m$  and  $n$  respectively. The  $V \otimes W$  is a  $nm$  dimensional space. The elements of  $V \otimes W$  are linear combinations of  $|u\rangle \otimes |w\rangle$ , where  $|u\rangle$  belongs to  $V$  and  $|w\rangle$  to  $W$ . Alternatively we can use the notation  $|u\rangle \otimes |w\rangle = |u, W\rangle$

By definition the tensor product satisfies the following properties

1) Assume  $|u\rangle \in V$  and  $|w\rangle \in W$  for an arbitrary scalar  $s$  we have

$$s(|u\rangle \otimes |w\rangle) = (s|u\rangle) \otimes |w\rangle = |u\rangle \otimes (s|w\rangle) \quad (2.1.17)$$

2) For arbitrary  $|u_1\rangle, |u_2\rangle \in V$  and  $|w\rangle \in W$  it holds that

$$(|u_1\rangle + |u_2\rangle) \otimes |w\rangle = |u_1\rangle \otimes |w\rangle + |u_2\rangle \otimes |w\rangle \quad (2.1.18)$$

Same relation holds for  $|u\rangle \in V$  and  $|w_1\rangle, |w_2\rangle \in W$

Furthermore assume that we have the linear operators  $\mathcal{A}, \mathcal{B}$  which act on  $V$  and  $W$  respectively. Then we define the tensor product of the operators  $\mathcal{A} \otimes \mathcal{B}$  by the following relation

$$(\mathcal{A} \otimes \mathcal{B})(|u\rangle \otimes |w\rangle) \equiv (\mathcal{A}|u\rangle) \otimes (\mathcal{B}|w\rangle). \quad (2.1.19)$$

Obviously due to the linearity of the tensor product the same relation is generalized for a linear combination of elements on  $V \otimes W$

$$(\mathcal{A} \otimes \mathcal{B})(\sum_i s_i |u_i\rangle \otimes |w_i\rangle) \equiv \sum_i s_i \mathcal{A}|u_i\rangle \otimes \mathcal{B}|w_i\rangle. \quad (2.1.20)$$

Furthermore one can easily define the inner product between elements of  $V \otimes W$ . Assume that  $U$  and  $W$  are inner product spaces, then we define the inner product as

$$\left( \sum_i a_i |u_i\rangle \otimes |w_i\rangle, \sum_j b_j |u'_j\rangle \otimes |w'_j\rangle \right) \equiv \sum_{i,j} a_i^* b_j \langle u_i | u'_j \rangle \langle w_i | w'_j \rangle. \quad (2.1.21)$$

Finally assume that the operators  $\mathcal{A}, \mathcal{B}$  can be represented as matrices of dimension  $n \times m, p \times q$  respectively. Then the matrix representation of the tensor product  $\mathcal{A} \otimes \mathcal{B}$  called Kronecker product is

$$A \otimes B \equiv \begin{pmatrix} A_{11}B & A_{12}B & \dots & A_{1n}B \\ A_{21}B & A_{22}B & \dots & A_{2n}B \\ \vdots & \vdots & \vdots & \vdots \\ A_{m1}B & A_{m2}B & \dots & A_{mn}B \end{pmatrix} \quad (2.1.22)$$

We close this section with an important theorem, The Schimidt decomposition.

**Theorem**(Schmidt Decomposition): Let  $\mathcal{U}$  and  $\mathcal{V}$  be vector spaces of dimensions  $n$  and  $m$  respectively (assume  $n \geq m$ ). For any vector  $v$  in the product space  $\mathcal{U} \otimes \mathcal{V}$ , there exist orthonormal sets  $\{u_1, \dots, u_n\} \subset \mathcal{U}$  and  $\{w_1, \dots, w_m\} \subset \mathcal{V}$  such that:

$$v = \sum_{i=1}^m s_i u_i \otimes w_i, \quad (2.1.23)$$

where  $s_i \geq 0$  and are uniquely determined by  $v$ .

**proof**

Suppose we have the orthonormal bases  $\{e_1, \dots, e_n\} \subset \mathcal{U}$  and  $\{f_1, \dots, f_m\} \subset \mathcal{V}$ . Any vector  $v$  in the product space  $\mathcal{U} \otimes \mathcal{V}$  can be written in the form

$$v = \sum_{i=1}^m a_{ij} u_i \otimes w_i, \quad (2.1.24)$$

where  $a_{ij}$  is the matrix element of the  $e_i f_j^T$ .

By the singular value decomposition theorem the matrix B can be written as

$$B = USW^T, \quad (2.1.25)$$

where U,W unitary and S a positive semidefinite diagonal matrix. If we let  $\{u_1, \dots, u_n$  and  $\{w_1, \dots, w_n\}$  and  $s_1, \dots, s_m$  the diagonal elements of S. we can rewrite matrix B as

$$B = \sum_{i=1}^m s_i u_i w_i^T. \quad (2.1.26)$$

Finally v can be rewritten as

$$v = \sum_{i=1}^m s_i u_i \otimes w_i \quad (2.1.27)$$

□

## 2.1.4 Pure and Mixed States

When the state of a quantum system can be represented by a linear superposition of basis vectors  $|n\rangle$ ,  $|\Psi\rangle = \sum_n c_n |n\rangle$  the system is said to be in a *pure state*. The density operator  $\rho$  for the system in a pure state is defined as

$$\rho = |\Psi\rangle\langle\Psi|. \quad (2.1.28)$$

Which can be rewritten as

$$\rho = \sum_n \sum_m c_n c_m^* |n\rangle\langle m| = \sum_{n,m} \rho_{nm} |n\rangle\langle m|. \quad (2.1.29)$$

Note that the diagonal matrix elements  $\rho_{nn}$  are called populations and denote the probability of finding the system in the state  $|n\rangle$ . The off-diagonal matrix elements are called coherences because they depend on the relative phase of  $c_n, c_m$ . In equilibrium we are concerned only with  $\rho_{nn}$  since equilibrium in statistical mechanics means complete loss of phase information. In quantum information the coherence is absolutely necessary, since decoherence means loss of the quantum information.

The density operator for the pure state has the following properties

- $Tr(\rho) = 1$
- $\rho^2 = \rho$

Let us assume now that individual systems have been mixed in such a way that they are inseparable. If the system is in a mixture of states  $|\Psi\rangle$ , not necessarily orthogonal to each other, with probabilities  $P_\Psi$  the density operator is then defined as

$$\rho = \sum_{\Psi} P_{\Psi} |\Psi\rangle \langle \Psi|. \quad (2.1.30)$$

Similarly with the pure state it holds that  $Tr(\rho) = 1$ . However  $\rho^2 \neq \rho$  and therefore this is a "diagnostic" tool to find out under a specific density operator whether or not it describes a pure state.

#### 2.1.4a Expectation value of an operator

When the system is described by a density matrix  $\rho$  the expectation value of an operator  $\mathcal{A}$  is

$$\begin{aligned} \langle \mathcal{A} \rangle &= Tr(\rho \mathcal{A}) = \sum_n (\rho \mathcal{A})_{nn} = \sum_{n,m} \rho_{nm}^{\Psi} \mathcal{A}_{mn} \\ &= \sum_{\Psi} \sum_{nm} P_{\Psi} \rho_{nm}^{\Psi} \mathcal{A}_{mn} = \sum_{\Psi} P_{\Psi} \langle \Psi | \mathcal{A} | \Psi \rangle. \end{aligned} \quad (2.1.31)$$

Furthermore if we rewrite our result in terms of the eigenvectors of the operator  $\mathcal{A}$   $|a_i\rangle$  we have that the probability for obtaining the result  $a_i$  in a single measurement is given by

$$P(a_i) = Tr(\rho \Pi_i), \quad (2.1.32)$$

where  $\Pi_i \equiv |a_i\rangle \langle a_i|$  and denotes the corresponding projection operator.

Let us examine now what happens for compound systems. Assume that we have the Hilbert space  $H$  which it is represented by the density operator  $\rho$ . Moreover assume that  $|n^A\rangle \in H_A$ ,  $|n^B\rangle \in H_B$  where  $H_A, H_B$  are the corresponding Hilbert spaces for the systems A,B respectively. For an operator  $\mathcal{A}$  which acts on  $H$  the expectation value is

$$\begin{aligned}
\langle \mathcal{A} \rangle &= Tr(\rho \mathcal{A}) = \sum_{n^A} \sum_{n^B} \langle n^A | \otimes \langle n^B | \rho \mathcal{A} | n^A \rangle \otimes | n^B \rangle & (2.1.33) \\
&= \sum_{n^A, m^A} \sum_{n^B, m^B} \langle n^A n^B | \rho | m^A m^B \rangle \langle m^A m^B | \mathcal{A} | n^A n^B \rangle,
\end{aligned}$$

where  $|AB\rangle \equiv |A\rangle \otimes |B\rangle$ . Obviously if we assume that the operator  $\mathcal{A}$  acts only on the subsystem A we get a full simplification of the above equation

$$\langle \mathcal{A} \rangle = Tr(\rho \mathcal{A}) = \sum_{n^A, m^A} \langle n^A | \rho^A | m^A \rangle \langle m^A | \mathcal{A} | n^A \rangle = Tr(\rho^A \mathcal{A}), \quad (2.1.34)$$

where

$$\rho^A = \sum_{n^B} \langle n^B | \rho | n^B \rangle = Tr_B(\rho) \quad (2.1.35)$$

is called the reduced density operator of system A, obtained by taking the trace with partial respect to system B.

### 2.1.4b Reduced Density Operator

Consider a compound system A+B each with a Hilbert space  $H_A, H_B$  is in a pure state  $|\Phi\rangle \in H_A \otimes H_B$  and therefore its density operator is  $\rho = |\Phi\rangle\langle\Phi|$ . The reduced density operator of system A is

$$\rho^A = \sum_{n^B} \langle n^B | \Phi \rangle \langle \Phi | n^B \rangle = \sum_{n^B} P_{n^B} |\Psi_{n^B}^A\rangle \langle \Psi_{n^B}^A|, \quad (2.1.36)$$

where the probabilities  $P_{n^B}$  are given by

$$P_{n^B} = |\langle n^B | \Phi \rangle|^2 \quad (2.1.37)$$

and the normalized state vector of system A are defined through

$$|\Psi_{n^B}^A\rangle = \frac{1}{\sqrt{P_{n^B}}} \sum_{n^A} |n^A\rangle \langle n^A n^B | \Phi \rangle. \quad (2.1.38)$$

Clearly  $|\Psi_{n^B}^A\rangle$  and the corresponding probabilities  $P_{n^B}$  depend on the particular basis  $\{|n^B\rangle\}$  we have used for tracing over the degrees of freedom of system B. Furthermore note that if the two systems A,B are uncorrelated

the total state is factorized as  $|\Phi\rangle = |\Psi^A\rangle \otimes |\Psi^B\rangle$  and therefore the reduced density operator of system A is

$$\rho^A = |\Psi^A\rangle\langle\Psi^A|. \quad (2.1.39)$$

If state of the compound system does not admit factorization into a product of states of its subsystems,  $|\Phi\rangle \neq |\Psi^A\rangle \otimes |\Psi^B\rangle$  is called an *entangled state*. However using the Schmidt decomposition (??) we can expand a pure state  $|\Phi\rangle$  of a compound state as

$$|\Phi\rangle = \sum_i s_i |\psi_i^A\rangle \otimes |\psi_i^B\rangle, \quad (2.1.40)$$

where  $\{|\psi_i^A\rangle\}$  and  $\{|\psi_i^B\rangle\}$  are orthonormal bases of system A and B respectively.

In this basis the reduced density operator for system A is diagonal,

$$\rho^A = \sum_i p_i |\psi_i^A\rangle\langle\psi_i^A| \quad , \quad p_i = s_i^2. \quad (2.1.41)$$

## 2.1.5 Time Evolution

One of the postulates of quantum mechanics is that the time evolution of a physical system is governed by the Schrödinger equation

$$i\hbar \frac{\partial |\Psi(t)\rangle}{\partial t} = \mathcal{H} |\Psi(t)\rangle. \quad (2.1.42)$$

For an isolated system  $\mathcal{H} = \mathcal{H}^0$  we can expand our wavefunction  $|\Psi\rangle$  in terms of the energy eigenvectors  $|E_n\rangle$  of  $\mathcal{H}^0$

$$|\Psi\rangle = \sum_n c_n(t) |E_n\rangle. \quad (2.1.43)$$

Solving the differential equation for  $c_n(t)$  we find that

$$|\Psi\rangle = \sum_n c_n(0) e^{-i\omega_n t} |E_n\rangle \quad , \quad \omega_n = E_n/\hbar. \quad (2.1.44)$$

Consider now the case where the Hamiltonian is time dependent and of the form  $\mathcal{H} = \mathcal{H}^0 + \mathcal{V}(t)$ . If we expand the system in the basis of the time-independent Hamiltonian  $\mathcal{H}^0$ .

$$|\Psi(t)\rangle = \sum_n c_n(t)|E_n\rangle = \sum_n \tilde{c}_n(t)e^{-i\omega_n t}|E_n\rangle. \quad (2.1.45)$$

The Schrödinger equation for the  $\tilde{c}$  coefficients gives

$$\frac{\partial \tilde{c}_n(t)}{\partial t} = \frac{1}{i\hbar} \sum_m \tilde{\mathcal{V}}_{nm} \tilde{c}_m(t) \quad , \quad \tilde{\mathcal{V}}_{nm} \equiv e^{i\omega_{nm}t} \langle E_n | \mathcal{V}(t) | E_m \rangle, \quad (2.1.46)$$

where  $\omega_{nm} = \omega_n - \omega_m$ . These equations govern the time evolution of the systems in the so-called interaction picture, in which the rapid oscillations of the coefficients of the state vector expansion in terms of the energy eigenstates  $|E_n\rangle$  were removed via the transformation

$$|\tilde{\Psi}\rangle = e^{\frac{i}{\hbar}\mathcal{H}^0 t} |\Psi(t)\rangle = \sum_n \tilde{c}_n(t) |E_n\rangle. \quad (2.1.47)$$

The Schrödinger equation (??) for  $|\tilde{\Psi}(t)\rangle$  then reads

$$i\hbar \frac{\partial |\tilde{\Psi}(t)\rangle}{\partial t} = \tilde{\mathcal{V}}(t) |\tilde{\Psi}(t)\rangle \quad , \quad \tilde{\mathcal{V}}(t) \equiv e^{\frac{i}{\hbar}\mathcal{H}^0 t} \mathcal{V}(t) e^{-\frac{i}{\hbar}\mathcal{H}^0 t} \quad (2.1.48)$$

For a system that does not offer an analytic solution to the problem one can use perturbation theory via the time evolution operator in the interaction picture  $\tilde{U}(t) = \mathcal{T} e^{-\frac{i}{\hbar} \tilde{\mathcal{V}} t}$ . The solution is then given by the Dyson series

$$\tilde{U}(t, t_0) = \sum_{n=0}^{\infty} \left(-\frac{i}{\hbar}\right)^n \int_{t_0}^t dt_1 \dots \int_{t_0}^{t_{n-1}} dt_n \tilde{\mathcal{V}}(t_1) \tilde{\mathcal{V}}(t_2) \dots \tilde{\mathcal{V}}(t_n). \quad (2.1.49)$$

Now consider that our system is described by the density operator  $\rho$ . The equation governing the time evolution of the system is the Liouville equation

$$i\hbar \frac{\partial \rho}{\partial t} = [\mathcal{H}, \rho]. \quad (2.1.50)$$

In the interaction picture

$$i\hbar \frac{\partial \tilde{\rho}}{\partial t} = [\tilde{\mathcal{V}}, \tilde{\rho}] \quad (2.1.51)$$

and for the matrix elements of  $\rho$

$$i\hbar \frac{\partial \tilde{\rho}_{nm}}{\partial t} = \sum_k [\tilde{\mathcal{V}}_{nk} \tilde{\rho}_{km} - \tilde{\rho}_{nk} \tilde{\mathcal{V}}_{km}]. \quad (2.1.52)$$

## 2.1.6 Qubits and Logical Gates

### 2.1.6a One Qubit

Suppose that we are dealing with a quantum machine with simply two configurations for each cell. Such a setup is called a qubit<sup>1</sup>. Mathematically qubit can be defined as

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle, \quad (2.1.53)$$

where  $\alpha, \beta \in \mathbb{C}$ .

It is convenient to set  $\alpha = \cos(\frac{\theta}{2})$ ,  $\beta = e^{i\phi} \sin(\frac{\theta}{2})$ , where  $0 \leq \theta \leq \pi$  and  $0 \leq \phi \leq 2\pi$ . This transform maps all of the single qubit states onto the surface of a sphere, i.e. we can interpret  $\theta$  as the azimuthal angle and  $\phi$  as the zenth angle in spherical polar coordinates. This sphere is called the Bloch sphere.

A confusing thing about the Bloch sphere is that single qubit states which are orthogonal are not orthogonal vectors on the Bloch sphere. For instance  $|0\rangle$  and  $|1\rangle$  but are represented on the Bloch sphere as  $\theta = 0$  and  $\theta = \pi$ . Another point which often confuses people is that at the abstract level of qubits, the directions on the Bloch sphere have no "physical" meaning. This is due to the fact that qubits can be any two level system. However often we will have to compare qubits and therefore relative phase i.e. directions on Bloch sphere will play a significant role. Moreover note that the qubit position on the Bloch sphere is expressed as

$$\vec{q} = (\cos \phi \sin \theta, \sin \phi \sin \theta, \cos \theta) \quad (2.1.54)$$

Having defined qubits it is convenient to define the fundamental transforms of qubits, the Pauli operators. The Pauli operators are the four operators

$$\sigma_0 = I = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \sigma_x = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \sigma_y = \begin{pmatrix} 0 & i \\ -i & 0 \end{pmatrix}, \quad \sigma_3 = \sigma_z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \quad (2.1.55)$$

The Pauli operators satisfy the following commutation relations

$$[\sigma_i, \sigma_j] = \epsilon_{abc} \delta_{ij} \sigma_j \quad (2.1.56)$$

---

<sup>1</sup>The word "qubit" was first used in the scientific literature by Ben Schumacher

and the following anticommutation relations

$$\{\sigma_i, \sigma_j\} = 0. \quad (2.1.57)$$

Hence we can rewrite a qubit state as a matrix element of SU(2)

$$M_q = \vec{q} \cdot \vec{\sigma} = \begin{pmatrix} \cos(\theta) & e^{-i\phi} \sin(\theta) \\ e^{i\phi} \sin(\theta) & -\cos(\theta) \end{pmatrix} \quad (2.1.58)$$

A general rotation of a qubit about axis  $\hat{n} = (n_x, n_y, n_z)$ , is built using the following unitary matrix

$$U_{\hat{n}}(\theta) = e^{-i\frac{\theta}{2}\hat{n}\cdot\vec{\sigma}} = \cos\left(\frac{\theta}{2}\right)I - i \sin\left(\frac{\theta}{2}\right)(\hat{n} \cdot \vec{\sigma}). \quad (2.1.59)$$

Now a qubit rotation by angle  $\theta$  about the arbitrary axis  $\hat{n}$  is expressed as the similarity transformation

$$M_{q'} = U_{\hat{n}}(\theta)M_qU_{\hat{n}}^\dagger(\theta) = U_{\hat{n}}(\theta)M_qU_{\hat{n}}(-\theta), \quad (2.1.60)$$

since it can be easily shown that  $U_{\hat{n}}^\dagger(\theta) = U_{\hat{n}}(-\theta)$

Analysing the above relation we obtain an equation for the qubit state SO(3) element  $\vec{q}$  rotated by angle an  $\theta$

$$\vec{q}' = \cos \theta \vec{q} + (1 - \cos \theta) \hat{n}(\hat{n} \cdot \vec{q}) + \sin \theta \hat{n} \times \vec{q} \quad (2.1.61)$$

or in component form this is written as

$$q'_i = R_{ij}(\theta)q_j, \quad (2.1.62)$$

where  $R_{ij}$  is a rotation matrix of the SO(3) group.

The careful reader could discover an ambiguity between the SO(3) representation and the SU(2) representation of the qubit state. If we rotate our system by  $2\pi$   $R(2\pi) = I$  but the SU(2) matrix element  $U(2\pi) = -I$ . So if we have a physical object where rotation in three dimensional space corresponds to our rotation of the Bloch sphere, we find that when we rotate the object by  $2\pi$  the qubit state acquires a global phase of -1. These types of objects we call them spinors. Mathematically this happens because the function

$\Phi : SU(2) \rightarrow SO(3)$  is a double cover, or two-to-one , surjective homomorphism.

