Entanglement and Energy level crossing of Spin and Fermi Hamilton Operators

by

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Abstract

Entanglement is a quantum resource with applications in quantum communication as well as quantum computing amongst others. Since quantum entanglement is such an abstract concept numerous mathematical measures exist. Some of these have a purely theoretic purpose whereas others play a role in describing the magnitude of entanglement of a system. In quantum systems energy level crossing may occur. Energy levels in quantum systems tend to repel each other so when any type of degeneracy occurs where the energy levels coalesce or cross it is of interest to us. Two such points of degeneracy are exceptional and diabolic points. When these occur it is useful to investigate these points in specific systems and observe level crossing. In this thesis we mainly investigate the relationship between entanglement, energy level crossing and symmetry as well as the exceptional and diabolic points of specific systems. We are especially interested in systems described by spin and Fermi operators.

Contents

List of Symbols and Notation

$:=$	is defined as
$\in$	belongs to (a set)
$\emptyset$	empty set
$A \subset B$	subset A of set B
$\mathbb{N}$	natural numbers excluding 0
$\mathbb{N}_0$	natural numbers including 0
$\mathbb{R}$	real numbers
$\mathbb{R}^+$	nonnegative real numbers
$\mathbb{R}^n$	n-dimensional Euclidean space
$\mathbb{C}$	complex numbers
$\mathbb{C}^n$	n-dimensional complex linear space
i	$\sqrt{-1}$
$\omega_n := e^{2\pi i/n}$	n-th root of unity where $n \in \mathbb{N}$
$\mathbb{Z}_n$	cyclic group of order n under addition modulo n
$\mathbb{F}$	field
$\mathcal{P}_n$	Pauli group over n qubits
$\mathcal{H}$	Hilbert space
$\mathbf{x}$	column vector in $\mathbb{C}^n$
$\mathbf{x}^T$	transpose of $\mathbf{x}$ (row vector)
$\mathbf{x}^*$	conjugate transpose of $\mathbf{x}$ (row vector)
$\|.\|$	norm
$\mathbf{x} \cdot \mathbf{y} \equiv \mathbf{x}^*\mathbf{y}$	scalar product (inner product) in $\mathbb{C}^n$
$\langle .\|.\rangle$	scalar product in Hilbert space
$\mathbf{x} \times \mathbf{y}$	vector (cross) product in $\mathbb{R}^3$
$A \otimes B$	Kronecker product of matrices A and B
$A \oplus B$	direct sum of matrices A and B
$\det(A)$	determinant of square matrix A
$\mathrm{tr}(A)$	trace of square matrix A
$[A, B] := AB - BA$	commutator for square matrices A and B

$[A,B]_+ := AB + BA$	anticommutator for square matrices A and B
A^T	transpose of matrix A
$\overline{A}$	conjugate of matrix A
$A^* = (\overline{A})^T$	conjugate transpose of matrix A
δ_{jk}	Kronecker delta with $\delta_{jk} = 1$ for $j = k$ and $\delta_{jk} = 0$ for $j \neq k$
$\widehat{H}$	Hamilton operator
$\widehat{N}$	number operator
U	unitary matrix
Π	projection matrix
P	permutation matrix
$\hbar$	$h/2\pi$ with h the Planck constant
ω	frequency
t	time

The Pauli spin matrices are used extensively and are given by

$$\sigma_1 := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 := \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 := \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

where we may also refer to σ_x, σ_y and σ_z, respectively. The spin matrices for describing a spin-$\frac{1}{2}$ system are given by

$$s_1 := \frac{\sigma_1}{2} = \frac{1}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad s_2 := \frac{\sigma_2}{2} = \frac{1}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad s_3 := \frac{\sigma_3}{2} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

The spin matrices for describing a spin-1 system are given by

$$S_1 := \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S_2 := \frac{1}{\sqrt{2}}\begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \quad S_3 := \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}.$$

The Bell basis in $\mathbb{C}^4$ is used extensively and is given by

$$|\phi^+\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad |\phi^-\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix},$$

$$|\psi^+\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \quad |\psi^-\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}.$$

Chapter 1

Introduction

Quantum entanglement is a type of quantum correlation and is a powerful resource in quantum communication. Quantum entanglement occurs when particles interact physically and the interaction is such that each member of the pair may be described by a shared quantum state. The state of the individual particles is not well defined and is not the same for each member of the pair. Entanglement plays a large role in quatum communication and computing. It may be described as a type of quantum superposition. According to the Copenhagen interpretation the shared state is indefinite until measured. There is a correlation between the results of measurements performed on the entangled pair even if they are separated by an arbitrary distance. This feature of quantum entanglement sparked discussion between physicists and research into this phenomenon started in 1935 with papers from Einstein, Podolsky and Rosen [30] introducing the EPR-paradox. This is a thought experiment designed to show that quantum mechanical theory was incomplete. This was followed by letters from Schrödinger [108], [109] where he coined the term entanglement. Many of these papers highlighted the counterintuitive nature of entanglement and it was only in 1964 when Bell [6] highlighted a flaw in previous assumptions thereby showing the validity of quantum entanglement as a theory. This phenomenon has been proven experimentally and is recognized as a fundamental feature of quantum mechanics. Research is now focused on exploiting this resource.