In the language of quantum information the unitary transformations are called logical gates. It is useful to introduce them with the help of the quantum circuit notation. The quantum circuit notation is a useful way to denote a set of actions that we apply to our quantum system. In the quantum circuit diagrams, time runs from left to right. a qubit is denoted by single line.

$$\alpha|0\rangle + |\beta\rangle \text{ —————} \quad (2.1.63)$$

the Walsh-Hadamard transform  $H$  is defined by

$$H|k\rangle \equiv \frac{1}{\sqrt{2}}(|0\rangle + (-1)^k|1\rangle) \quad (2.1.64)$$

or in matrix form as

$$H = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{2}} \\ \frac{1}{\sqrt{2}} & -\frac{1}{\sqrt{2}} \end{pmatrix} \quad (2.1.65)$$

As an example consider a qubit initialized in the  $|0\rangle$  state the application of the Hadamard transform is sketched as follows

$$|0\rangle \text{ —————} \boxed{H} \text{ —————} \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) \quad (2.1.66)$$

All gates are represented by a box and all qubit states by a straight line. Other logical gates are the unity transform  $I$ , the Pauli matrices operations (??)  $X = \sigma_x, Y = \sigma_y, Z = \sigma_z$ , the NOT operation  $U_{NOT}$  and the Phase operation  $U_{Phase}$

$$U_{NOT} \equiv |0\rangle\langle 1| + |1\rangle\langle 0| \quad (2.1.67)$$

$$U_{Phase} \equiv |0\rangle\langle 0| + i|1\rangle\langle 1| \quad (2.1.68)$$

### 2.1.6b Two Qubits

The general state of a two qubit system is given by the quantum state

$$|\psi\rangle = \alpha_{00}|00\rangle + \alpha_{10}|10\rangle + \alpha_{01}|01\rangle + \alpha_{11}|11\rangle, \quad (2.1.69)$$

where  $\alpha_{ij} \in \mathbb{C}$  and  $|\alpha_{00}|^2 + |\alpha_{10}|^2 + |\alpha_{01}|^2 + |\alpha_{11}|^2 = 1$

When we have two qubits, we should think that we have two separate physical systems, each with a two level system. If we perform a unitary transformation  $U$  on only one of these physical subsystems, then the unitary we are implementing is of the form  $U \otimes I_2$  or  $I_2 \otimes U$  depending on which subsystem the transformation acts. In general one can act to the two qubits simultaneously, but with a process that does not couple the two qubits and our unitaries will be of the form  $U \otimes V$ . Finally we can consider transformations that allow the two qubits to interact quantum mechanically, then we are able to enact unitaries which cannot be expressed in the form  $U \otimes V$ . An example of such a unitary, and one which is of some significance is the controlled-NOT operation,

$$U_{CNOT} \equiv |0\rangle\langle 0| \otimes I_2 + |1\rangle\langle 1| \otimes U_{NOT}. \quad (2.1.70)$$

In quantum circuit notation is

$$U_{NOT} = \begin{array}{c} \text{---} \bullet \text{---} \\ | \\ \text{---} \oplus \text{---} \end{array} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (2.1.71)$$

Since the controlled-NOT cannot be written as an action on either of these qubits along, we write it as a two qubit gate: a gate with two quantum wires input and two quantum wires output. This should be contrasted with an evolution like  $U \otimes V$  which we denote in quantum circuit notation by

$$U \otimes V = \begin{array}{c} \text{---} \boxed{U} \text{---} \\ \text{---} \boxed{V} \text{---} \end{array} = \begin{pmatrix} U_{00}V_{00} & U_{00}V_{01} & U_{01}V_{00} & U_{01}V_{01} \\ U_{00}V_{10} & U_{00}V_{11} & U_{01}V_{10} & U_{01}V_{11} \\ U_{10}V_{00} & U_{10}V_{01} & U_{11}V_{00} & U_{11}V_{01} \\ U_{10}V_{10} & U_{10}V_{11} & U_{11}V_{10} & U_{11}V_{11} \end{pmatrix} \quad (2.1.72)$$

Within the class of two qubit states, an important distinction to make is between states that can be expressed as separate single qubit wave functions  $|\phi\rangle \otimes |\psi\rangle$ ,  $|\phi\rangle = \alpha|0\rangle + \beta|1\rangle$  and  $|\psi\rangle = \gamma|0\rangle + \delta|1\rangle$ , and those who cannot be expressed like this. The first are called *separable states* and the latter are

called *entangled states*. the most elegant way to show whether or not a two qubit state is separable is by the Schmidt decomposition as explained in a previous section.

## 2.1.7 Quantum Fidelity

Before the definition of the fidelity let us define a mathematical tool, the Schatten norm.

### Definition:

For any operator  $\mathcal{A} \in L(\mathcal{H}_1, \mathcal{H}_2)$ <sup>2</sup> and any real number  $p \geq 1$ , one defines the *Schatten p-norm* of  $\mathcal{A}$  as:

$$\|\mathcal{A}\|_p \equiv [Tr((\mathcal{A}^\dagger \mathcal{A}))]^{1/p}. \quad (2.1.73)$$

We also define

$$\|\mathcal{A}\|_\infty = \max\{\|\mathcal{A}u\| : u \in \mathcal{H}_1, \|u\|=1\}. \quad (2.1.74)$$

The "distance" measure for two states  $|\psi\rangle$  and  $|\phi\rangle$  is just  $F = \langle \psi | \phi \rangle$ . Suppose that we want to measure the "distance" between a pure state  $|\psi\rangle$  and a mixed state with density operator  $\rho$ . The simplest way would be an inner product of the operator with the pure state. Hence

$$F = \langle \psi | \rho | \psi \rangle. \quad (2.1.75)$$

With the physical examples in mind and the definition of Schatten p-norm we could generalize fidelity for two general density operators  $\rho, \sigma$  as a Schatten 1-norm

Given two positive semidefinite operators (or specifically for density operators)  $\rho, \sigma \in Pos(\mathcal{H})$  we define Fidelity as :

$$F(\rho, \sigma) \equiv \|\sqrt{\rho}\sqrt{\sigma}\|_1^2 \quad (2.1.76)$$

or equivalently

$$F(\rho, \sigma) \equiv \left[ Tr \sqrt{\sqrt{\rho}\sigma\sqrt{\rho}} \right]^2. \quad (2.1.77)$$

---

<sup>2</sup> $L(\mathcal{H}_1, \mathcal{H}_2)$  is the space of all linear, bounded operators such that  $\mathcal{A} : \mathcal{H}_1 \rightarrow \mathcal{H}_2$

Note the similarity with classical fidelity which is defined as

$$F(\{p_i\}, \{q_i\}) = \left[ \sum_{i=1}^N \sqrt{p_i q_i} \right]^2, \quad (2.1.78)$$

where  $\{p_i\}, \{q_i\}$  with  $i=1,2,\dots,N$  are probability distributions.

Note that if we choose two density operators that are simultaneously diagonalizable  $\rho = \sum_i r_i |i\rangle\langle i|$  and  $\sigma = \sum_i s_i |i\rangle\langle i|$ , we obtain the classical fidelity.

### 2.1.7a Basic Properties of Quantum Fidelity

The properties of Fidelity are a subject of research in Mathematics. Here we present the most useful properties of fidelity based on [?, ?]

- **Bounds of Fidelity**

Fidelity takes the bounds

$$0 \leq F(\rho, \sigma) \leq 1, \quad (2.1.79)$$

where  $F(\rho, \sigma) = 1$  iff  $\rho = \sigma$  and  $F(\rho, \sigma) = 0$  iff  $\text{supp}(\rho) \perp \text{supp}(\sigma)$ .

- **Symmetry**

$$F(\rho, \sigma) = F(\sigma, \rho). \quad (2.1.80)$$

- **unitary invariance**

$$F(\rho, \sigma) = F(U\rho U^\dagger, U\sigma U^\dagger), \quad (2.1.81)$$

where U are unitary operators

- **Concavity**

$$F(\rho, \alpha\rho_1 + (1 - \alpha)\rho_2) \geq \alpha F(\rho, \rho_1) + (1 - \alpha)F(\rho, \rho_2), \quad (2.1.82)$$

for  $\alpha \in [0, 1]$ .

- **multiplicativity**

Let  $\rho_1, \rho_3 \in Pos(\mathcal{H}_1)$  and  $\rho_2, \rho_4 \in Pos(\mathcal{H}_2)$  it holds that

$$F(\rho \otimes \rho_2, \rho_3 \otimes \rho_4) = F(\rho_1, \rho_3)F(\rho_2, \rho_4). \quad (2.1.83)$$

• **Uhlmann's Theorem**

Let  $\mathcal{H}_1$  and  $\mathcal{H}_2$  be complex Euclidean spaces and  $\rho, \sigma \in Pos(\mathcal{H}_1)$  be semidefinite operators, both having at most rank equal to  $dim(\mathcal{H}_2)$ , and let  $|\psi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2$ , be any purification of  $\rho$ . It holds that[?]

$$F(\rho, \sigma) = \{max|\langle\psi|\phi\rangle|^2 : |\phi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2, Tr_{\mathcal{Y}}(|\phi\rangle\langle\phi|) = \sigma\} \quad (2.1.84)$$

**proof:**

Since the rank of  $\rho, \sigma$  is at most  $dim(\mathcal{H}_2)$  there exists operators  $P, Q \in \mathbb{L}(\mathcal{H}_1, \mathcal{H}_2)$  for which  $P^\dagger P = \Pi_\rho$  and  $Q^\dagger Q = \Pi_\sigma$ . The equations

$$Tr_{\mathcal{H}_1}(vec(\sqrt{\rho}P^\dagger)vec(\sqrt{\rho}P^\dagger)^\dagger) = \rho \quad (2.1.85)$$

$$Tr_{\mathcal{H}_1}(vec(\sqrt{\sigma}Q^\dagger)vec(\sqrt{\sigma}Q^\dagger)^\dagger) = \sigma \quad (2.1.86)$$

Therefore  $vec(\sqrt{\rho}P^\dagger)$  and  $vec(\sqrt{\sigma}Q^\dagger)$  are purifications of  $\rho, \sigma$ , respectively.

Note that we found some specific purifications, but not "all of them". But of course we can reproduce the others using Unitary transformations. Therefore

$$|\Psi\rangle = (\mathbb{I}_{\mathcal{H}_1} \otimes U)vec(\sqrt{\rho_1}P) = vec(\sqrt{\rho_1}PU^T) \quad (2.1.87)$$

$$|\Phi\rangle = (\mathbb{I}_{\mathcal{H}_1} \otimes V)vec(\sqrt{\rho_2}Q) = vec(\sqrt{\rho_2}QV^T) \quad (2.1.88)$$

for some unitary operators  $U, V \in U(\mathcal{H}_2)$

Hence the maximization of the statement becomes

$$max|\langle(vec(\sqrt{\rho_1}PU^T), vec(\sqrt{\rho_2}QV^T))\rangle| = max|\langle U^T \bar{V} P \sqrt{\rho_1}, \sqrt{\rho_2} Q^\dagger \rangle| \quad (2.1.89)$$

Since max run over all unitary operators we can choose the above equation to be  $\| P\sqrt{\rho}\sqrt{\sigma}Q^\dagger \|$ .

Finally using the fact that P,Q have a spectra of at most 1 we get

$$\| \sqrt{\rho}\sqrt{\sigma} \| = \| P^\dagger P \sqrt{\rho}\sqrt{\sigma}Q^\dagger Q \| \leq \| \sqrt{\rho}\sqrt{\sigma} \|, \quad (2.1.90)$$

and thus the equality holds.

Finally we get

$$\| P\sqrt{\rho}\sqrt{\sigma}Q^\dagger \| = F(\rho, \sigma). \quad (2.1.91)$$

□

• **generalization of concavity**

Let  $\rho_1, \dots, \rho_n$  and  $\sigma_1, \dots, \sigma_n \in Pos(\mathcal{H}_1)$  be positive semidefinite operators, it holds that

$$F\left(\sum_{i=1}^n \rho_i, \sum_{i=1}^n \sigma_i\right) \geq \sum_{i=1}^n F(\rho_i, \sigma_i). \quad (2.1.92)$$

**proof:**

Let  $\mathcal{H}_2$  be a Hilbert space of dimension at least of  $Pos(\mathcal{H}_1)$  and choose  $|\psi_1\rangle, \dots, |\psi_n\rangle, |\phi_1\rangle, \dots, |\phi_n\rangle \in \mathcal{X} \otimes \mathcal{Y}$  satisfying  $Tr(|\psi_i\rangle\langle\psi_i|) = \rho_i$  and  $Tr(|\phi_i\rangle\langle\phi_i|) = \sigma_i$  and also  $\langle\psi_i|\phi_i\rangle = F(\rho_i, \sigma_i)$  for each  $i=1, \dots, n$ . Such vectors always exist by Uhlmann's theorem.

Suppose we define  $|\Psi\rangle, |\Phi\rangle \in \mathcal{H}_1 \otimes \mathcal{H}_2 \otimes \mathbb{C}^n$

$$|\Psi\rangle = \sum_{i=1}^n |\psi_i\rangle \otimes e_i, \quad |\Phi\rangle = \sum_{i=1}^n |\phi_i\rangle \otimes e_i. \quad (2.1.93)$$

Taking the Trace over  $\mathcal{H}_2 \otimes \mathbb{C}^n$  we get

$$Tr_{\mathcal{H}_2 \otimes \mathbb{C}^n}(|\Psi\rangle\langle\Psi|) = \sum_{i=1}^n \rho_i, \quad Tr_{\mathcal{H}_2 \otimes \mathbb{C}^n}(|\Phi\rangle\langle\Phi|) = \sum_{i=1}^n \sigma_i. \quad (2.1.94)$$

Using again the Uhlmann's theorem we get

$$F\left(\sum_{i=1}^n \rho_i, \sum_{i=1}^n \sigma_i\right) \geq |\langle\Psi|\Phi\rangle| = \sum_{i=1}^n F(\rho_i, \sigma_i). \quad (2.1.95)$$

□

## 2.2 Entropy In Quantum Information

### 2.2.1 Shannon Entropy

Consider an ensemble  $X$  of letters  $\{x_1, x_2, \dots, x_n\}$  occurring with probabilities  $p(x_i)$ . This ensemble is our source, from which messages of  $N$  letters are drawn. We are concerned with messages of very large  $N$ . For such messages, we know that typical sequences of letters will contain  $Np(x_i)$  of letter  $x_i$ ,  $Np(x_j)$  of  $x_j$  and so on. The number of distinct typical sequences of letters is then given by

$$M = \frac{N!}{(Np(x_1))!(Np(x_2))!\dots(Np(x_n))!} \quad (2.2.1)$$

since  $N \rightarrow \infty$  we can use the stirling approximation  $\ln(n!) = n \ln n - n$

Therefore  $M = 2^{NH(X)}$ , where  $H(X)$  is the Shannon entropy for the ensemble  $X$ . With this example we have shown how the Shannon entropy arises naturally from a typical information problem

**Definition** (Shannon Entropy): Suppose we have an ensemble  $X = \{x, p(x)\}$ , where  $x$  describes the possible values  $\{x_1, \dots, x_n\}$  and  $p(x)$  is the probability distribution function. The Shannon entropy is defined as

$$H(X) \equiv - \sum_x p(x) \log_2(p(x)) \quad (2.2.2)$$

The Shannon entropy  $H(X)$  quantifies how much information is conveyed, on the average, by a "letter" drawn from the ensemble  $X$ , for it tells us how many bits (the minimum of bits) are required (asymptotically as  $N \rightarrow \infty$ , where  $N$  is the number of letters drawn) to encode that information.

**Definition**(Joint Entropy): Suppose we have the ensembles  $X = \{x, p(x)\}$  and  $Y = \{y, p(y)\}$  the joint entropy is defined as

$$H(X, Y) \equiv - \sum_{x,y} p(x, y) \log_2 p(x, y) \quad (2.2.3)$$

The joint entropy measures our total uncertainty about the pair  $(X, Y)$ . Suppose we know the value of  $Y$ , so we have acquired  $H(Y)$  bits of information about the pair,  $(X, Y)$ . The remaining uncertainty about the pair  $(X, Y)$ ,

is associated with our remaining lack of knowledge about X, even given that we know Y.

Furthermore we can define the entropy of X if we know Y as  $H(X|Y) \equiv H(X, Y) - H(Y) = \langle -\log_2(\frac{p(x|y)}{p(y)}) \rangle$  (*conditional entropy*)

**Definition**(Mutual Information): Suppose we have the ensembles  $X = \{x, p(x)\}$  and  $Y = \{y, p(y)\}$  the mutual information is defined as

$$I(X, Y) \equiv H(X) - H(X|Y) = H(Y) - H(Y|X) = \langle \log_2(\frac{p(x, y)}{p(x)p(y)}) \rangle \quad (2.2.4)$$

The mutual information  $I(X, Y)$  quantifies how correlated two messages are or in other words, how much can we learn about the message Y if we know the message X. In the case of bits  $I(X, Y)$  quantifies the number of additional bits per letter needed to specify both x and y if y is known

Finally note that if  $p(y|x)$  describes a noisy channel the mutual information describes the amount of information per letter that can be transmitted through the channel.

### 2.2.1a Basic Properties of Shannon Entropy

:

- $H(X) \geq 0$
- (Maximum-Minimum value)  $H(X) \in [0, \log_2 N]$ , where N is the number of different realizations
- $H(X, Y) = H(Y, X)$
- $H(Y|X) \geq 0$  equality holds iff  $Y=f(X)$

- *subadditivity*:  $H(X, Y) \leq H(X) + H(Y)$  equality holds iff  $X, Y$  are independent random variables
- $H(Y|X) \leq H(Y)$
- *strong subadditivity*  $H(X_1, X_2, \dots, X_n) \leq \sum_{i=1}^n H(X_i)$ , equality holds iff the variables are independent
- $H(X|Y, Z) \leq H(X|Y)$

### 2.2.1b An Example of Data Compression

:

Suppose that Alice is a sender and Bob is a receiver. Suppose further that a noiseless bit channel connects Alice to Bob. Bob receives "0" if Alice transmits "0" and Bob receives "1" if Alice transmits "1". Alice would like to use the noiseless channel to communicate information to Bob. Suppose that an information source randomly chooses from four symbols  $\{a, b, c, d\}$  and selects them with a skewed probability distribution:

$$\begin{aligned}
 P(a) &= \frac{1}{2} & (2.2.5) \\
 P(b) &= \frac{1}{8} \\
 P(c) &= \frac{1}{4} \\
 P(d) &= \frac{1}{8}
 \end{aligned}$$

Furthermore we assume that the source of information chooses each variable randomly with the above probabilities.

In the first Place Alice encodes the four symbols in the following coding scheme:

$$a \rightarrow 00 \quad , \quad b \rightarrow 01 \quad , \quad c \rightarrow 10 \quad , \quad d \rightarrow 11 \quad (2.2.6)$$

For this coding scheme the expected length is equal to two-bits. On the other hand Alice could also use the following scheme to encode the four symbols

$$a \rightarrow 0 \quad , \quad b \rightarrow 110 \quad , \quad c \rightarrow 10 \quad , \quad d \rightarrow 111 \quad (2.2.7)$$

The above scheme has the advantage that any coded sequence is uniquely decodable. For example, suppose that Bob obtains the following sequence

$$00010110010011110101011 \quad (2.2.8)$$

This message can be considered as a sequence of

$$0 - 0 - 0 - 10 - 11 - 0 - 0 - 10 - 0 - 11 - 110 - 110 - 10 - 10 - 11 \quad (2.2.9)$$

which is equivalent to the following message

$$aaacdaacaabadbbccd \quad (2.2.10)$$

In this coding scheme the expected length is  $7/4$  bits which is shorter than the two bits of the previous encoding scheme. In fact this coding scheme is the optimal since the entropy for this example is

$$H(x) = -P(a) \log_2 P(a) - P(b) \log_2 P(b) - P(c) \log_2 P(c) - P(d) \log_2 P(d) = 7/4 \quad (2.2.11)$$

## 2.2.2 Von Neumann Entropy

**Definition**(Von Neumann Entropy): For a density matrix  $\rho$  the Von Neumann entropy is defined as

$$S(\rho) = -Tr(\rho \log_2 \rho) \quad (2.2.12)$$

equivalently if we diagonalize  $\rho$ ,  $\rho = \sum_k \lambda_k |k\rangle \langle k|$  the Von Neumann entropy is  $S(\rho) = H(K)$  for the ensemble  $K = \{k, \lambda_k\}$

The Interpretation of the Von Neumann entropy is analogous to Shannon entropy but in a quantum context. Suppose that Alice generates a quantum state  $|\psi_Y\rangle$  in her lab according to some probability density  $p_Y(y)$  of a random variable  $Y$ . Suppose further that Bob has not yet received the state from

Alice and does not know which one she sent. The expected density operator from Bob's point of view is then

$$\rho = \sum_y p_Y(y) |\psi_Y\rangle \langle \psi_Y| \quad (2.2.13)$$

The entropy  $S(\rho)$  quantifies Bob's uncertainty about the "message" (state) Alice sent. his expected information gain is  $S(\rho)$  qubits upon receiving and measuring the state that Alice sent. Although Shannon's entropy and Von Neumann entropy seem to have the same interpretation there is a significant quantitative difference. Consider Alice that generates a sequence of  $|\psi_1\rangle \otimes |\psi_2\rangle \otimes \dots \otimes |\psi_n\rangle$  of quantum states according to the following ensemble

$$Y = \{(1/4, |0\rangle), (1/4, |1\rangle), (1/4, |+\rangle), (1/4, |-\rangle)\} \quad (2.2.14)$$

Suppose that Alice and Bob share a perfect classical channel. If she employs Shannon's classical noiseless coding protocol, she should transmit classical data to Bob at a rate of two classical channel uses per source state (the Shannon entropy of the uniform distribution  $n=4$  is two bits)  $|\psi_1\rangle$  in order for him to reliably recover the classical data needed to reproduce the sequence of states that Alice transmitted

for the uniform distribution the density matrix is the maximally entangled

$$\rho = \frac{1}{4} [|0\rangle\langle 0| + |1\rangle\langle 1| + |+\rangle\langle +| + |-\rangle\langle -|] \quad (2.2.15)$$

The calculation of Von Neumann entropy gives  $S(\rho) = 1$  bit Suppose now that Alice and Bob share a noiseless quantum channel between them (this is a channel that can preserve quantum coherence without any interaction with an environment). Then Alice only needs to send qubits at a rate of one channel use per source symbol if she employs a protocol known as Schumacher compression. Bob can then reliably decode the qubits that Alice sent. In general it can be proven that  $H(X) \geq S(\rho_X)$  for any ensemble  $X$  with the equality occurring when the density operator is in diagonal form.

### 2.2.2a Mathematical Properties of Von Neumann Entropy

**Positivity:**  $S(\rho) \geq 0 \forall \rho$  (density operators)

**Minimum Value:** The minimum value of Von Neumann entropy is zero and occurs iff the density operator describes a pure state.

**Maximum Value:** The maximum value of Von Neumann entropy is  $S_{max}(\rho) = \log_2 N$ , where  $N$  is the dimension of the Hilbert space and occurs iff  $\rho = \frac{1}{N} \sum_i |\psi_i\rangle\langle\psi_i|$ , with  $\{\psi_i\}$   $i=1,2,\dots,N$  forming an orthonormal basis

**Concavity:** The entropy is concave in the density operator:

$$S(\rho) \geq \sum_x p_X(x) S(\rho_x) \quad (2.2.16)$$

where  $\rho = \sum_x p_X(x) \rho_x$

**Unitary Invariance:**  $S(\rho) = S(U\rho U^\dagger)$

### 2.2.2b Joint Von Neumann Entropy

**Definition**(Joint Von Neumann Entropy): Suppose we have a composite bipartite system  $A+B$  which can be described by the density operator  $\rho^{AB}$  the Joint Von Neumann entropy is defined as:

$$S(A, B) \equiv -Tr(\rho^{AB} \log_2(\rho^{AB})) \quad (2.2.17)$$

The joint Von Neumann entropy will reveal major differences from the classical definition of entropy. Hence it is crucial to study some properties of the joint entropy

#### pure bipartite system

For two ensembles  $X, Y$  we recall that  $H(X, Y) \geq H(X) + H(Y), \forall X, Y$ . In the quantum world this is not always the case. Consider a bipartite system  $A+B$  which is described by the pure state  $|\psi\rangle^{AB}$ . The Von Neumann entropy for a pure state is zero, therefore

$$S(AB) = 0 \quad (2.2.18)$$

Moreover suppose that we perform a Schmidt decomposition(??) on the pure state of the composite system AB  $|\psi\rangle^{AB}$

$$|\psi\rangle^{AB} = \sum_i s_i |\phi\rangle^A \otimes |\phi\rangle^B \quad (2.2.19)$$

Next we perform a purification on the bipartite state to find the marginal density operators  $\rho^A, \rho^B$

$$\rho^A = Tr_B(|\psi\rangle^{AB} \langle\psi|^{AB}) = \sum_i s_i^2 |\phi\rangle^A \langle\phi|^A \quad (2.2.20)$$

$$\rho^B = Tr_A(|\psi\rangle^{AB} \langle\psi|^{AB}) = \sum_i s_i^2 |\phi\rangle^B \langle\phi|^B \quad (2.2.21)$$

Hence it is obvious that the corresponding Von Neumann entropies will be equal

$$S(A) = S(B) \quad (2.2.22)$$

With this example we reveal a fundamental difference between the classical and the quantum world.

### independent quantum systems

Suppose we have two independent quantum systems  $H_A, H_B$  which are described by the density operators  $\rho, \sigma$ . Then the Von Neumann entropy for the total composite system  $H_A \otimes H_B$  is

$$S(\rho \otimes \sigma) = S(\rho) + S(\sigma) \quad (2.2.23)$$

Let us diagonalize  $\rho$  in the orthonormal basis  $\{|\psi_i\rangle\} \subset H_A$   $i = 1, 2, \dots, N_A$  and  $\sigma$  in the orthonormal basis  $\{|\phi_i\rangle\} \subset H_B$   $i = 1, \dots, N_B$

$$\rho = \sum_{i=1}^{N_A} p_i |\psi_i\rangle \langle\psi_i| \quad (2.2.24)$$

$$\sigma = \sum_{i=1}^{N_B} s_i |\phi_i\rangle \langle\phi_i| \quad (2.2.25)$$

Then the Von Neumann entropy reduces to the Shannon entropy, and thus using the identity  $H(X, Y) = H(X) + H(Y)$  for uncorrelated ensembles we conclude that

$$S(\rho \otimes \sigma) = S(\rho) + S(\sigma) \quad (2.2.26)$$

□

### Joint Von Neumann entropy of a classical-quantum state

Suppose we have two systems a classical  $H_{cl}$  and a quantum system  $H_q$ . The classical system is described by the ensemble  $X = \{p(x)|x\rangle\}$  and a quantum system which is described by a superposition of the density operators  $\rho_x^B$ . The total density operator is described by

$$\rho^{XB} = \sum_x p_X(x)|x\rangle\langle x| \otimes \rho_x^B \quad (2.2.27)$$

the density operators can be written as

$$\rho_x^B = \sum_y p_{Y|X}(y|x)|y_x\rangle\langle y_x| \quad (2.2.28)$$

Then

$$S(XB) = -Tr \left[ \sum_x p_X(x)|x\rangle\langle x| \otimes \rho_x^B \log_2 \left( \sum_x p_X(x)|x\rangle\langle x| \otimes \rho_x^B \right) \right] \quad (2.2.29)$$

expanding in the density operators  $\rho_x^B$

$$S(XB) = -Tr \left[ \sum_x p_X(x)|x\rangle\langle x| \otimes \sum_y p_{Y|X}(y|x')|y_{x'}\rangle\langle y_{x'}| \quad (2.2.30)$$

$$\times \log_2 \left( \sum_{x'} p_X(x')|x'\rangle\langle x'| \otimes \sum_{y'} p_{Y|X}(y'|x')|y'_{x'}\rangle\langle y'_{x'}| \right) \right] \quad (2.2.31)$$

Using the identity  $f(A) = f(\sum_i a_i|i\rangle\langle i|) = \sum_i f(a_i)|i\rangle\langle i|$  we get

$$S(XB) = - \sum_{x,y,x',y'} p_X(x)p_{Y|X}(y|x) \log_2(p_X(x')p_{Y|X}(y'|x')) \quad (2.2.32)$$

$$\times \text{Tr} \left[ |x\rangle\langle x|x'\rangle\langle x'| \otimes |y_x\rangle\langle y_x| \right] \quad (2.2.33)$$

Evaluating the Trace, using the identity  $\text{Tr}(A \otimes B) = \text{Tr}(A)\text{Tr}(B)$  we obtain

$$S(XB) = - \sum_{x,y} p_X(x)p_{Y|X}(y|x) \log_2(p_X(x)p_{Y|X}(y|x)) \quad (2.2.34)$$

$$= H(X) + \sum_x p_X(x)S(\rho_x) \quad (2.2.35)$$

Finally we have shown that the joint entropy of a classical(X)-quantum(B) state is

$$S(XB) = H(X) + \sum_x p_X(x)S(\rho_x) \quad (2.2.36)$$

**Definition**(Conditional Von Neumann Entropy): The conditional Von Neumann entropy  $S(A|B)$  of a bipartite quantum state  $\rho^{AB}$  is defined as

$$S(A|B) = S(AB) - S(B) \quad (2.2.37)$$

One major property of the conditional Von Neumann Entropy is the following theorem

**Theorem**(conditioning does not decrease entropy): suppose we have a quantum bipartite system  $\rho^{AB}$ . Then it holds that

$$S(A) \geq S(A|B) \quad (2.2.38)$$

### Conditional Quantum Entropy for Classical-Quantum States

using the previous result we can calculate the conditional entropy for a quantum-classical system

$$S(B|X) = S(XB) - S(X) \quad (2.2.39)$$

$$= S(X) + \sum_x p_X(x)S(\rho_x) - S(X) \quad (2.2.40)$$

$$= \sum_x p_X(x)S(\rho_x) \quad (2.2.41)$$

Note that another fundamental difference between the classical and quantum definition of entropy is that the conditional quantum entropy can be

negative. For example consider a bipartite system with a state  $|\Phi\rangle^{AB}$  shared by Alice and Bob. Moreover suppose that the source generates random states with equal probability. Therefore the marginal state of Bob is the maximal entangled state  $\rho = \frac{1}{N} \sum_i |i\rangle\langle i|$ . Hence the Joint entropy is zero since the total state is a pure state but the entropy of Bob is equal to since since the  $\log_2 2 = 1$ . Therefore

$$S(A|B) = S(AB) - S(B) = 0 - 1 = -1 \quad (2.2.42)$$

**Definition**(Coherent Information): For a bipartite system AB with the density operator  $\rho^{AB}$  the coherent information is defined as

$$I(A, B) \equiv S(B) - S(AB) \quad (2.2.43)$$

**Theorem:** Suppose that Alice and Bob share a bipartite state  $\rho^{AB}$ . The following bound applies to the absolute value of the conditional entropy  $S(A|B)$ :

$$|S(A|B)| \leq \log_2 N \quad (2.2.44)$$

where N is the dimension of a Hilbert space

**Definition**(Von Neumann mutual Entropy): The quantum mutual information of a bipartite state  $\rho^{AB}$  is as follows:

$$I(A, B) \equiv S(A) + S(B) - S(AB) \quad (2.2.45)$$

**Theorem:** The Von Neumann mutual entropy for a bipartite quantum system  $\rho^{AB}$  is always positive

$$I(A; B) \geq 0 \quad (2.2.46)$$

### 2.2.3 Von Neumann Entropy as a Measurement of Entanglement

Quantifying entanglement is a field of research in its own, since quantifying entanglement in a multipartite system is conceptually a difficult task and the existing proposes are not well defined. In this section we pay attention only to bipartite system due to the fact that the existing measures for entanglement are conceptually well understood.

### 2.2.3a Pure bipartite systems

We have already mentioned that a pure bipartite state  $|\psi_{AB}\rangle$  is entangled if and only if it cannot be written as a tensor product of pure states of the parts, but the question is how can we quantify entanglement and what properties should have a good entanglement measure  $E$ . Obviously 1) the measure  $E$  should be invariant under local unitary operations, 2) it should be a continuous function and 3) it should be additive, when several copies of the system are present:  $E(|\psi_{AB}\rangle \otimes |\phi_{AB}\rangle) = E(|\psi_{AB}\rangle) + E(|\phi_{AB}\rangle)$ . The best candidate that satisfies all three criterion is the von Neumann entropy of the reduced density matrices[?] (??)

$$E(\psi) = S(\rho_A) = S(\rho_B) = - \sum_i s_i^2 \log(s_i^2). \quad (2.2.47)$$

Therefore the answer to the question of how entangled a pure state is, is given by the von Neumann entropy of the reduced density operator. We can simplify this expression by using the concept of concurrence  $\mathcal{C}(\psi)$  [?, ?]

$$E(\psi) = E(\mathcal{C}(\psi)), \quad (2.2.48)$$

where  $\mathcal{C}$  is defined as

$$\mathcal{C}(\psi) = \langle \psi | \tilde{\psi} \rangle, \quad (2.2.49)$$

with  $|\tilde{\psi}\rangle = \sigma_y |\psi\rangle$  (*spin-flip transformation*).

### 2.2.3b Entanglement in mixed states

Let us see how entanglement can be defined for a mixed state. In general there are three important measures of entanglement, the entanglement cost  $E_C$ , the distillable entanglement  $E_B$  and the entanglement of formation  $E_F$ . In this section we will use only the  $E_F$  measure. We have already quantified entanglement for pure states with the use of the Von Neumann entropy, and naively one should expect that it would be the same definition for mixed states which is not true due to the infinite number of possible decompositions of a density matrix. The only thing that we can do is to solve this ambiguity by taking the minimum over all possible decompositions, simply because if there is a decomposition where the average is zero, this state can be created

locally without the need of any entangled pure state. The entanglement of formation of a state  $\rho$  is therefore defined as

$$E_F(\rho) \equiv \min \sum_j p_j S(\rho_{A,j}), \quad (2.2.50)$$

where the minimum is taken over all realizations of the state  $\rho_{AB} = \sum_j p_j |\psi_j\rangle\langle\psi_j|$ .

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^\dagger (\sigma_y \otimes \sigma_y) \quad (2.2.51)$$

For two qubits systems we can find an analytic expression for  $E_F$

$$E_F(\rho) = - \sum_{\sigma=\pm} \frac{\sqrt{1 + \sigma \mathcal{C}^2(\rho)}}{2} \ln \frac{\sqrt{1 + \sigma \mathcal{C}^2(\rho)}}{2} \quad (2.2.52)$$

where  $\mathcal{C}(\rho)$  is a generalization of the concept of concurrence [?] using the spin flip transformation for mixed states

$$\tilde{\rho} = (\sigma_y \otimes \sigma_y) \rho^\dagger (\sigma_y \otimes \sigma_y). \quad (2.2.53)$$

The hermitian matrix  $R \equiv \sqrt{\rho} (\sigma_y \otimes \sigma_y) \rho^\dagger (\sigma_y \otimes \sigma_y) \sqrt{\rho}$  has eigenvalues  $\lambda_1^2 \geq \dots \lambda_4^2$  and concurrence is defined as

$$\mathcal{C}(\rho) \equiv \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\}. \quad (2.2.54)$$

## 2.3 Spin Chain Model

Bulk materials often have a large collection of spins permanently coupled to each other. The mutual interaction of these spins makes them prefer alignment or anti-alignment with respect to each other, resulting in diverse phenomena such as ferromagnetism or anti-ferromagnetism. A spin model is a large class of such materials in which the spins are arranged in a d-dimensional lattice and permanently coupled to each other.

A general Hamiltonian of a d-dimensional spin lattice can be described by

$$\mathcal{H} = \sum_{i,j} [J_{ij}^x S_i^x S_j^x + J_{ij}^y S_i^y S_j^y + J_{ij}^z S_i^z S_j^z] - \sum_i \vec{H}_i \cdot \vec{S}_i, \quad (2.3.1)$$

where the vector  $\vec{J}_{ij}$  is the two body interaction between the lattice points and  $\vec{H}$  a one body parameter. The  $S_i^\alpha$  (??) are the generators of the SU(2) group (Pauli matrices) in the lattice point  $i$  satisfying the following relations

$$[S_i^a, S_j^b] = \epsilon_{abc} \delta_{ij} S_j^c. \quad (2.3.2)$$

Note that for different values of  $\vec{J}$  we get different models of interest.

### 2.3.1 Spin-1/2 models with short range interactions

A model hamiltonian for a set of localized spins interacting[?] with nearest neighbour exchange coupling on a d-dimensional lattice is the XY model

$$\begin{aligned} \mathcal{H} = & \frac{J}{2} \sum_{\langle i,j \rangle} [(1 + \gamma) S_i^x S_j^x + (1 - \gamma) S_i^y S_j^y] \\ & + J\Delta \sum_{\langle i,j \rangle} S_i^z S_j^z - \sum_i h_i S_i^z. \end{aligned} \quad (2.3.3)$$

A positive exchange coupling favours antiferromagnetic ordering in the xy plane. The parameters  $\gamma$  and  $\Delta$  account for the anisotropy in the exchange z-direction.

For d-dimensional spin models with  $d > 1$  it is difficult to find exact solutions. On the contrary for  $d=1$  the model is solvable in several cases.

a)  $\Delta = 0$  *Quantum XY model*

For  $\gamma = 1$  we get the quantum Ising model while the XX model is obtained for  $\gamma = 0$ . In the isotropic case the model possesses an additional symmetry resulting in the conservation<sup>3</sup> of the magnetization  $S^z = \sum_i S_i^z$  along the z-axis or in the language of Quantum Information the number of qubits is conserved.

---

<sup>3</sup>Note that

$$[\mathcal{H}, A] = i\hbar \frac{dA}{dt}, \quad (2.3.4)$$

A very interesting feature of this model is a mapping between the spin chain model and a free spinless fermion model via a procedure called the Jordan-Wigner transformation[?]. specifically the Hamiltonian becomes

$$\mathcal{H} = \sum_{i,j} \left[ c_i^\dagger A_{ij} c_j + \frac{1}{2} (c_i^\dagger B_{ij} c_j^\dagger + h.c) \right] + \frac{1}{2} \sum_i A_{ii}, \quad (2.3.5)$$

with  $c_i$  fermionic operators. The two matrices A,B are defined as  $A_{jk} = \gamma J(\delta_{k,j+1} + \delta_{j,k+1}) - h_z \delta_{j,k}$  and  $B_{jk} = \gamma J(\delta_{k,j+1} - \delta_{j,k+1})$ .

### 2.3.2 Jordan-Wigner Transformation

Let us discuss analytically the Winger-Jordan transformation[?] we introduced previously for the XY model.

Again we consider the XY model

$$\mathcal{H} = \frac{1}{2} \sum_{\langle i,j \rangle} J_{ij} [(1 + \gamma) S_i^x S_j^x + (1 - \gamma) S_i^y S_j^y] - \sum_i h_i S_i^z. \quad (2.3.6)$$

Let us introduce the spin raising and lowering operators

$$S_i^+ = S_i^x + i S_i^y \quad (2.3.7)$$

$$S_i^- = S_i^x - i S_i^y. \quad (2.3.8)$$

These operators obey the algebra:

$$\{S_i^+, S_i^-\} = 1 \quad , \quad \{S_i^+, S_i^+\} = \{S_i^-, S_i^-\} = 0 \quad (2.3.9)$$

$$[S_i^+, S_j^-] = 0 \quad , \quad [S_i^+, S_j^+] = [S_i^-, S_j^-] = 0 \quad , \quad i \neq j. \quad (2.3.10)$$

After this transformation the Hamiltonian becomes:

$$\mathcal{H} = \sum_{\langle i,j \rangle} J_{ij} [(S_i^+ S_j^- + S_i^- S_j^+) + \gamma (S_i^+ S_j^+ + S_i^- S_j^-)] - 2 \sum_i h_i S_i^+ S_j^-. \quad (2.3.11)$$

In fact for many purposes this simple transformation is enough to obtain the equations of motions, but ultimately we search for transformation that

eventually can diagonalize the Hamiltonian (??) and thus solve the problem from a theoretical point of view. Unfortunately this transformation cannot lead us to a diagonalization of the problem at least with linear transformations since the ladder operators don't obey the same commutation relations globally in the lattice. The solution of the problem was given by Jordan and Wigner in 1928 by introducing the following operators.

$$c_k = e^{\pi i \sum_{j=1}^{k-1} S_j^+ S_j^-} S_k^- \quad c_k^\dagger = S_k^+ e^{-\pi i \sum_{j=1}^{k-1} S_j^+ S_j^-}. \quad (2.3.12)$$

We will show explicitly that these operators obey fermionic algebra globally

$$\{c_i^\dagger, c_j\} = \delta_{ij}, \quad \{c_i, c_j\} = \{c_i^\dagger, c_j^\dagger\} = 0 \quad (2.3.13)$$

First we observe that  $[S_i^+ S_i^-, S_j^+ S_j^-] = 0$ . Using the Baker-Campbell-Hausdorff identity  $e^{\mathcal{A}+\mathcal{B}} = e^{\mathcal{A}} e^{\mathcal{B}} e^{-[\mathcal{A}, \mathcal{B}]/2}$  we obtain

$$e^{\pm \pi i \sum_{j=1}^{k-1} S_j^+ S_j^-} = \prod_{j=1}^{k-1} e^{\pm \pi i S_j^+ S_j^-}. \quad (2.3.14)$$

Furthermore it holds that  $(S_i^+ S_i^-)^2 = S_i^+ S_i^-$  and therefore the exponential is fully simplified to

$$e^{\pm \pi i S_j^+ S_j^-} = 1 - 2S_j^+ S_j^-. \quad (2.3.15)$$

Finally observe that  $\{S_i^+, 1 - 2S_i^+ S_i^-\} = \{S_i^-, 1 - 2S_i^+ S_i^-\} = 0$ . With these relations the equal site anticommutator is

$$\{c_i^\dagger, c_i\} = 1, \quad (2.3.16)$$

while for  $j > i$

$$\{c_i^\dagger, c_j\} = S_i^- e^{\pi i \sum_{m=1}^{i-1} S_m^+ S_m^-} S_m^+ S_m^- e^{-\pi i \sum_{m=1}^{j-1} S_m^+ S_m^-} S_j^+ + S_i^+ e^{\pi i \sum_{m=1}^{j-1} S_m^+ S_m^-} e^{-\pi i \sum_{m=1}^{i-1} S_m^+ S_m^-} S_m^+ S_j^- \quad (2.3.17)$$

$$= S_i^+ e^{-\pi i \sum_{m=i}^{j-1} S_m^+ S_m^-} S_j^- + S_j^+ e^{\pi i \sum_{m=i}^{j-1} S_m^+ S_m^-} S_i^- \quad (2.3.18)$$

$$= (S_i^- S_i^+ - S_j^+ S_j^-) e^{\pi i \sum_{m=i}^{j-1} S_m^+ S_m^-} = 0. \quad (2.3.19)$$

Similarly for  $i > j$ . We have shown that the c-operators obey fermionic algebra. The next step is to rewrite our Hamiltonian (??) in term of c.

The inverse transformation is

$$S_j^- = e^{-\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m} c_j \quad S_j^+ = e^{\pi i \sum_{m=1}^{j-1} c_m^\dagger c_m} c_j^\dagger. \quad (2.3.20)$$

By complete analogy with the previous

$$e^{\pm \pi i \sum_{m=1}^{k-1} S_m^+ S_m^-} = \prod_{m=1}^{k-1} e^{\pm \pi i c_m^\dagger c_m} = \prod_{m=1}^{k-1} (1 - 2c_m^\dagger c_m). \quad (2.3.21)$$

Therefore with simple algebra calculations we obtain we obtain that

$$S_i^- S_{i+1}^+ = c_i c_{i+1}^\dagger \quad (2.3.22)$$

$$S_{i+1}^+ S_i^- = c_{i+1}^\dagger c_i. \quad (2.3.23)$$

where the calculation is made only over nearest neighbours.

Similarly for the operators  $S_i^- S_{i+1}^-$  and  $S_{i+1}^+ S_i^+$  we obtain

$$S_i^+ S_{i+1}^+ = c_i^\dagger c_{i+1}^\dagger \quad (2.3.24)$$

$$S_{i+1}^- S_i^- = c_{i+1} c_i. \quad (2.3.25)$$

Note that for this calculations we have used the fact that the operator  $\sum_{m=1}^{i-1} c_m^\dagger c_m$  takes only integer values. In fact the operator  $\mathcal{N} = \sum_{m=1}^N c_m^\dagger c_m$  is the number operator

Rewriting our Hamiltonian (??) in terms of the c-operators we obtain

$$\mathcal{H} = \sum_{i,j} \left[ c_i^\dagger A_{ij} c_j + \frac{1}{2} (c_i^\dagger B_{ij} c_j^\dagger - c_i B_{ij} c_j) \right] + \frac{1}{2} \sum_i A_{ii}. \quad (2.3.26)$$

The two matrices A,B are defined as  $A_{ij} = \gamma J_{ij} (\delta_{i,j+1} + \delta_{i,j-1}) - h_z i \delta_{i,j}$  and  $B_{ij} = \gamma J_{ij} (\delta_{i,j-1} - \delta_{i,j+1})$ .

The final step is to diagonalize this Hamiltonian via a Bogoliubov transformation[?]

$$u_k = \sum_i \left( g_{ki} c_i + h_{ki} c_i^\dagger \right) \quad (2.3.27)$$

$$u_k^\dagger = \sum_i \left( g_{ki} c_i^\dagger + h_{ki} c_i \right). \quad (2.3.28)$$

Using the equation of motion technique  $[\mathcal{H}, u_k^\dagger] = E_k u_k^\dagger$ , where  $E_k$  is the matrix that diagonalizes the Hamiltonian (??) we get

$$\mathbf{A}g_k + \mathbf{B}h_k = E_k g_k \quad (2.3.29)$$

$$\mathbf{B}g_k - \mathbf{A}h_k = E_k h_k. \quad (2.3.30)$$

Letting  $\phi_{ki} = g_{ki} + h_{ki}$  and  $\psi_{ki} = g_{ki} - h_{ki}$

$$(\mathbf{A} + \mathbf{B})\phi_k = E_k \psi_k \quad (2.3.31)$$

$$(\mathbf{A} - \mathbf{B})\psi_k = E_k \phi_k \quad (2.3.32)$$

which implies,

$$(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})\phi_k = E_k^2 \phi_k \quad (2.3.33)$$

$$(\mathbf{A} + \mathbf{B})(\mathbf{A} - \mathbf{B})\psi_k = E_k^2 \psi_k \quad (2.3.34)$$

Moreover if we let  $\psi_k = E_k^{-1}(\mathbf{A} + \mathbf{B})\phi_k$  the only remaining thing to do is to find the eigenvectors  $E_k^2$  and the eigenstates  $\phi_k$  of  $(\mathbf{A} - \mathbf{B})(\mathbf{A} + \mathbf{B})$ . The solution can be found due to translational invariance

$$E_k = (1 - (1 - \gamma^2) \sin^2 k)^{1/2} \quad (2.3.35)$$

$$\phi_{ki} = \sqrt{\frac{2}{N}} \sin(ki), k > 0 \quad \phi_{ki} = \sqrt{\frac{2}{N}} \cos(ki), k < 0 \quad (2.3.36)$$

and thus

$$\psi_{ki} = \frac{1}{E_k} (\cos(k)\phi_{ki} + \sin(k)\phi_{-ki}) \quad (2.3.37)$$

where  $k = \frac{2\pi n}{N}$ ,  $k \in [-\pi, \pi)$ ,

The diagonalized form of the Hamiltonian (??) describes the spectrum of spinless free fermions with energies  $E_k$

$$\mathcal{H} = \sum_k E_k (u_k^\dagger u_k - \frac{1}{2}). \quad (2.3.38)$$

### 2.3.3 Magnetism and Quantum Information correspondence

The ground state of a one-dimensional ferromagnetic spin-1/2 chain is the all-up state

$$|\Psi_G\rangle = |\uparrow\rangle_1 \otimes |\uparrow\rangle_2 \otimes \dots \otimes |\uparrow\rangle_N = |\uparrow\uparrow \dots \uparrow\rangle \quad (2.3.39)$$

where the states  $|\uparrow\rangle_i$  and  $|\downarrow\rangle_i$  are eigenstates of the  $S_i^-, S_i^+$  operators. Without an external magnetic field this state is of course degenerate with the all-down state. An excited state can be created by flipping a single spin,  $S_i^- |\uparrow\uparrow \dots \uparrow\rangle$ . This state breaks translational invariance but by a superposition of such states we restore the symmetry.

$$|\Psi_k\rangle = \sum_{j=1}^N e^{ikj} S_j^- |\uparrow\uparrow \dots \uparrow\rangle \quad , \quad k = \frac{2\pi m}{N}, m = 0, 1, \dots, N-1 \quad (2.3.40)$$

Note that periodic boundary conditions have assumed. This state is called "spin wave" state in magnetism while in quantum information science is called "twisted W state". Since a single spin wave is a stationary space it cannot be used to transmit information. To that end, temporal structure has to be introduced by generating pulses, therefore the inverse Fourier transform may be applied to write  $S_j^- |\uparrow\uparrow \dots \uparrow\rangle$  as a superposition of  $|\Psi_k\rangle$ .

The correspondence between quantum information and magnetism is straightforward, since by thinking the  $|\uparrow\rangle$  and  $|\downarrow\rangle$  in the qubit basis as  $|0\rangle$  and  $|1\rangle$ . Therefore the ground state of a ferromagnet can be considered as  $|\mathbf{0}\rangle = |000\dots 0\rangle$  in the computational basis and the state  $S_j^- |\uparrow\uparrow \dots \uparrow\rangle$  is interpreted as one of the N computational basis states with a single non-zero qubit at site j

$$S_j^- |\uparrow\uparrow \dots \uparrow\rangle \equiv |\mathbf{j}\rangle. \quad (2.3.41)$$



# Chapter 3

## Quantum State Transfer: Introduction and known results

### 3.1 Mathematical Definition of Perfect State Transfer

Perfect action [?] is defined by starting with a single qubit state  $\rho_{qubit}$  on some input mode A, with  $\rho_{in}$  the state of the rest of the many-qubit system, and requiring that after evolution for some time  $t_0$  under a fixed Hamiltonian  $\mathcal{H}$ , the output state

$$e^{-i\mathcal{H}t_0}(\rho_{qubit}^A \otimes \rho_{in})e^{i\mathcal{H}t_0} = \rho_{qubit}^B \otimes \tilde{\rho}_{out} \quad (3.1.1)$$

is produced, thereby transmitting the input qubit state to another site, B.

If the system is in the 1th excitation subspace of Hilbert space, then

$$(\alpha|0\rangle + \beta|1\rangle)_A \otimes |0\rangle^{\otimes(N-1)} \mapsto |\Psi\rangle_{out} \otimes (\alpha|0\rangle + e^{i\phi}\beta|1\rangle)_B. \quad (3.1.2)$$

The evolution of the 1-excitation subspace is described by an  $N \times N$  matrix,  $H$ .

Let us denote the excitation on the  $n$ th qubit of a length,  $N$ , spin chain as

$$|\mathbf{n}\rangle \equiv |0\rangle^{\otimes n-1}|1\rangle|0\rangle^{\otimes(N-n)} \quad (3.1.3)$$

In this basis the Hamiltonian can be expressed as

$$\mathcal{H} = \sum_{n < m} (J_{nm} |\mathbf{n}\rangle\langle\mathbf{m}| + J_{nm}^* |\mathbf{m}\rangle\langle\mathbf{n}|) + \sum_{n=1}^N B_n |\mathbf{n}\rangle\langle\mathbf{n}|. \quad (3.1.4)$$

In a diagonal form,  $\mathcal{H}$  can be written as

$$\mathcal{H} = \sum_{n=1}^N \lambda_n |\lambda_n\rangle \langle \lambda_n|, \quad (3.1.5)$$

where  $\lambda_n$  is an energy eigenvalue and  $|\lambda_n\rangle$  the corresponding eigenvector of  $\mathcal{H}$

### 3.1.1 Conditions for perfect transfer

Let us prove the necessary and sufficient conditions for perfect state transfer in the first excitation Hilbert subspace. Assume that Alice wants to transmit the state of her qubit say  $|A\rangle$  to Bob's qubit  $|B\rangle$  and that we have a transfer time  $\tau_c$  and a transfer phase  $\phi_0$  [?]

$$|\langle A|\lambda_n\rangle| = |\langle B|\lambda_n\rangle|. \quad (3.1.6)$$

For all  $n$ , and on the eigenvalues

$$\lambda_n \tau_c = -\phi_0 - \phi_n + 2\pi f(n) \quad , \quad f : \mathbb{Z} \rightarrow \mathbb{Z}, \quad (3.1.7)$$

where

$$\phi_n = \arg \left( \frac{\langle \lambda_n|B\rangle}{\langle \lambda_n|A\rangle} \right). \quad (3.1.8)$$

From the above equation it can be easily seen that the energy eigenvalues give rise to commensurate energies [?] (energy functions proportional to integers)

$$\lambda_n = [2\pi f(n) + n]\omega + \omega_0 \quad (3.1.9)$$

#### 3.1.1a Proof of necessity

Requiring that there exists a  $\tau_c$  and  $\phi_0$  such that

$$e^{-i\mathcal{H}\tau_c}|A\rangle = e^{i\phi_0}|B\rangle. \quad (3.1.10)$$

By taking the overlap with an eigenvector

$$e^{-i\lambda_n\tau_c}\langle \lambda_n|A\rangle = e^{i\phi_0}\langle \lambda_n|B\rangle. \quad (3.1.11)$$

Therefore

$$|\langle A|\lambda_n\rangle| = |\langle B|\lambda_n\rangle|, \quad (3.1.12)$$

for all  $n$ . Moreover the phases must also match

$$\lambda_n \tau_c = -\phi_0 - \phi_n + 2\pi f(n) \quad , \quad f : \mathbb{Z} \rightarrow \mathbb{Z}. \quad (3.1.13)$$

### 3.1.1b Proof of sufficiency

Suppose that a suitable  $\tau_c$  and  $\phi_0$  exist. So,

$$e^{-i\mathcal{H}\tau_c}|A\rangle = \sum_n |\lambda_n\rangle \langle \lambda_n|A\rangle e^{-i\lambda_n \tau_c}. \quad (3.1.14)$$

We can now supply the conditions on  $\lambda_n$

$$\begin{aligned} e^{-i\mathcal{H}\tau_c}|A\rangle &= \sum_{\langle \lambda_n|A\rangle \neq 0} |\lambda_n\rangle \langle \lambda_n|A\rangle e^{i(\phi_0 + \phi_n - 2\pi f(n))} \\ &= \sum_{\langle \lambda_n|A\rangle \neq 0} |\lambda_n\rangle \langle \lambda_n|A\rangle e^{i\phi_0} \frac{\langle \lambda_n|B\rangle}{\langle \lambda_n|A\rangle} \\ &= e^{i\phi_0}|B\rangle. \end{aligned} \quad (3.1.15)$$

The major advantage is that we can adjust the coupling strengths simply by specifying the desired spectrum.

### 3.1.1c Mirror symmetry and perfect state transfer

In the previous discussion we have set conditions in order to achieve perfect state transfer and showed that the energy eigenvalues must be integer functions (commensurate energies). We didn't discuss what is the proper form of the Hamiltonian in order to satisfy the PST conditions. The following statements make clear what Hamiltonians can provide us rigorous PST [?].

#### Statement:

In order to transfer an excitation in a 1 dimensional  $N$ -qubit XX open chain, The coupling strengths must be mirror symmetric, i.e. :

$$J_n^2 = J_{N-n}^2 \quad (3.1.16)$$

$$B_n = B_{N+1-n} \quad (3.1.17)$$

for all  $n=1,2,\dots,N$

**Proof:**

Assume that the spectrum of the Hamiltonian is  $\{|\lambda_n\rangle, \lambda_n\}$ ,  $n=1,2,\dots,N$

$$|1\rangle = \sum_{n=1}^N \alpha_n |\lambda_n\rangle \quad , \quad \alpha_n = \langle \lambda_n | 1 \rangle \quad (3.1.18)$$

$$|N\rangle = \sum_{n=1}^N \beta_n |\lambda_n\rangle \quad , \quad \beta_n = \langle \lambda_n | N \rangle. \quad (3.1.19)$$

We want to transfer  $|1\rangle \rightarrow |N\rangle$ . Hence

$$e^{-i\mathcal{H}\tau_c} |1\rangle = e^{i\phi_0} |N\rangle \quad , \quad \forall n \quad (3.1.20)$$

Therefore it must be also true that

$$e^{-i\lambda_n \tau_c} \alpha_n = e^{i\phi_0} \beta_n \quad , \quad \forall n \quad (3.1.21)$$

raising  $\mathcal{H}$  to an integer power  $m$ , we get

$$\langle 1 | H^m | 1 \rangle = \sum_{n=1}^N \lambda_n^m |\alpha_n|^2 = \langle N | H^m | N \rangle \quad (3.1.22)$$

taking various values of  $m$  we conclude that.

$$J_n^2 = J_{N-n}^2 \quad (3.1.23)$$

$$B_n = B_{N+1-n} \quad (3.1.24)$$

With the above relations it is easy to show that the Hamiltonian  $\mathcal{H}$  commutes with the symmetry operator

$$S = \sum_{i=1}^N |n\rangle \langle N+1-n|. \quad (3.1.25)$$

Therefore the space is divided into symmetric and antisymmetric subspaces with eigenvectors  $|\lambda_n^s\rangle$  and  $|\lambda_n^a\rangle$  respectively.

**Statement:**

A necessary and sufficient condition for perfect state transfer in a symmetric chain is that there should exist a time  $\tau_c$  and a phase  $\phi_0$  such that  $e^{-i\tau_c\lambda_n^s} = e^{i\phi_0}$  and  $e^{-i\tau_c\lambda_n^a} = -e^{i\phi_0}$  for all eigenvectors  $\langle \lambda_n | 1 \rangle \neq 0$

**Proof:**

Let us decompose  $|1\rangle$  and evolve it with the time operator

$$|1\rangle = \sum_{n=1}^N [a_n^s |\lambda_n^s\rangle + a_n^a |\lambda_n^a\rangle]. \quad (3.1.26)$$

Therefore

$$\begin{aligned} e^{-iH\tau_c} |1\rangle &= \sum_{n=1}^N [e^{-i\lambda_n^s \tau_c} a_n^s |\lambda_n^s\rangle + e^{-i\lambda_n^a \tau_c} a_n^a |\lambda_n^a\rangle] \\ &= e^{i\phi_0} \sum_{n=1}^N [a_n^s |\lambda_n^s\rangle - a_n^a |\lambda_n^a\rangle] = e^{i\phi_0} S |1\rangle \end{aligned} \quad (3.1.27)$$

Note that if state transfer occurs in time  $\tau_c$  there is a revival of the state on the input spin at times  $2k\tau_c$ ,  $k$  integer and perfect state transfer at all times  $(2n+1)\tau_c$ .

□

**3.1.2 Fidelity Formula for Arbitrary Graphs**

Assume that we have a Hamiltonian of the form

$$\mathcal{H} = \frac{1}{2} \sum_{i=1}^{N-1} J_i (S_i^x S_{i+1}^x + S_i^y S_{i+1}^y) - \sum_{i=1}^N B_i \cdot S_i^z. \quad (3.1.28)$$

Suppose that Alice places a pure state  $|\psi\rangle = a|0\rangle + b|1\rangle$  and that Bob picks up the spin at the optimum time  $\tau_c$ . The fidelity (the quality of transfer) becomes [?]

$$F = \langle \psi_{in} | \rho_{out}(\tau_c) | \psi_{in} \rangle. \quad (3.1.29)$$

Note that a fidelity of  $2/3$  can be achieved if Alice communicated Bob classically. Thus we would like to obtain  $F$  greater than  $2/3$  in our quantum communication spin.

Time evolving the initial state for the whole system

$$U(t)|\Psi(0)\rangle = e^{-i\mathcal{H}t}(\alpha|\mathbf{0}\rangle + \beta|\mathbf{1}\rangle) \Rightarrow |\Psi(t)\rangle = \alpha|\mathbf{0}\rangle + \beta \sum_{j=1}^N f_{1j}(t)|\mathbf{j}\rangle, \quad (3.1.30)$$

where the  $|\mathbf{j}\rangle$  is a class of states with flipped the  $j$ th spin and  $f_{1j}(t) \equiv \langle \mathbf{j} | e^{-i\mathcal{H}t} | \mathbf{1} \rangle$ .

The reduced density operator is

$$\begin{aligned} \rho_{out}(t) &= Tr_{1,2,\dots,N-1}(|\Psi(t)\rangle\langle\Psi(t)|) \\ &= (1 - |\beta|^2|f_{1N}(t)|^2)|0\rangle\langle 0| + |\beta|^2|f_{1N}(t)|^2|1\rangle\langle 1| \\ &\quad + \alpha\beta^*f_{1N}(t)^*|0\rangle\langle 1| + \alpha^*\beta f_{1N}(t)|1\rangle\langle 0|. \end{aligned} \quad (3.1.31)$$

Hence defining  $f_{1j}(t) = \sqrt{p(t)}e^{i\phi}$ , we obtain

$$\begin{aligned} F_\psi(|\beta|^2, p, \phi) &= 1 + |\beta|^2[-1 - p + 2\sqrt{p}\cos(\phi)] \\ &\quad + [2p - 2\sqrt{p}\cos(\phi)|\beta|^4]. \end{aligned} \quad (3.1.32)$$

Finally averaging over all possible input states (over the Bloch sphere) the fidelity is

$$\bar{F}(p, \phi) = \frac{1}{2} + \frac{p}{6} + \frac{\sqrt{p}\cos(\phi)}{3}. \quad (3.1.33)$$

## 3.2 Quantum Communication Protocols

The coupling  $J_{ij}$  can be carefully chosen to obtain a spin chain which accomplishes perfect quantum state transfer. As mentioned in the previous section quantum state transfer can be achieved if [?]

i) The couplings are mirror symmetric  $J_n^2 = J_{N-n}^2, B_n = B_{N+1-n}$ .

ii) The couplings are engineered to give rise to energies which are proportional to integers (commensurate energies) i.e.  $E_k \sim k, k(k+1), k^2$  etc.

If the two conditions are satisfied then there exists a time  $\tau_c$  that will mirror invert the spin state.

$$|\psi\rangle = \sum c_j |j\rangle \Rightarrow e^{-iH\tau_c} |\psi\rangle = \sum c_j |N - j + 1\rangle. \quad (3.2.1)$$

The mirror inversion implies that in time  $\tau_c$  a spin flip at first site of the spin chain will be perfectly transferred to the Nth site.

Next we shall proceed to the study of the two different types of quantum communication protocols: a) passive protocols, the ones that they do not change over time and b) the protocols that are time dependent.

### 3.2.1 Passive protocols

#### 3.2.1a Spin coupling protocol

The spin coupling protocol for an XX open chain (XY model with  $\gamma = 0$ ) was proposed by Christandl et al. and simultaneously by Nikolopoulos et al. [?, ?] and has drawn much attention. In fact together with the optimal coupling protocol has been declared the most faithful protocol to achieve state transfer. The most natural way to introduce this scheme is to consider a relabelling of the nth qubit excitation state  $|n\rangle$  as  $|m\rangle$  where  $m = -\frac{1}{2}(N - 1) + n - 1$ , which remind us the eigenstates of the z-axis Pauli matrix for a spin  $(N - 1)/2$  particle.

Therefore for an XX Hamiltonian  $\mathcal{H} = \sum_n \frac{J_n}{2} [\sigma_n^x \sigma_{n+1}^x + \sigma_n^y \sigma_{n+1}^y]$  the matrix elements become

$$\begin{pmatrix} 0 & J_1 & 0 & \dots & 0 \\ J_1 & 0 & J_2 & \dots & 0 \\ 0 & J_2 & 0 & \dots & 0 \\ \vdots & \vdots & \vdots & \ddots & J_{N-1} \\ 0 & 0 & 0 & J_{N-1} & 0 \end{pmatrix} \quad (3.2.2)$$

The above matrix is identical to the matrix representation of the Hamiltonian H of a spin particle  $S = (N - 1)/2$  with  $H = \lambda S^x$ . In this case the matrix elements are equal to  $J_n = \frac{\lambda}{2} \sqrt{n(N - n)}$ .

The time evolution operator is  $U(t) = e^{-i\lambda S^x t}$ , and thus the probability amplitude for transferring the state from the first site to the  $j$ th site is

$$A_j(t) = \langle j|U(t)|1\rangle \binom{N-1}{j-1}^{1/2} [-i \sin\left(\frac{\lambda t}{2}\right)]^{(j-1)} \cos\left(\frac{\lambda t}{2}\right)^{(N-j)}. \quad (3.2.3)$$

Hence the probability amplitude for the  $N$ th site is

$$A_N(t) = \left[-i \sin\left(\frac{\lambda t}{2}\right)\right]^{N-1}, \quad (3.2.4)$$

with perfect state transfer occurring for the first time at  $\tau_c = \frac{\pi}{\lambda}$ .

Finally note that the energy spectrum is commensurate linear.

### 3.2.1b Optimal coupling protocol

The previous protocol was a bit imaginative and of course is not an obvious selection for a quantum communication protocol. The simplest communication protocol would be a homogeneous chain. Unfortunately this protocol cannot achieve perfect state transfer for chain lengths greater than  $N=3$  [?] due to the dispersive quantum dynamics which makes probability amplitude to decrease exponentially with  $N$  and the transferring time to increase linearly with  $N$ . Therefore one should modulate the chain in order to achieve perfect state transfer, with the simplest modulation to be the control of the two boundary spins [?, ?]. The boundary spins can be engineered to  $J_1 = J_N = \alpha J$  with  $\alpha$  being in two different regimes:

i) *The optimal coupling regime* ( $\alpha \sim \frac{1}{N^6}$ ) If we scale  $\alpha \sim 1/N^6$  the initial state corresponds to a wave packet with approximately Lorentzian probability distribution in the wavenumbers  $k$  optimised to possess an almost equidistant spectrum  $E_k$  in the middle of the energy band, resulting in a quasidisersionless fast transfer with high fidelity

ii) *The weak coupling regime* ( $\alpha \ll 1$ ) In that regime the transmitted state appears roughly periodically at the receiving end of the chain. In fact the eigenvalues responsible for the transfer are determined analytically and it is found that for very small values of  $\alpha$  compared to  $J_i$ ,  $i \neq 1, N$  only two

or three (when  $N$  is odd) closely-spaced energy levels in the center of the spectrum are important. Oscillations between these states determine the quality of transfer. Furthermore the transfer time is  $\tau_c \sim 1/\alpha^2$  for  $N$  even and  $\tau_c \sim 1/\sqrt{N}\alpha^{-1}$  and fidelity decreases from unity by a factor of  $\alpha^2 N$ .

## 3.2.2 Active Protocols

### 3.2.2a Adiabatic protocol

Let us assume that we have spin chain with and odd number of sites  $N$  and that each individual coupling can be manipulated independently. In this case the XX Hamiltonian possesses a coherent population trap (CPT) [?, ?] eigenstate

$$|\Psi^{(0)}\rangle = \frac{1}{\sqrt{N_0}} [J_2 J_4 \dots J_{N-1} |1\rangle - J_1 J_4 \dots J_{N-1} |3\rangle + \dots + (-1)^{\mathcal{J}} J_1 J_3 \dots J_{N-1} |N\rangle], \quad (3.2.5)$$

$$\mathcal{J} \equiv \frac{1}{2}(N-1), \quad (3.2.6)$$

with eigenvalue  $\lambda^0 = 0$ . Thus the amplitude of initial state  $A_1$  is proportional to the product of all the even-numbered couplings, while the amplitude of final state  $A_N$  is given by the product of all the odd-numbered couplings, divided by the normalization constant  $N_0 = (J_2 J_4 \dots J_{N-1})^2 + \dots + (J_1 J_4 \dots J_{N-2})^2$ . The above make clear what procedure we should follow in order to achieve state transfer. First we switch on only the even-numbered couplings to make  $|\Psi^{(0)}\rangle = |1\rangle$ . This is then followed by switching-on all the odd-numbered couplings, while the even-numbered ones decrease, which will result in a complete transfer to the state  $|N\rangle$ . Since the two coupling sets will overlap in time the transfer will complete in  $\tau_c$ , when  $J_{odd} \gg J_{even} \simeq 0$  with  $A_N(\tau_c) = (-1)^{\mathcal{J}}$ .

Finally note that the adiabatic scheme holds true only if, during the transfer process, the non adiabatic transitions out of  $|\Psi^{(0)}\rangle$  are negligible, which requires that the rate of change of the coupling strengths be small compared to the energy separation between  $|\Psi^{(0)}\rangle$  and all the other eigenstates. Hence if the rate of change of the coupling strengths is assumed to be the same and denoted as  $\Gamma$  the condition  $J_{even,odd}^{max} \gg \Gamma$  should be satisfied

### 3.2.2b Sequential SWAP protocol

The SWAP protocol [?] is the most straightforward approach to the state transfer between the two ends of a chain. The procedure is to apply a sequence of SWAP operations implemented by  $\pi$  pulses between the pairs of neighbouring sites. Initially the couplings  $J_i$  are set to zero, we switch  $J_1$  coupling for time  $\pi/(2J_1)$ , then we switch  $J_2$  coupling for time  $\pi/(2J_2)$ , etc, until the  $N$ th site is reached. The corresponding state amplitude is  $A_j(t_{j-1}) = -i \sin(J_{i-1}t_{j-1})A_{j-1}(t_{j-2})$ . Furthermore we can pulse all the couplings to the maximal possible coupling  $J_{max}$ , and thus the total time becomes  $t_{out} = (N - 1)\pi/2J_{max}$ , with the  $N$ th state amplitude  $A_N(t_{out}) = (-i)^{N-1}$  and the  $\phi_0 = (-\pi/2)(N - 1)(mod 2\pi)$ .

### 3.2.3 Wave-packet encoding

So far we have encoded the information as a single spin flip at the one end. An alternative would be to encode the signal in a spatial wavepacket [?, ?] with a well defined group velocity. The most robust wavepacket is the Gaussian wave-packet state,

$$|G(j_0, k)\rangle = \sum_j e^{-\frac{(j-j_0)^2}{L^2} - ik_0j} |j\rangle. \quad (3.2.7)$$

The wavepacket extends in a block of  $L$  sites around  $j_0$ . For appropriate choice of  $k_0$  one can choose  $L \sim N^{1/3}$ , so that the wavepacket travels with a negligible dispersion for short times.

Let us consider a problem where we have a ring (closed) XY model. Alice controls a block  $L$  of spins, then she encodes the  $|1\rangle$  state of the qubit she intends to transmit on  $|G(j_A, k)\rangle$ , where  $j_A$  belongs to the subset of  $L$ . Bob located at any distant site along the ring can receive almost the entire wave-packet by using a sufficiently long subset of spins ( $\sim N^{1/3}$ ) to receive the state. The fidelity is proportional to the amplitude  $|\langle G(j_A, k) | G(j_B, k) \rangle|^2$  which can be as high as 95 percent for  $N$  up to 5000. The solution for the open ended chain came from Haselgrove [?], using the singular value decomposition on the time evolution operator and choosing an initial state that quickly evolves to a Gaussian wavepacket. This allow us to avoid the distortion and spread

of the Gaussian wavepacket in an open chain from the reflection of the endpoints. In fact Haselgrove showed that choosing the optimal state encoding is a simple matter of performing a singular value decomposition on a modified evolution matrix.

### 3.3 Entangled States in State Transfer

Entangled states play a very significant role in the field of quantum information since they play a fundamental role in transmitting information. In this section we will mention some basic features of entanglement in state transfer. We begin by describing a famous protocol for state transfer called *quantum teleportation* and then we continue with an alternate criterion for the success of a transmitted information, based on the entanglement that can be transferred through a spin chain protocol.

#### 3.3.1 Quantum Teleportation

Assume that we have two distant parties, customarily called Alice and Bob, wish to exchange some quantum information [?]. Specifically Alice needs to communicate to Bob one qubit of information

$$|\psi\rangle = a|0\rangle + b|1\rangle. \tag{3.3.1}$$

Furthermore suppose that Alice does not know the state of qubit she needs to send to Bob. A measurement on the qubit will not disclose all the information about the two coefficients and also will destroy the qubit state. Moreover from the No-cloning theorem Alice cannot clone a qubit in order to perform many measurements and infer its state with high precision.

To overcome this obstacles Alice and Bob should share a pair of qubits in the entangled state  $|B_{00}\rangle = \frac{1}{\sqrt{2}}(|0^A\rangle|0^B\rangle + |1^A\rangle|1^B\rangle)$ . In fact we could choose any of the four Bell states.

The initial state of the three qubits is given by

$$|\Phi\rangle = |\psi\rangle \otimes |B_{00}\rangle. \tag{3.3.2}$$

If Alice applies the CNOT (??) transformation  $U_{CNOT}$  to her qubits we get

$$(U_{CNOT} \otimes I_2) |\Phi\rangle = \frac{1}{\sqrt{2}} [a|0\rangle \otimes (|0^A\rangle \otimes |0^B\rangle + |1^A\rangle \otimes |1^B\rangle) + b|1\rangle \otimes (|1^A\rangle \otimes |0^B\rangle + |0^A\rangle \otimes |1^B\rangle)] \quad (3.3.3)$$

Applying the Hadamard transformation H (??) to the qubit she intends to transmit we get

$$|\Psi\rangle = \frac{1}{2} [ |00^A\rangle \otimes (a|0^B\rangle + b|1^B\rangle) + |01^A\rangle \otimes (a|1^B\rangle + b|0^B\rangle) + |1^A0\rangle \otimes a(|0^B\rangle - b|1^B\rangle) + |11^A\rangle \otimes (a|1^B\rangle - b|0^B\rangle) ] . \quad (3.3.4)$$

Alice measures the two qubits in her possession and communicates the result to Bob with two classical bits of information. Bob then receives from Alice a two-bit message and instantaneously knows what unitary transformation to perform in order to achieve the original  $|\psi\rangle$  state. Finally we should mention that nor atoms nor energy is transmitted from the one place to the other but only the state (the information) is transmitted from Alice to Bob. Finally note that entanglement is crucial to quantum teleportation, since if we do not work with entangled states we cannot achieve teleportation[?]

### 3.3.2 Entanglement as Figure of Merit

The fidelity tells us if our quantum channel is good enough to faithfully transmit information. A different figure of merit for judging the performance of the spin chain as a quantum communication channel is the entanglement[?]

Assume that we have one of the four Bell states<sup>1</sup>

$$|B_{00}\rangle = \frac{1}{\sqrt{2}} (|0^A\rangle|0^B\rangle + |1^A\rangle|0^B\rangle). \quad (3.3.5)$$

Let us look at the transmission of the state of one member of a pair of particles in the entangled state  $|B_{00}\rangle$ . Alice prepares two qubits in the state  $|B_{00}\rangle$ , keeps one of them (say A) and places the other on the first site of the

---

<sup>1</sup>Our analysis does not depend on which Bell state we will choose.

chain. Bob waits for an optimal time  $\tau_c$  and then picks up the qubit N from the chain. The joint state of Alice's qubit A and Bob's qubit is given by

$$\rho_{1N}(\tau_c) = \frac{1}{2} [(1 - |f_{rs}(\tau_c)|^2)|00\rangle\langle 00|_{1N} + (|10\rangle + |f_{rs}(\tau_c)||01\rangle)(\langle 10| + |f_{rs}(\tau_c)||01|_{1N})], \quad (3.3.6)$$

where  $\mathcal{C} = |f_{rs}(\tau_c)|$  is the concurrence (??) .

The above relations help us to estimate the entanglement that can be transferred, which is very useful especially for very large chains that fail to achieve a fidelity greater than  $2/3$ . For example for an open homogeneous chain without disorder we find that the concurrence for large spin chains is

$$\mathcal{C} \sim 1.35/N^{1/3}, \quad (3.3.7)$$

which is a slow decrease of the concurrence for an increase in chain length N. Hence entanglement distribution is possible even for spin chains that fail to overcome the classical value of fidelity. Let us mention that the entanglement distribution has been recently analysed for the spin coupling protocol by Lorenz et al.[?].

### 3.4 Perfect State transfer

There are several known quantum communication protocols that can achieve PST and some of them we overview in the previous section, but studies seem to converge that the two most robust channels are the spin-coupling protocol and the optimal coupling protocol for exchanging quantum Information. In this section we introduce the reader to some basic noiseless results for these two channels.

Our analysis pertains to XX Spin Chain Hamiltonians can be transformed via a Wigner-Jordan transformation(??) to the Hubbard Hamiltonian for non-interacting spinless fermions or hard-core bosons:

$$\mathcal{H} = - \sum_k \varepsilon_k a_k^\dagger a_k + \frac{1}{2} \sum_{n=1}^{N-1} J_n [a_{n+1}^\dagger a_n + a_n^\dagger a_{n+1}]. \quad (3.4.1)$$

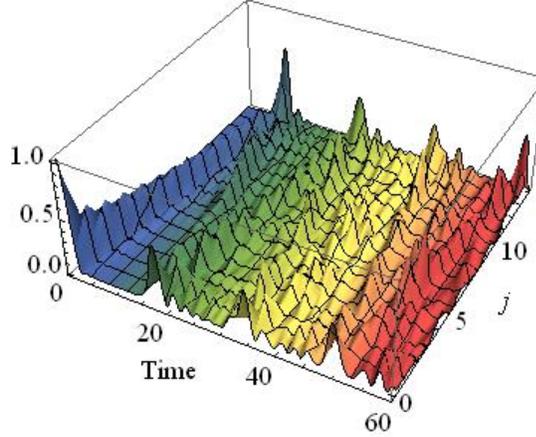


Figure 3.1: Probability amplitude in a chain of  $N=15$  for the case of the homogeneous protocol. The communication failure is obvious since the  $N$ th site probability amplitude is  $P_N(\tau_c) \simeq 0.8$  in the first maximum

The total wavefunction reads  $|\Psi(t)\rangle = \sum_{k,\alpha} A_k^\alpha(t) |k_\alpha\rangle$ , where  $|k_\alpha\rangle = a_{k\alpha}^\dagger |0_1 0_2 \dots 0_N\rangle$  denotes the state with one electron having spin  $\alpha = \uparrow, \downarrow$  at the  $j$ -th spin site. The equations of motion are

$$i \frac{dA_k^\alpha}{dt} = \varepsilon_k A_k^\alpha + J_{k-1} A_{k-1}^\alpha + J_{k+1} A_{k+1}^\alpha, \quad (3.4.2)$$

Fig.1 shows the total communication failure of the homogeneous chain even for relatively small chains,  $N=15$ , since the Probability amplitude is significantly decreased at the state transfer time  $t = \tau_c$ . Fig.2 shows the main difference between the most robust channels, the spin coupling protocol and the optimal protocol, which makes clear the significant role of commensurate energy spectrum for state perfect transfer even for already optimized models since the probability amplitude of the  $N$ th site slowly decreases over each period in terms of  $\tau_c$ . Of course this is not devastating since we do not account latter times than  $\tau_c$  and thus the maximum probability amplitude is always close to unity even for large  $N$ . However the transfer time for the optimized protocol is relatively shorter,  $\tau_c^{spin} \sim \frac{\pi}{2} \tau_c^{opt}$ .

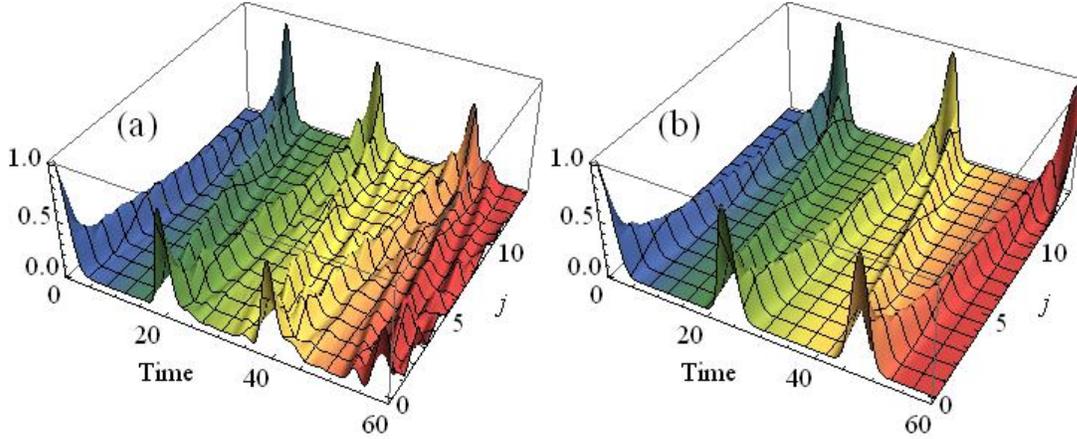


Figure 3.2: Probability amplitude in a chain of  $N=15$  for the case of (a) spin-coupling protocol and (b) the optimal protocol. All parameters are normalized to  $J_{max}$

### 3.5 State Transfer in the presence of disorder

PST is an idealized situation where decoherence and disorder is not present or totally negligible, and thus Fidelity is unity. Unfortunately in a realistic environment our physical system (e.g. a quantum dots array) will have decreased change of successfully transmitting the information between the two ends of our channel due to the presence of disorder, and thus the fidelity will be less than unity. In this section we compare the two most prominent communication protocols i.e. the spin-coupling protocol and the optimal protocol in the presence of off-disorder for the purpose of extracting conclusions about the reliability of these two protocols and ultimately to decide which is the most faithful to transmit information.

#### 3.5.1 Static and Dynamic Disorder

In a realistic system the introduction of disorder is inevitable due to manufacturing errors, thermal and quantum fluctuations. For example if we implement our model to a quantum dots array [?] the loss of information quality is due to hyperfine interactions and exchange coupling fluctuations. Generally disorder is divided in two types [?], *static* and *dynamic*.

### 3.4.1a Static disorder

Static disorder in the couplings within the transfer channel is described by  $J_k \rightarrow J_k + \Delta J_k(t)$  with  $\Delta J_k(t)$  being a random variable. There are two possible disorder models: a) *relative static disorder*, where each coupling is allowed to fluctuate by a certain fraction of its ideal size,  $\Delta J_k(t) = J_k \delta_k$  and b) *absolute static disorder*, where all couplings may fluctuate within a certain fixed range which we measure in terms of the maximum coupling  $J_{max}$ ,  $\Delta J_k(t) = J_{max} \delta_k$ .  $\delta_k$  is a dimensionless uncorrelated random variable which is usually characterized by the Gaussian or the uniform distribution. It is obvious that the absolute disorder is expected to be more damaging than the relative one.

### 3.4.1b Dynamic disorder

The dynamic disorder can be introduced as a time-dependent coupling and energy fluctuation  $\Delta J_k(t)$  and  $\Delta E_k(t)$ . As in the static disorder case there exist the *relative dynamic disorder* and the *absolute dynamic disorder*. In this case the dimensionless parameter  $\delta_k(t)$  has two main properties: i) disorder in each site is independent from the other sites and ii) in each site k the disorder is correlated in time such that the frequency spectrum behaves as  $S(f) = \sigma_J / f^a$ , where  $\sigma_J$  is the standard deviation and a the type of noise. For instance a=0 represents the white noise, a=1 represents the pink noise, a=2 is known as the Brownian motion and  $a = \infty$  is the static noise. The noise generator is given by the discrete Fourier transform [?, ?],

$$s(t) = \frac{1}{M} \sum_{k=0}^{M-1} S(f_k) e^{i2\pi(f_k - \eta_k)t}. \quad (3.5.1)$$

Finally note that the dynamic disorder can be considered as static disorder if the couplings are varying much slower than the transfer time.

## 3.5.2 State transfer in the presence of Noise: Known results

As mentioned earlier perturbations due either to manufacturing imperfections or to interactions with the environment are the main source of problems for transmitting an input state through a quantum channel. This section

is devoted to the presentation of some known results [?] of the behaviour of the two spin chain communication protocols in the presence of disorder. The main tool to decide whether or not state transfer is successful is the transmission fidelity and usually to compactify the computational analysis in smaller data we use the transmission fidelity averaged over all possible input states  $|\psi_{in}\rangle$  on the Bloch sphere,  ${}^2\bar{F}$ . For the rest of the text The symbol  $\langle \cdot \rangle$  is omitted but it should be clear that in the presence of randomness all physical quantities are represented as the mean value of a statistical variable.

Let us introduce the disorder by making the following transformation

$$\begin{aligned} J_k &\rightarrow J_k + \Delta J_k \\ \varepsilon_k &\rightarrow \varepsilon_k \end{aligned} \tag{3.5.2}$$

For simplicity we haven't considered in this section disorder in the diagonal elements (energies) while for the non-diagonal elements we consider both relative  $\Delta J_k = J_k \delta_k$  and absolute  $\Delta J_k = J_{max} \delta_k$  disorder, where  $\delta_k$  is an uncorrelated and uniformly distributed variable. Differences in the results between a uniform distribution and a Gaussian distribution with mean zero, exist, but we do not expect qualitative differences<sup>3</sup> and therefore they should be considered insignificant. Obviously for the optimal scheme the two types of noise can be taken as equivalent since the chain is homogeneous apart from the two ends.

Fig.3 is taken from the work of Zwick et al [?] and compares compactly the two communication protocols. As expected the relative disorder is much more detrimental than the absolute disorder. Moreover the spin coupling protocol for perturbations  $\varepsilon_J \leq 0.1$ , ( $\varepsilon_J$  is the standard deviation of the Gaussian variable) and relative static disorder always performs better than the optimal scheme for all N. However if absolute static disorder is assumed there exists a region with  $\varepsilon_J \simeq 0.05$  where the optimal performs better. Also

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<sup>2</sup>Note that in the perfect case, one can always set the phase  $\phi$  to zero with the use of a proper magnetic field, but in the presence of disorder the phase becomes  $\Delta\phi = \phi_{ideal} - \phi_{dis}$ .

<sup>3</sup>Another source of differentiation in the numerical results is the library from where the random generator is taken

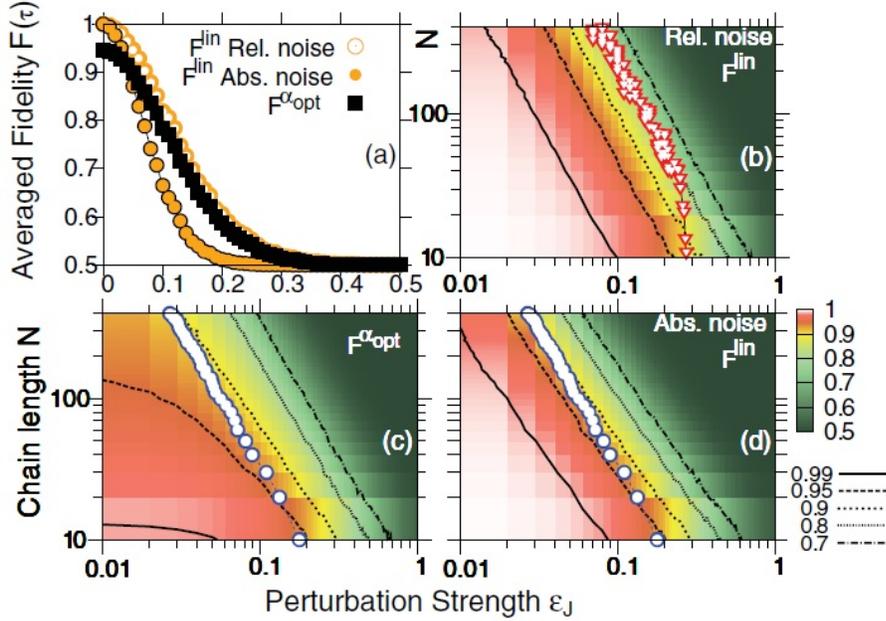


Figure 3.3: Average fidelity at transfer time  $\tau$  and  $N=200$  as a function of the perturbation strength  $\epsilon_J$  of the exchange coupling. For the spin-coupling scheme (linear) Relative (open circles) and Absolute (orange circles) disorder are considered. The optimal scheme is presented by black squares. The density plots present the spin-coupling scheme for relative and absolute disorder and the optimal scheme with respect to the number of sites  $N$  and the perturbation strength  $\epsilon_J$ . The white circles and triangles indicate the contours where the fidelity of the two models are equal.

Fig.3 indicates that there exists a region where the optimal protocol becomes more efficient than the spin coupling protocol and the separation of the two regions is proportional to the type of disorder that we use. Moreover the averaged fidelity is decreased significantly for large  $N$  and  $\epsilon_J \geq 0.06$  which makes the physical realization of state transfer rather difficult, as an example consider a channel of averaged fidelity  $\bar{F} \simeq 0.8$ . Although the fidelity as an absolute value is quite satisfying, it cannot be considered as a certain communication channel since it has a transmission error of 0.2 which means that about every 20 messages will be faulty transmitted.

## 3.6 Motivation

Although we acquired an insight from the previous section about the two protocols behaviour it is clear that the result of this comparison is inconclusive and in fact inadequate since it has considered only off diagonal disorder and has made conclusions based on the fidelity averaged over the Bloch sphere which is a moderate approach to the problem. Nikolopoulos [?] showed that a more accurate measure for the transfer quality should be the fidelity  $F_\psi$  which is a function of the input state  $\psi$ . This study is the motivation for further comparing the two protocols carefully in order to lead us to the final decision in the question of which protocol should be used in an experiment for certain levels of noise. Additionally studies that analyse the behaviour of a system in terms of the averaged fidelity tend to overestimate or underestimate the signal quality and thus may give a false image about the possibilities of a quantum channel in various regions of disorder. Therefore an open question is how much the two measures of fidelity differ for the two protocols and what are the implications of than for an experiment.



# Chapter 4

## Quantum State Transfer: Robustness of Spin Chains

In this chapter we present a study motivated by the papers of Nikolopoulos [?] and Zwick et al [?]. We present the behaviour of the two protocols in the presence of both diagonal and off-diagonal relative static disorder and in terms of  $F_\psi$  for various spin chain numbers. The system is again described by the Hamiltonian (??) and the equations of motion are (??).

### 4.1 Introducing the Diagonal Disorder

The disorder will be introduced with the form of **relative static disorder** by making the following transformation

$$\begin{aligned} J_k &\rightarrow J_k(1 + \delta_k) \\ \varepsilon_k &\rightarrow \varepsilon_k(1 + \eta_k) \end{aligned} \tag{4.1.1}$$

where  $\delta_k$  is an uncorrelated Gaussian ensemble. We prefer *relative disorder* due to the fact that the spin coupling channel with *absolute static disorder* cannot compete the optimal scheme and thus a comparison of the optimal and the spin coupling scheme in these terms is useless.

Introducing diagonal disorder has proven a interesting feature since not only the fidelity behaves differently at the two types of noise but also the models themselves have different disorder susceptibilities. Specifically Fig.4

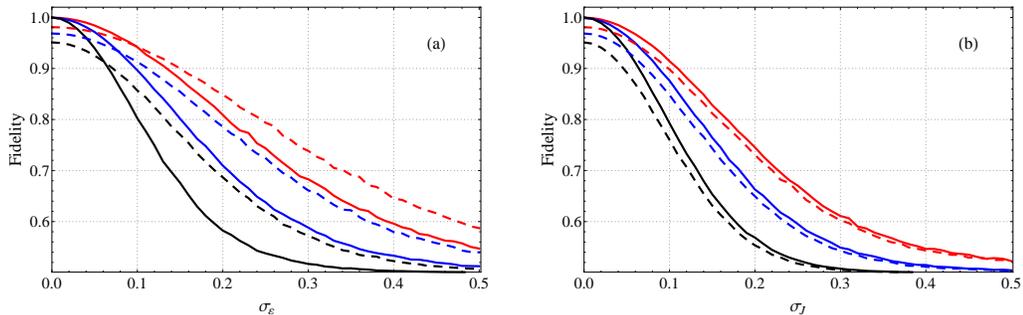


Figure 4.1: The Fidelity  $\bar{F}(\tau_c)$  for the optimal protocol(dashed lines) and the spin coupling protocol (solid lines) as a function of (a)  $\sigma_\varepsilon$  disorder for  $\sigma_J = 0$  and (b)  $\sigma_J$  disorder for  $\sigma_\varepsilon = 0$  for  $N=15$ (red), $N=25$ (blue) and  $N=50$ (black) number of spin sites

shows that the off-diagonal disorder  $\sigma_J$  seems to be more catastrophic than the diagonal disorder. Furthermore the spin coupling protocol is slightly more robust in the off diagonal noise than the optimal protocol, for example the spin coupling scheme has mean fidelity  $\bar{F}(\tau_c) \simeq 0.7$  at  $\sigma_J = 0.16$  while the optimal at  $\sigma_J = 0.13$ . On the contrary the optimal scheme is more robust to the diagonal noise than the spin coupling scheme since  $\bar{F}(\tau_c) \simeq 0.7$  at  $\sigma_\varepsilon = 0.21$  and the same value for the other protocol occurs at  $\sigma_\varepsilon = 0.15$ . Obviously the differences are quite small and thus only a combined feature of the two noises can give us further answers about the quality of information that the two different types of "noisy" channels can transmit. The behaviour of the mean fidelity obeys a simple scaling law which was found by a numerical fit to the data

$$\bar{F}(\tau_c) = [F_0 e^{-k_J N \sigma_J^2 - k_\varepsilon N \sigma_\varepsilon^2} + \frac{1}{2}], \quad (4.1.2)$$

where  $F_0, k_J, k_\varepsilon$  are parameters that depend on the protocol. For the spin-coupling protocol  $F_0 = 0.5$ ,  $k_J \simeq 1.07$  and  $k_\varepsilon \simeq 0.7$  while for the optimal protocol  $F_0 = \frac{|A_N(\tau_c)|^2}{3} + \frac{|A_N(\tau_c)|}{6}$ ,  $k_J \simeq 1.2$  and  $k_\varepsilon \simeq 0.46$ . This scaling law was firstly analysed in [?]

From fig.5 and 6 we see that in terms of the mean fidelity  $\bar{F}$  the two models can be characterized as almost equivalent for moderate spin chains ( $N \leq 25$ ) with the optimal scheme gaining ground for large  $\sigma_\varepsilon$  while the

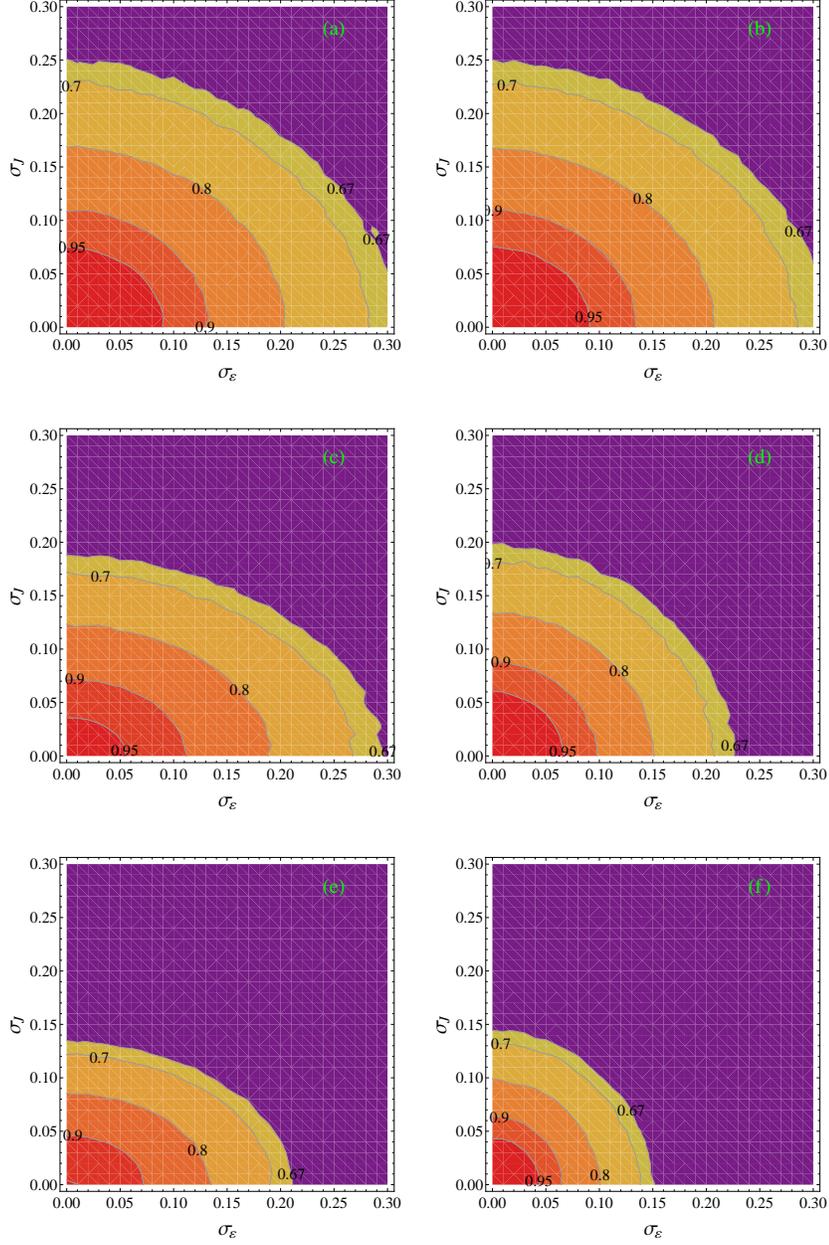


Figure 4.2: The  $\bar{F}(\tau_c)$  fidelity in the presence of  $\sigma_J, \sigma_\epsilon$  noise for the optimal(left figures) and spin-coupling scheme(right figures) for  $N=15$ ,  $N=25$  and for  $N=50$  number of spin sites. Note that the contours plotted correspond to  $\bar{F}(\tau_c)$

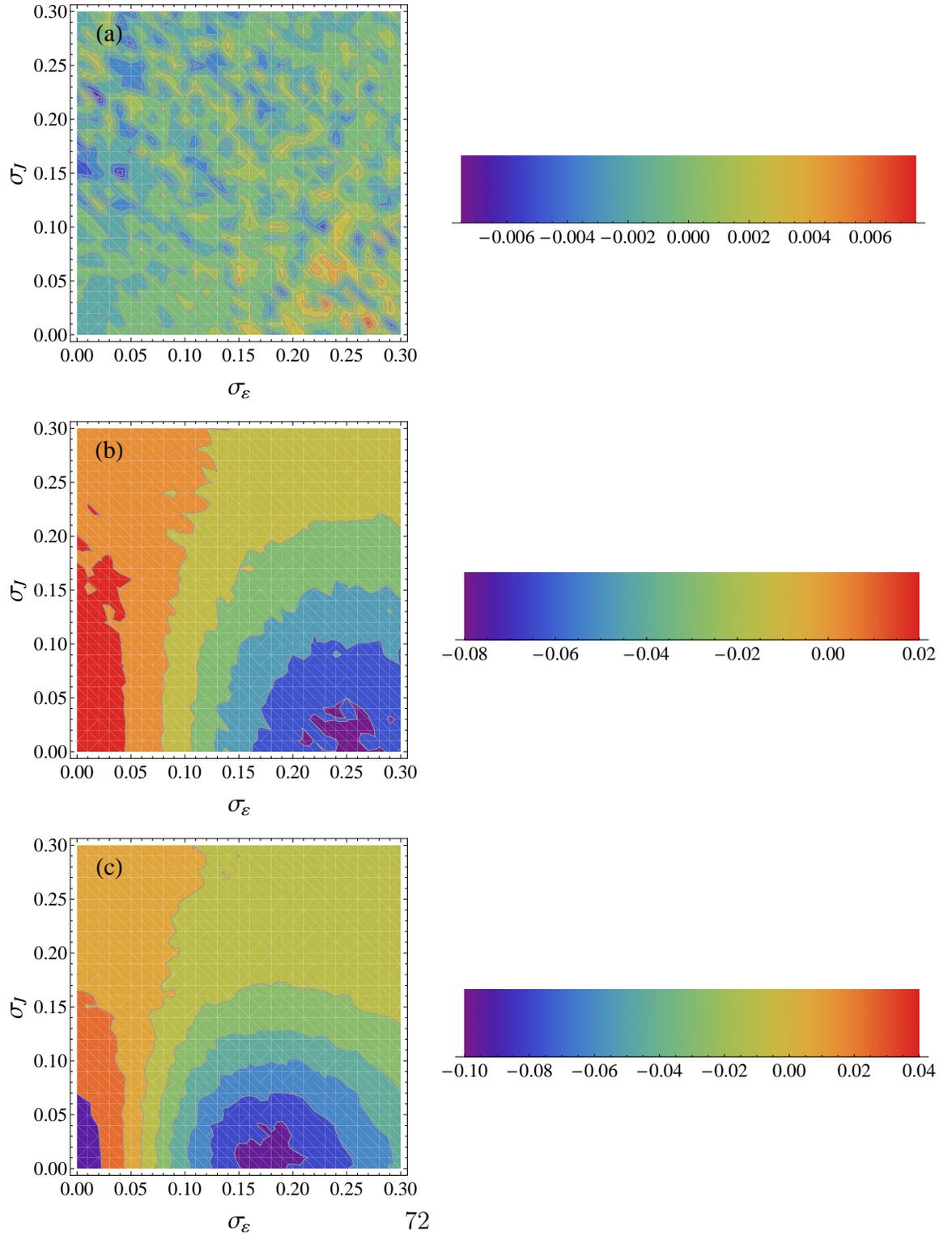


Figure 4.3: The Fidelity differences  $\bar{F}_{spin} - \bar{F}_{optimal}$  at time  $\tau_c$  for the two protocols as functions of  $\sigma_J$  and  $\sigma_\epsilon$  for  $N=15$ (top),  $N=25$ (middle) and  $N=50$ (bottom) number of spin sites

spin coupling seems to be slightly more robust in the region  $\sigma_\varepsilon$  close to zero and  $\sigma_J$  any value. Note that for  $N \geq 20$  there exists a "boundary" region that divides the dominant regions of the protocols. Although quantitatively for moderate spin chains we do not see big differences for large spin chains  $N > 100$  the dominant regions will become clear. For an experimentalist the most valuable region coincides with the "boundary" region which occurs for  $\Omega = (\sigma_\varepsilon \sim 0.08 - 0.15, \sigma_J \sim 0.08 - 0.15)$  due to the fact that this is a realistic feature for the disorder expected in a carefully designed experiment. In fact disorder greater than 0.2 is a pessimistic approach while disorder smaller than 0.08 is almost unreachable for a respectable number of spin sites.

## 4.2 Reliable Measures of Information Quality

In the previous section we have compared the two models with respect to the mean  $\bar{F}$  fidelity. Let us compare the two models with the  $F_\psi$  fidelity. Why  $F_\psi$  could make us difference? The  $F_\psi$  fidelity gives the exact value of fidelity for a specific input state  $|\psi\rangle$  and thus it can reveal if there are regions of disorder that highly overestimate/underestimate the quality of information that can be transferred which subsequently allow us to further compare the two models.

$$F_\psi(|\beta|^2, p, \phi) = 1 + |\beta|^2[-1 - p + 2\sqrt{p} \cos(\phi)] + [2p - 2\sqrt{p} \cos(\phi)]|\beta|^4. \quad (4.2.1)$$

From the analytical formula of Fidelity  $F_\psi$  we see that for  $|\beta|^2$  close to zero, fidelity goes to unity even for  $p, \cos(\phi) \neq 1$  and for  $|\beta|^2$  close to one, fidelity takes its minimum value. A specific  $|\beta|^2$  which is of particular interest is the one that minimizes fidelity [?] which is found to be

$$|\beta|_{min}^2 = \begin{cases} \frac{1+p-\sqrt{p} \cos(\phi)}{4(p-2\sqrt{p} \cos(\phi))} & |\beta|_{min}^2 \in [0, 1] \\ 1 & otherwise \end{cases} \quad (4.2.2)$$

From fig.7-10 we clearly see that the quality of transfer is totally dependent on the input state we used. For  $|\beta|^2 \in [0, 0.4]$  the two protocols can be considered as robust even for  $\sigma_\varepsilon, \sigma_J$  disorder greater than 0.2. On the contrary for  $|\beta|^2 \in [0.6, 1.0]$  the two protocols start to lose their robustness

and the region of quantum state transfer i.e.  $F_\psi > 0.67$  become smaller as the  $|\beta|^2$  approaches the  $|\beta|_{min}^2$ . Similarly with the previous section we see that the optimal scheme is more robust for small  $\sigma_J$  and big  $\sigma_\epsilon$  while the spin coupling is slightly more robust in the opposite direction. Again for small spin chains (N=15) the differences between the two models are insignificant with the only exception a small region where the optimal scheme behaves better by a percentage in the range 10 – 17%. For larger values of (e.g. for the case of N=50 depicted in Fig ) the differences in the performance of the two protocols are considerably larger and they grow up to 25% in specific regions. Moreover we see that the area and the magnitude of the differences in the performance of the two models are connected in an ascending manner to the input state.

By comparing the  $\bar{F}(\tau_c)$  and the  $F_\psi(\tau_c)$  given by (??) and (??) respectively, one starts to doubt about how precisely the averaged fidelity can inform us about the Robustness of a spin chain protocol due to the fact that depending the input state we will use the  $\bar{F}(\tau_c)$  significantly overestimates/underestimates the information quality. An interesting test that we can conduct to check if quantum state transfer occurs is the following. Assume that we have a counter that "clicks" every time the fidelity measurement we have chosen ( $\bar{F}(\tau_c)$  and the  $F_\psi(\tau_c)$  or others) is above the classical limit of 0.67 and this works given the disorder and the protocol. By repeating the experiment many times one can obtain statistics about the probability of success for achieving quantum state transfer. Mathematically this is defined as  $P(F > 0.67 | \sigma_\epsilon, \sigma_J, protocol)$  which is the probability for a chain of given disorder and protocol operating as a quantum channel (i.e.  $F > 0.67$ ). Fig.11 presents the difference  $P(F_{min} > 0.67) - P(\bar{F} > 0.67)$  between the minimum fidelity and the Bloch sphere averaged fidelity. First of all, one sees immediately that the average fidelity always overestimates or underestimates (depending on the input state) the performance of both protocols. A second observation is that even for moderate disorder ( $\sim 0.2$ ), this overestimation is of the order of 0.5. It is only for very small values of disorder that the deviations in the predictions of the two models are of the order of 0.1.

An obvious conclusion is that the  $\bar{F}(\tau_c)$  fidelity significantly underestimates the information quality for  $|\beta|^2 \in [0, 0.4]$  and overestimates the information

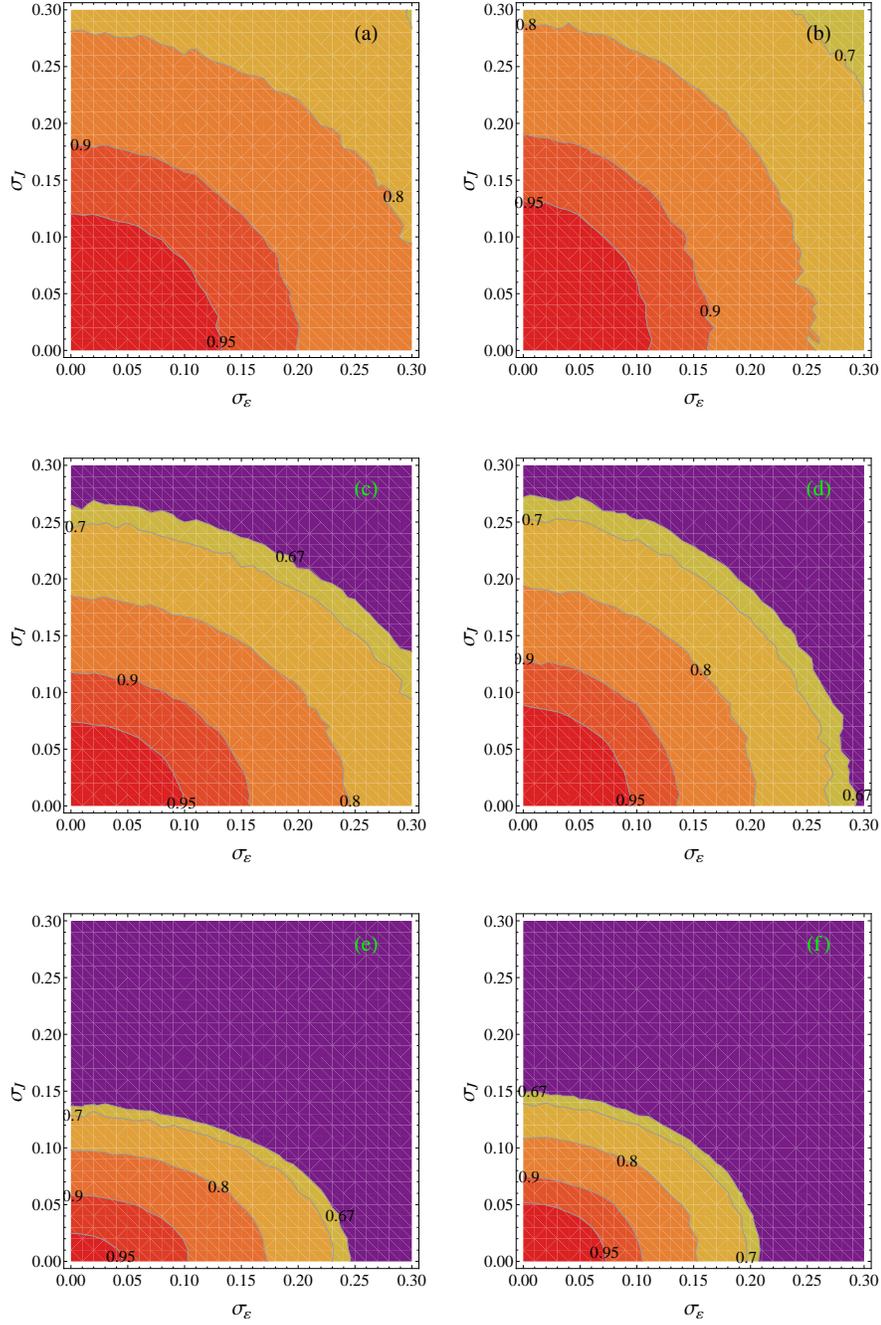


Figure 4.4:  $F_\psi(\tau_c)$  fidelity for  $|\beta|^2 = 0.4$ (top),  $|\beta|^2 = 0.6$ (middle) and  $|\beta|^2_{min}$ (bottom) for the optimal protocol(left) and the spin-coupling protocol(right) for a spin chain of length  $N=15$

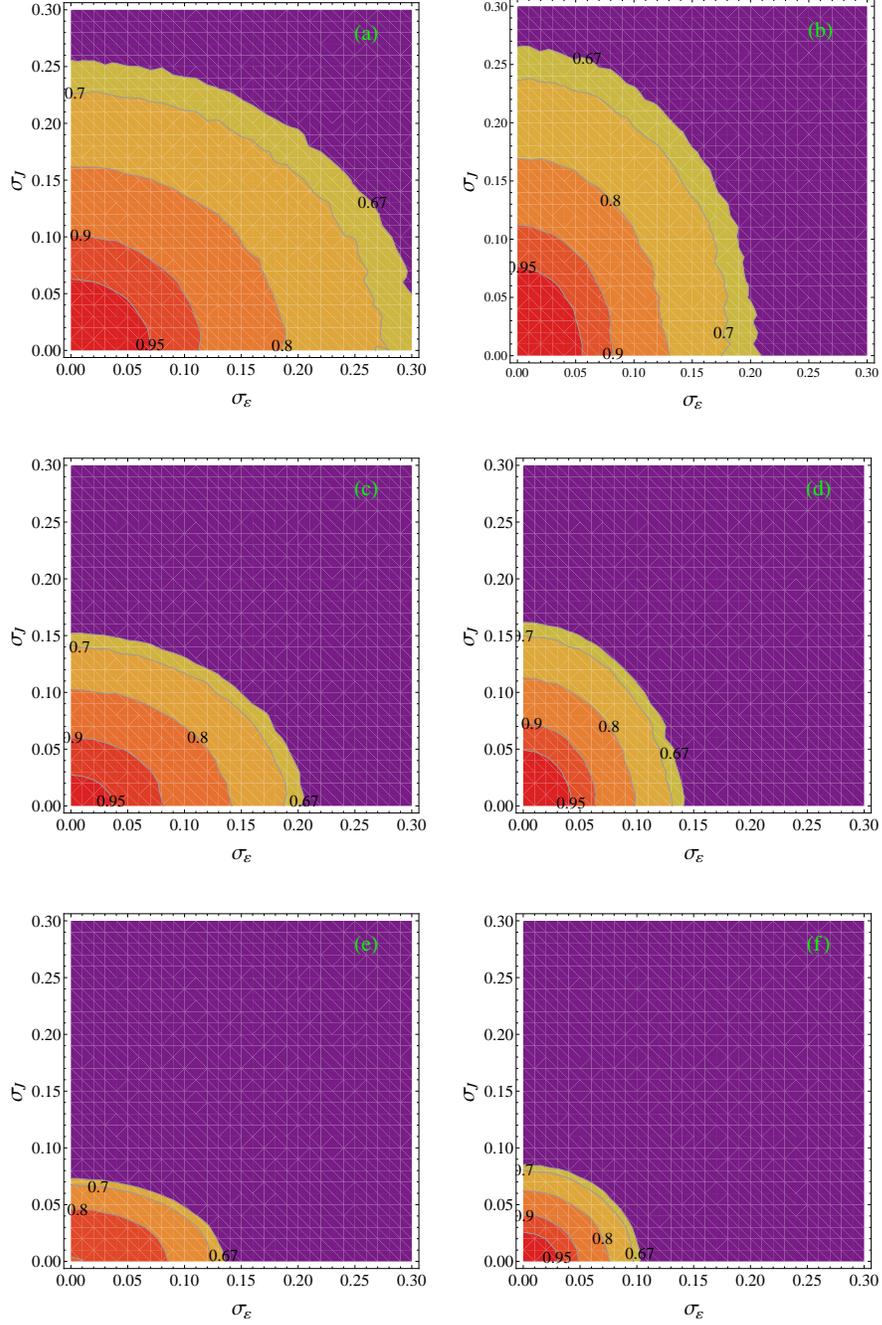


Figure 4.5:  $F_\psi(\tau_c)$  fidelity for  $|\beta|^2 = 0.4$ (top),  $|\beta|^2 = 0.6$ (middle) and  $|\beta|_{min}^2$ (bottom) for the optimal protocol(left) and the spin-coupling protocol(right) for a spin chain of length  $N=50$

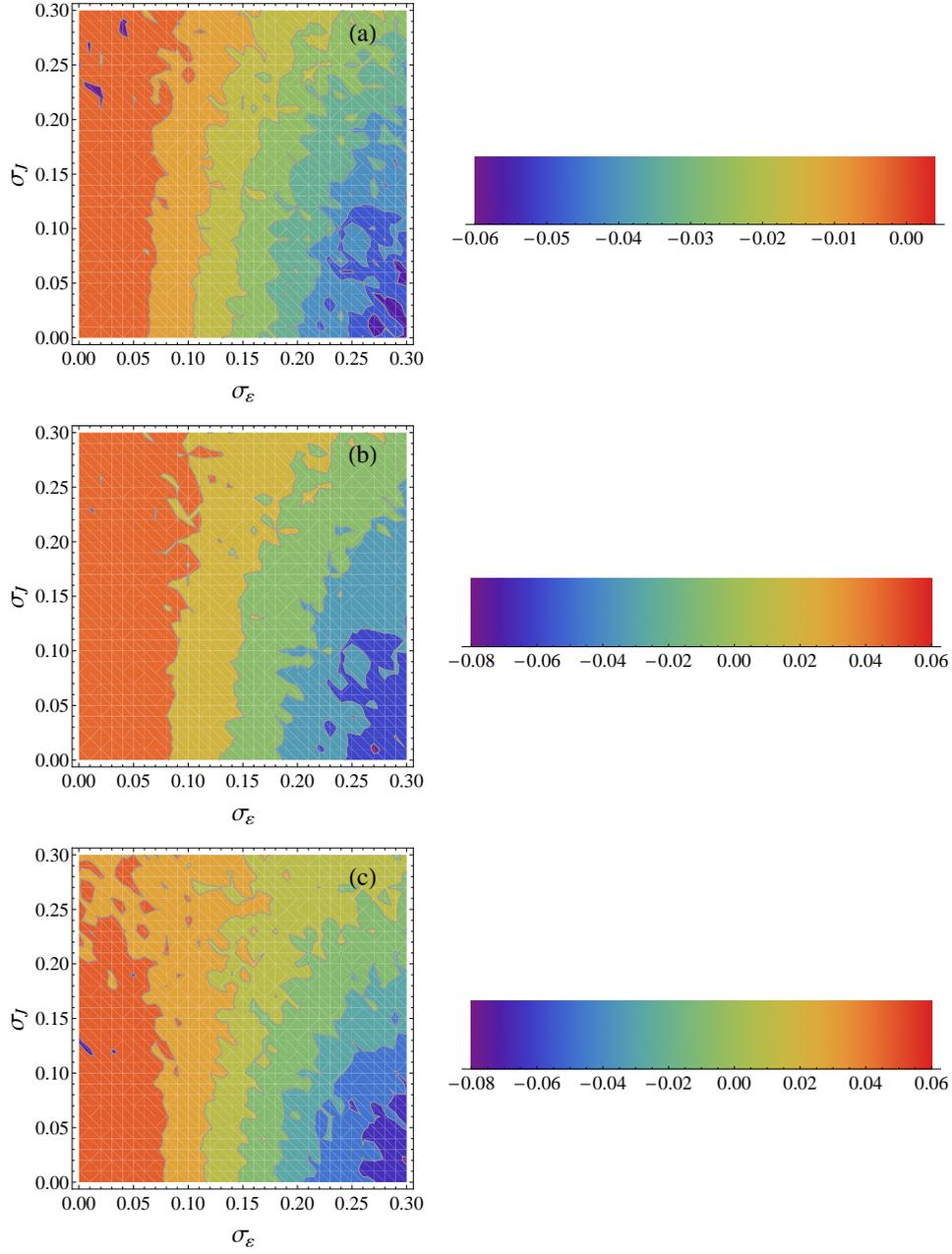


Figure 4.6:  $F_\psi(\tau_c)_{spin} - F_\psi(\tau_c)_{optimal}$  for  $|\beta|^2 = 0.4$  (top),  $|\beta|^2 = 0.6$  (middle) and  $|\beta|^2_{min}$  (bottom) for a spin chain of length  $N=15$

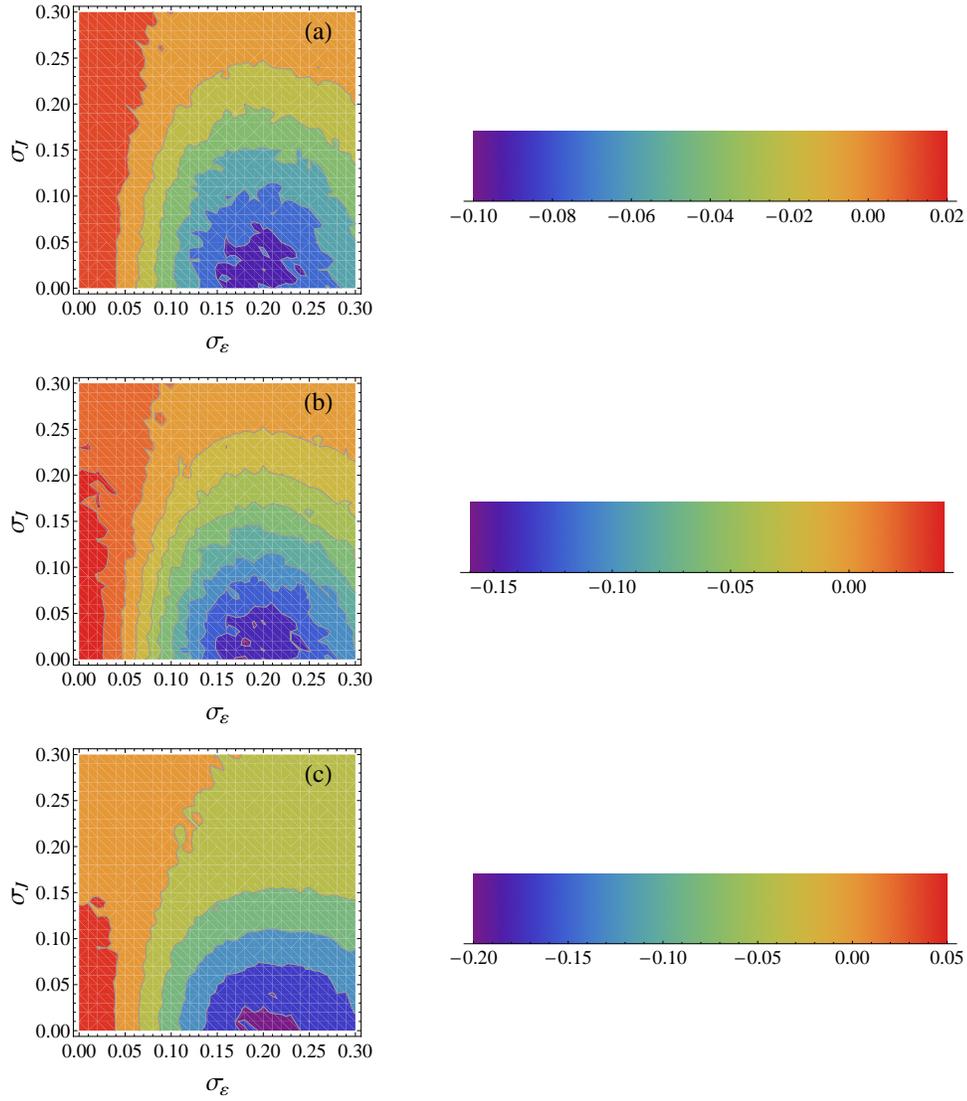


Figure 4.7:  $F_\psi(\tau_c)_{spin} - F_\psi(\tau_c)_{optimal}$  for  $|\beta|^2 = 0.4$  (top),  $|\beta|^2 = 0.6$  (middle) and  $|\beta|_{min}^2$  (bottom) for a spin chain of length  $N=50$

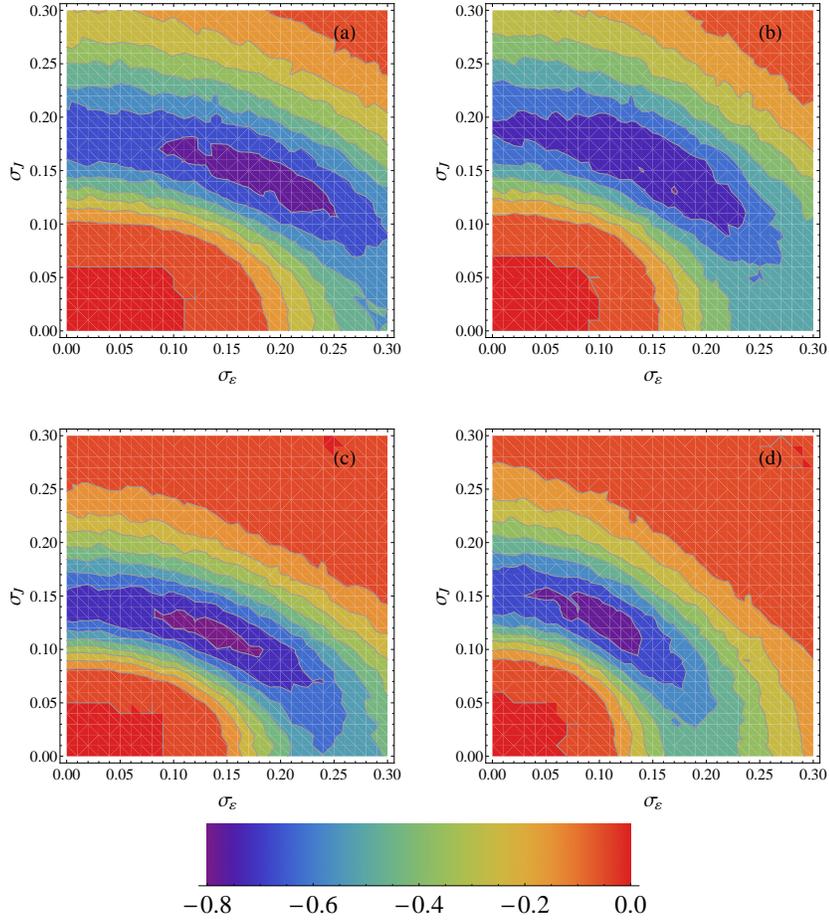


Figure 4.8:  $P(F_{min} > 0.67) - P(\bar{F} > 0.67)$  for the optimal protocol (left) and the spin coupling protocol(right) for number of spin sites  $N=15$ (top) and  $N=25$ (bottom)

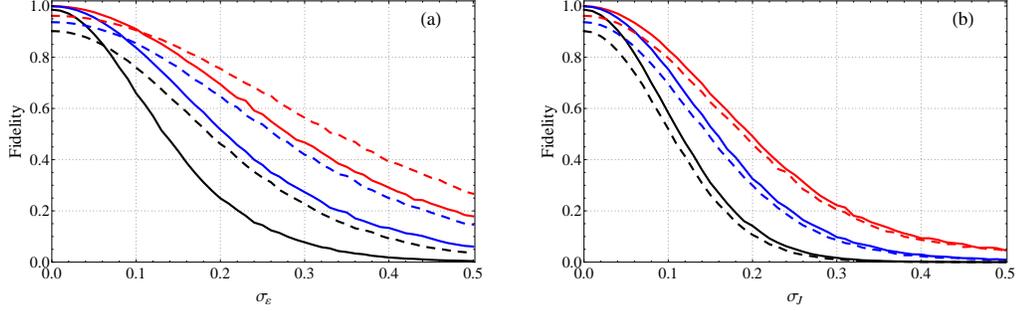


Figure 4.9: The Fidelity  $F_{min}(\tau_c)$  for the optimal protocol (dashed lines) and the spin coupling protocol (solid lines) as a function of (a)  $\sigma_\epsilon$  disorder for  $\sigma_J = 0$  and (b)  $\sigma_J$  disorder for  $\sigma_\epsilon = 0$  for  $N=15$  (red),  $N=25$  (blue) and  $N=50$  (black) number of spin sites

quality for  $|\beta|^2 \in [0.6, 1.0]$  therefore the Bloch averaged fidelity cannot be a reliable measure for the information quality since it cannot provide us a consistent decision whether or not the protocol fails to transmit information. A more reliable measure could be the  $F_{min}(\tau_c)$  fidelity since it satisfies basic three criterion: a) it is state independent b) it quantifies the information and c) it provides a lower bound for the fidelity. Although the lower bound it provides is rather loose, as we see from comparisons of the minimum fidelity to fidelities of different states (i.e  $F_\psi$ ) this measure can never fail since we cannot find a state with lower fidelity .

Similarly with the approximate relation of the state-averaged fidelity as a function of the disorder we find that for the  $F_{min}$

$$F_{min}(\tau_c) = [2\langle b \rangle_{min}^2 F_0 e^{-k_J N \sigma_J^2 - k_\epsilon N \sigma_\epsilon^2} + (1 - \langle |b|^2 \rangle_{min})], \quad (4.2.3)$$

where the parameters are again found by a numerical fit on the data. For the spin-coupling protocol  $F_0 = 0.5$ ,  $k_J \simeq 1.07$  and  $k_\epsilon \simeq 0.8$  while for the optimal protocol  $F_0 = \frac{|A_N(\tau_c)|^2}{3} + \frac{|A_N(\tau_c)|}{6}$ ,  $k_J \simeq 1.2$  and  $k_\epsilon \simeq 0.40$ . Furthermore note that  $\bar{|b|}_{min}^2$  is defined as the minimum state averaged over all disorder  $\sigma_\epsilon, \sigma_J$  configurations. In general one can assume an approximate relation for all  $|b|^2$

$$F_\psi(\tau_c) = [2|b|^2 F_0 e^{-k_J N \sigma_J^2 - k_\epsilon N \sigma_\epsilon^2} + (1 - |b|^2)], \quad (4.2.4)$$

### 4.3 Conclusions and further directions

We have presented a statistical analysis on the performance of Quantum state transfer Hamiltonians for the two protocols in the presence of static diagonal and off diagonal disorder. It has been shown that the Bloch averaged fidelity, usually employed in the literature for related studies, may fail to accurately describe the performance of the Hamiltonian for a large class of input states and it may lead us to faulty conclusions about the success of the transfer. As a solution to this ambiguity we recommend using the minimum fidelity which is typically employed for  $|\beta|^2 \simeq 0.94 - 1.0$  as a lower bound for the quality of transfer. Although it is not a tight bound and the quality of transfer can be considerably higher for small  $|\beta|^2$ , it is not misleading since it pertains to the "worst case scenario".

Additionally this study has shown that the optimal protocol is less susceptible to the diagonal disorder while the spin coupling is "slightly" less susceptible to the off diagonal disorder. In general we can characterize the optimal protocol more robust in a combined background of diagonal and off-diagonal disorder for medium size spin chains ( $N \geq 15$ ). For very small spin chains ( $N \leq 15$ ) the two protocols are almost equivalent and for very large spin chains  $N > 100$  the differences of the protocols will start to decrease until they become negligible due to the rapid decrease of fidelity with  $N$ .

In the present analysis we have considered only single-qubit states as most of related studies up to now do. Of course as mentioned in chapter 2, handling entangled states in a quantum system is of great importance in quantum information which should be explored in order to expand our general knowledge about the act of state transfer and as an alternative to the single-qubit state transfer, especially when the latter fails to achieve fidelities greater than  $2/3$ . Therefore an extension of this research would be to study the efficiency of transferring entangled states for the two quantum protocols in the presence of disorder, using previous results of Nikolopoulos et al. [?] and Karbach et al. [?]. Finally another interesting problem would be to study the effect of dissipation and decoherence for the two communication protocols which is one of the most important problems in quantum communication especially for large spin chains.



# Chapter 5

## Physical Implementations of Quantum Computing

### 5.1 Nuclear magnetic resonance

NMR quantum computing is one of the most mature technologies for implementing quantum computation. It utilizes the motion of spins of nuclei in custom-designed molecules manipulated by resonance frequency pulses[?, ?, ?]. The motion is on microscopic scale governed by the Schrodinger equation (??) in quantum mechanics. In fact liquid NMR receives more attention due to its technological maturity. NMR quantum computing is accomplished by using the spin-up and spin-down states of a  $\frac{1}{2}$  spin nucleus. A molecule with several nuclear spins may work as a quantum computer where each spin constitutes a qubit. The qubits are configured with different resonance frequencies and can be distinguished from each other. In a low viscosity liquid, dipolar coupling between nuclei is averaged out by the random motion of the molecules. The J-coupling dominates the spin-spin interaction, which is an indirect through-bond electronic interaction. As an example we could construct three qubits with a Hydrogen nucleus and two  $^{13}\text{C}$  nucleus which form a Trichloroethylene(TCE) molecule[?].

#### 5.1.1 Logical gates

A very interesting feature is the construction of the logical gates by controlling the applied magnetic field and the couplings between the nucleus. We

shall show how this can be achieved for one a qubit state and two a qubit state.

### one qubit logical gates

The Hamiltonian for a single qubit is [?]

$$H = -\vec{\mu} \cdot \vec{B}, \quad (5.1.1)$$

where  $\vec{m}$  is the magnetic moment and  $\vec{B} = B_0\mathbf{e}_z + B_1(e_x\cos(\omega t) + e_y\sin(\omega t))$ .

When  $B_1 = 0$  the Hamiltonian becomes  $H = \frac{\omega_0}{2}\sigma_z$

Suppose that the initial state is  $|\psi\rangle = a|0\rangle + b|1\rangle$ . Using the time evolution operator we get

$$e^{-i\frac{\omega_0}{2}\sigma_z}|\psi\rangle = \begin{pmatrix} e^{-i\frac{\omega_0}{2}t} & 0 \\ 0 & e^{i\frac{\omega_0}{2}t} \end{pmatrix} |\psi\rangle = R_z(\omega_0 t)|\psi\rangle \quad (5.1.2)$$

Therefore if we choose  $B_1 = 0$  we can construct the  $R_z(\omega_0 t)$  gate which is a rotation around z axis.

When  $B_1 \neq 0$  the Hamiltonian is given by

$$H = \frac{\omega_0}{2}\sigma_z + \frac{\omega_1}{2}(\sigma_x\cos(\omega t) + \sigma_y\sin(\omega t)) \quad (5.1.3)$$

To solve the Schrödinger equation we put the states to be rotating in a frame around z axis at frequency  $\omega$  there for state  $|\psi(t)\rangle = e^{-i\frac{\omega}{2}\sigma_z}|\phi(t)\rangle$ .

The schrödinger equation becomes

$$i\frac{\partial}{\partial t}|\phi(t)\rangle = \left( \frac{\omega_0 - \omega}{2}\sigma_z + \frac{\omega_1}{2}\sigma_x \right) |\phi(t)\rangle, \quad (5.1.4)$$

and the time evolution operator is  $U(t) = e^{-i(\frac{\omega_0 - \omega}{2}\sigma_z + \frac{\omega_1}{2}\sigma_x)t}$

this represents the rotation around the  $\mathbf{n}$  axis

$$\mathbf{n} = \frac{1}{\sqrt{1 + \left(\frac{\omega_1}{\omega_0 - \omega}\right)^2}} \left( \mathbf{e}_z + \frac{\omega_1}{\omega_0 - \omega} \mathbf{e}_x \right). \quad (5.1.5)$$

If  $\omega$  is much smaller compared to the others then we get

$$|\psi(t)\rangle = R_z(\omega_0 t)R_x(\omega_1 t)|\psi(0)\rangle. \quad (5.1.6)$$

Finally note that if the magnetic field acquires a phase  $\theta$  the magnetic field is  $\vec{B} = B_0 e_z + B_1(e_x \cos(\omega t + \theta) + e_y \sin(\omega t + \theta))$  and the time evolution operator becomes

$$U(t) = e^{-i(\frac{\omega_0 - \omega}{2} \sigma_z \cos(\theta) + \frac{\omega_1}{2} \sigma_x \sin(\theta))t} = \begin{pmatrix} \cos(\frac{\omega_1 t}{2}) & -i \sin(\frac{\omega_1 t}{2}) e^{-i\theta} \\ -i \sin(\frac{\omega_1 t}{2}) e^{i\theta} & \cos(\frac{\omega_1 t}{2}) \end{pmatrix} \quad (5.1.7)$$

This gate is called Rabi rotation gate

### • two qubit logical gates

We have analysed one qubit logical gates and thus we are ready to proceed in a more interesting case, the two qubit case, where we have two qubits entangled. The construction of a two-qubit gate requires the coupling of two spins. In a liquid sample of NMR, J-coupling is the dominating coupling between spins. Under the assumption that the resonance frequency difference between the coupled spins is much larger than the strength of the coupling, the total Hamiltonian of a two spin system without transverse magnetic field may be given as

$$H = \frac{\omega_1}{2} \sigma_z^1 + \frac{\omega_2}{2} \sigma_z^2 + \frac{J}{2} \sigma_z^1 \sigma_z^2. \quad (5.1.8)$$

The time evolution matrix takes the form

$$U(t) = \begin{pmatrix} e^{-i(\frac{\omega_1}{2} + \frac{\omega_2}{2} + \frac{J}{2})t} & 0 & 0 & 0 \\ 0 & e^{-i(\frac{\omega_1}{2} - \frac{\omega_2}{2} - \frac{J}{2})t} & 0 & 0 \\ 0 & 0 & e^{-i(\frac{-\omega_1}{2} + \frac{\omega_2}{2} - \frac{J}{2})t} & 0 \\ 0 & 0 & 0 & e^{-i(\frac{-\omega_1}{2} - \frac{\omega_2}{2} + \frac{J}{2})t} \end{pmatrix} \quad (5.1.9)$$

Therefore the rotations around z and x axis are

$$R_z^1(\pi/4) = \begin{pmatrix} e^{-i\frac{\pi}{4}} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\pi}{4}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\pi}{4}} & 0 \\ 0 & 0 & 0 & e^{i\frac{\pi}{4}} \end{pmatrix} \quad R_z^2(-\pi/4) = \begin{pmatrix} e^{i\frac{\pi}{4}} & 0 & 0 & 0 \\ 0 & e^{-i\frac{\pi}{4}} & 0 & 0 \\ 0 & 0 & e^{i\frac{\pi}{4}} & 0 \\ 0 & 0 & 0 & e^{-i\frac{\pi}{4}} \end{pmatrix} \quad (5.1.10)$$

$$R_y^1(\pi/4) = \frac{\sqrt{2}}{2} \begin{pmatrix} 1 & -1 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 0 & 1 & -1 \\ 0 & 0 & 1 & 1 \end{pmatrix} \quad R_y^2(-\pi/4) = \frac{\sqrt{2}}{2} \begin{pmatrix} 1 & 1 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 0 & 0 & 1 & 1 \\ 0 & 0 & -1 & 1 \end{pmatrix} \quad (5.1.11)$$

In the whole process we have supposed that we can turn off whenever we want the the J-couplings and operate independently the two spins. Practically this is not an easy operation and in fact is one of the major difficulties of the NMR quantum computation which is solvable with a special technique called refocusing. We apply a soft  $\pi$  pulse on the spare spin that we don't want to change at the middle point of the operation time duration while we are working on the target spin. The effect of the  $\pi$  pulse is that the coupling before the pulse cancels the one after the pulse, and thus we decouple our system. Finally we send another  $\pi$  pulse and we re-couple our system as it was in the beginning.

Mathematically this procedure can be expressed with the following statement

Assume that the Hamiltonian is  $H = \frac{\omega_1}{2}\sigma_z^1 + \frac{J}{2}\sigma_z^1\sigma_z^2 + A$ , where  $A = A(\sigma_z^2)$  then we have the following relation

$$e^{-iAt} = -R_x^1(\pi)e^{-iHt/2}R_x^1(\pi)e^{-iHt/2} \quad (5.1.12)$$

the above theorem tells us that both the chemical shift evolution (precession) and the J-coupling effect on spin 1 are removed and only the term  $\omega_2/over{2}\sigma_z^2$  remains. We obtain a z-rotation of spin 2 while freezing spin 1. By combining it with several hard pulses, we can also achieve any arbitrary rotation on spin 2 with the motion of spin 1 frozen. Similar computation shows that a hard  $\pi$  pulse applied at the middle point of the time duration cancels the chemical shift evolution of both spins. This can be seen by checking the following identity

$$e^{-iHt/2}R_x^1(\pi)R_x^2(\pi)e^{-iHt/2} = \begin{pmatrix} 0 & 0 & 0 & e^{-iJt/2} \\ 0 & 0 & e^{iJt/2} & 0 \\ 0 & e^{iJt/2} & 0 & 0 \\ e^{-iJt/2} & 0 & 0 & 0 \end{pmatrix} \quad (5.1.13)$$

Another hard  $\pi$  pulse can rotate two spins back, so we have achieved an evolution which has only the J-coupling effect, denoted by  $\mathbb{R}(\theta)$

$$\mathbb{R}(\theta) = \begin{pmatrix} e^{-i\theta t/2} & 0 & 0 & 0 \\ 0 & e^{i\theta t/2} & 0 & 0 \\ 0 & 0 & e^{i\theta t/2} & 0 \\ 0 & 0 & 0 & e^{-i\theta t/2} \end{pmatrix} \quad (5.1.14)$$

Combining these Rotations we can construct the CNOT transformation

$$W_{CNOT} = e^{-i\frac{\pi}{4}}R_z^1\left(\frac{\pi}{2}\right)R_y^2\left(-\frac{\pi}{2}\right)R_z^2\left(-\frac{\pi}{2}\right)\mathbb{R}\left(\frac{\pi}{2}\right)R_y^2\left(\frac{\pi}{2}\right) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix} \quad (5.1.15)$$

In ideal situation this simple pulse designing works perfectly. In practice decoherence causes the loss of quantum information with time, thus we must perform all operation within a short range of time, constrained by the energy relaxation time and the phase randomization time. An area of research is to find the shortest path between the identity matrix and a point in the space of  $SU(N)$  allowed by the system[?], and thus minimize the time needed to perform these operations.

## 5.2 Quantum Dots chain

Quantum dot chains look promising in the context of transmitting quantum information because of the relatively long relaxation time of the electron spins and the coherent manipulation they offer. Furthermore Quantum dot

chains have the practical advantage that we can easily manipulate the exchange couplings between neighbouring dots.

In general a quantum dot chain is a nanocrystal made of semiconductor materials small enough to exhibit quantum properties. As an example consider a linear array of nearly identical quantum dots which are electrostatically confined in a two-dimensional electron gas by means of metallic gates on top of a semiconductor heterostructure say GaAs/AlGaAs. The Hamiltonian of the system is described by the extended Mott-Hubbard Model [?],

$$H = \sum_{j,\alpha} \epsilon_{j\alpha} a_{j\alpha}^\dagger a_{j\alpha} + \frac{1}{2} \sum_j U n_j (n_j - 1) + \sum_{i<j,\alpha} t_{ij,\alpha} (a_{i\alpha}^\dagger a_{j\alpha} + H.c) + \sum_{i,j} V_{ij} n_i n_j. \quad (5.2.1)$$

The first term of the Hamiltonian is the kinetic term while the second term is a coulomb repulsion between the electrons of the j-th quantum dot. The other two terms describe interactions between quantum dots. In fact The third our well known tunnel effect and the fourth term is an interdot electrostatic interaction.

- $U = \frac{e^2}{8\pi\epsilon_r\epsilon_0} \int d^3\vec{r} d^3\vec{r}' |\Psi_{j\alpha}(\vec{r})|^2 |\Psi_{j\alpha}(\vec{r}')|^2 / |\vec{r} - \vec{r}'| \simeq e^2/C_g$ , with  $C_g = 8\epsilon_r\epsilon_0$  being the self-capacitance for a 2D disc-shaped quantum dot

- $a_{j\alpha}^\dagger, a_{j\alpha}$  creates/destroys a an electron in state  $\alpha$ (orbital and spin) with energy  $\epsilon_{j\alpha}$ . and electronic orbit  $\Psi_{j\alpha}\vec{r}$ .

- $t_{ij,\alpha} = \frac{\hbar}{2m^*} \int d^3\vec{r} \Psi_{i\alpha}^*(\vec{r}) \nabla^2 \Psi_{j\alpha}(\vec{r})$ , where  $m^*$  is the electron effective mass

- $V_{ij} \simeq U(C/C_g)^{|i-j|}$ , where C is the interdot capacitance

The problem is simplified if we assume that the Coulomb repulsion and the single electron spacing  $\Delta\epsilon$  is much larger than the tunneling rates  $U > \Delta\epsilon \gg t_{ij,a}$ . Then only the equivalent states are coupled to each other.

Similarly to the case of NMR the engineering of the couplings and the use of external fields (for example magnetic field) can construct one and two qubit gates, and thus perform mathematical operations which lead us to the realization of a quantum computer.

### 5.2.1 one qubit gates

Suppose that we have doped each quantum dot with a single electron occupying the ground state with proper voltage application to the metal gates. In this case our qubit is described by

$$\begin{aligned} |\uparrow\rangle &\equiv |0\rangle \\ |\downarrow\rangle &\equiv |1\rangle. \end{aligned} \tag{5.2.2}$$

where the quantization z-axis is taken perpendicular to the surface. If we apply a static magnetic field  $\vec{B}(x) = B_{\perp}(x)\vec{k}$  with large gradient along the x direction, we can achieve a Zeeman split in the degenerate spin states of the electron for each quantum dot. The energy split of the electron in the jth dot is  $\Delta E_j = 2\mu_B g_e B_{\perp}(x_j)$ . Using an ac magnetic field we create a driven two level system which is resonant in the frequency  $\omega_{j\uparrow\downarrow} = (E_{j\uparrow} - E_{j\downarrow})/\hbar$ . The characteristic spin-up spin-down state oscillations that occur are described by the Rabi frequency  $\Omega = \mu_e B_{\parallel}^{ac}/\hbar$ . Therefore proper choice of the phase and time duration  $\tau$  of the ac magnetic field, one can construct any unitary transformation[?]  $U_{\uparrow\downarrow}(\theta)$  with  $\theta = 2\Omega\tau$ .

### 5.2.2 two qubit gates

To construct a two-qubit gate we shall consider two neighbouring but relatively distant quantum dots A and B, each containing a single electron in the ground state [?, ?]. If the external magnetic field is zero the two spin states of the electron are degenerate, which in turn we set them as the zero point energy. The interaction(tunnelling elements) between the two electrons can be manipulated with the gate voltage. If the gate voltage is high the tunnelling is suppressed exponentially with the voltage and thus interaction is switched "off". On the other hand the interaction can be turned "on" if we lower the central barrier for a certain "switching" time  $\tau_s$ . Therefore our model can be approximated by

$$H(t) = J(t)\sigma_A^z\sigma_B^z, \tag{5.2.3}$$

where  $J(t) = t_{AB}^2(\tau_s)/U$ ,  $U$  denotes the charging energy of a single dot.

The time evolution operator is given by  $U(t) = \mathcal{T}exp(-i \int_0^t H(t') dt')$ . If  $J(t) = J_0$  for time  $\tau_s$  then  $U(t) = e^{-iJ_0\sigma_A^z\sigma_B^z\tau_s}$

The act of the time evolution operator with the choice  $J_0\tau_s = \pi \text{mod} 2\pi$   $U(t)|1^A 0^B\rangle = |0^A 1^B\rangle$ , and thus realizes the SWAP gate. Furthermore if the interaction is switched on for the shorter time  $\tau_s/2$  then  $U(\tau_s/2) = \sqrt{U(\tau_s)}$  which realizes the  $\sqrt{SWAP}$  gate. Finally using this result we can construct the CNOT gate as a composite object

$$W_{CNOT} = e^{i\pi/2\sigma_A^z} \sqrt{U(\tau_s)} e^{-i\pi/2\sigma_B^z} e^{i\pi\sigma_A^z} \sqrt{U(\tau_s)}. \quad (5.2.4)$$

Note that the above approximation is valid if the following criteria is satisfied

- $\Delta E \gg K_B T$ , where  $\Delta E$  is the energy spacing and  $T$  is the temperature. This ensures that the temperature cannot provide sufficient energy for transitions to higher-lying orbital states.
- $\tau_s \gg \Delta E/\hbar$  meaning that the switching time  $\tau_s$  to be such that the action of the Hamiltonian is "adiabatic enough" to prevent transitions to higher orbital levels.
- $t_{AB}(t_0) > U$  or all  $t$  in order for the Heisenberg approximation to be accurate
- $t_{decoherence} \gg \tau_s$  this ensures that all the operations within  $\tau_s$  can be done without significant "loss" of information.

### 5.3 Cold Atoms chain

Cold atoms are atoms maintained at nearly  $T=0$  K usually trapped and pre-cooled via laser cooling in a magneto-optical trap. To reach the lowest possible temperature, further cooling is performed using evaporative cooling

in a magnetic or optical trap. For bosonic atoms this state is a Bose-Einstein condensate and for fermionic atoms this is a degenerate Fermi gas. In order to be able to manipulate and control atomic qubits it is necessary to know the position of each of the atoms precisely. While random filling of optical lattices from laser cooled atoms and a superfluid filling of a lattice (with large particle number fluctuations as discussed above) do not provide sufficient knowledge on the position of the atoms a Mott Insulator state is ideally suited for this purpose. All the lattice sites are filled, i.e. each lattice site contains a qubit and the fluctuations in the occupation numbers are very small. For an appropriate choice of internal atomic states the optical lattice allows to trap both of them and thus can hold a quantum register for storing quantum information.

The Hamiltonian is a Bose-Hubbard model

$$H = -J \sum_{\langle i,j \rangle} a_i^\dagger a_j + \frac{U}{2} \sum_i n_i(n_i - 1) - \mu \sum_i n_i \quad (5.3.1)$$

In the Superfluidity phase i.e.  $T=0$  and the interactions are very small compared to  $J$ , the Hamiltonian becomes

$$H = -J \sum_{\langle i,j \rangle} a_i^\dagger a_j. \quad (5.3.2)$$

In the Mott Insulator state i.e.  $T=0$  and the interactions are large compared to  $H$ , the Hamiltonian becomes

$$H = \frac{U}{2} \sum_i n_i(n_i - 1). \quad (5.3.3)$$

## 5.4 Conditions for the realization of a quantum computer

A quantum computer would be a major technological advantage not because it simply speeds up the computational processes but because it changes completely the perspective for computing. In fact a quantum computer does not

speed up all the algorithms. For example obtaining the  $n$ th iterate of a function  $f(f(\dots f(x)))$  is not sped up at all, while on the contrary the factorization of an  $n$ -digit number (Shor's algorithm) is sped up exponentially. Moreover the amount of data required to communicate can be reduced quadratically. The crucial difference between classical based computer and quantum computers is that quantum computers introduce new tasks that have no classical counterparts like quantum cryptography and winning strategies in some games which are not available classically.

Unfortunately the realization of a quantum computer is a very difficult task since it requires almost the exact control of the conditions in a many-body system. However it is important to have some requirements[?] that will further guide us on which physical systems can be useful to construct a quantum computer.

- A scalable physical system with well characterized qubits
- The ability to initialize the state of the qubits to a simple fiducial state, such as  $|0_1\dots 0_N\rangle$
- Long relevant decoherence times, much longer than the gate operation time
- A universal set of quantum gates
- A qubit-specific measurement capability
- The ability to faithfully transmit quantum states from one place to another over short or long distances, depending the task.

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