Historically energy level crossing and symmetries was first discussed by Hund [56] in 1927 and the non-crossing rule was quantitatively formulated in 1929 by von Neumann and Wigner [147], proving the theorem put forward by Hund. This concept plays a large role in atomic chemistry, spectroscopy and quantum chemistry. Energy levels in quantum systems tend to repel each other so when any type of degeneracy occurs where the energy levels coalesce or cross it is of interest to us. Two such points of degeneracy are exceptional and diabolic points. When these occur it is useful to investigate these points in specific systems and observe level crossing. It is of importance to consider exceptional

points of hermitian and non-hermitian operators as have been studied by Kato [60] amongst others. Diabolic points were introduced by Berry in 1984 [11] where they play a large role in molecular magnets and interest in their study has increased when Berry noted that they behave as magnetic monopoles in parameter space. These points have also been studied by Teller [139].

In this thesis we mainly investigate the relationship between entanglement, energy level crossing and symmetry as well as the exceptional and diabolic points of specific systems. We are especially interested in systems described by spin and Fermi operators. In chapter 2 we introduce the mathematical concepts of Hilbert spaces, tensor products and group theory as these will be exploited in further chapters. In chapter 3 we provide some historical background on quantum theory introducing the postulates of quantum mechanics and giving a brief overview of the Schrödinger picture compared to the Heisenberg picture. In chapter 4 we introduce linear operators and investigate the properties of various normal matrices. We introduce the eigenvalue problem and investigate spin Hamilton operators and Hamilton operators of Fermi operators. In chapter 5 we introduce the concept of bipartite and multipartite entanglement as well as some applicable measures of entanglement. In chapter 6 we investigate the properties and differences of exceptional and diabolic points. We note that at an exceptional point the eigenvalues merge or coalesce and at a diabolic point the eigenvectors merge with bifurcations occuring at these points. We classify these singularities for both hermitian and non-hermitian Hamilton operators. We consider conservation laws, level crossings and symmetries. In chapter 7 we provide some sample Maxima programs implementing some of the concepts discussed throughout.

Chapter 2

Mathematical Preliminaries

2.1 Hilbert Spaces

An *abstract space* is a set of elements satisfying certain axioms. By changing the axioms, different spaces may be obtained. These abstract spaces help us to generalize various concepts. Hilbert spaces have been investigated by various authors such as Balakrishnan [3], Collatz [22], Debnath and Mikusiński [25], Jain [58], Kreyszig [69], Prugovečki [96], Richtmyer [100], Steeb [119], [120], [123], Weidmann [149], Yosida [157]. In this chapter we introduce the concept of Hilbert spaces as well as some useful applications. Hilbert spaces enable us to generalize the concept of the dot product and orthogonality to arbitrary vector spaces.

2.1.1 Definitions

An *inner product space* (also known as a pre-Hilbert space) is a vector space X with an *inner product* defined on X, where an inner product on X is a mapping from $X \times X$ into the scalar field of X. With every pair of vectors x and y there is associated a scalar written as $\langle x, y\rangle$ that satisfies the following properties

1. $\langle x + y, z\rangle = \langle x, z\rangle + \langle y, z\rangle$
2. $\langle \alpha x, y\rangle = \alpha \langle x, y\rangle$
3. $\langle x, y\rangle = \overline{\langle y, x\rangle}$
4. $\langle x, x\rangle \geq 0$ and $\langle x, x\rangle = 0 \Leftrightarrow x = 0$

for $x, y, z \in X$ and α a scalar. An inner product on X defines a *norm* on X

$$\|x\| \ = \ \sqrt{\langle x, x\rangle}.$$

From this we know the inner product also defines a *metric* on X

$$d(x,y) \;=\; \|x-y\| \;=\; \sqrt{\langle x-y, x-y\rangle}.$$

A *Hilbert space* is a complete inner product space. All inner product spaces are normed spaces but not all normed spaces are inner product spaces. Mathematically a Hilbert Space is a set $\mathcal{H}$ of elements or vectors that satisfies the following conditions

(a) If $x, y \in \mathcal{H}$ then there is a unique element $x + y \in \mathcal{H}$ where the addition operation $(+)$ is invertible, commutative and associative.

(b) If $c \in \mathbb{C}$ then for any $x \in \mathcal{H}$ there is an element $cx \in \mathcal{H}$ and the multiplication of elements by complex numbers thereby defined satisfies the distributive conditions $c(x + y) = cx + cy$ and $(c_1 + c_2)x = c_1x + c_2x$.

(c) Hilbert spaces $\mathcal{H}$ possess a zero element 0 characterized by the property that $0 + x = x$ for all elements $x \in \mathcal{H}$.

(d) For each pair of vectors $x, y \in \mathcal{H}$ there is a complex number $\langle x, y\rangle$ termed the inner product or scalar product of x with y. This satisfies the properties introduced above.

(e) If $\{x_n\}$ is a sequence in $\mathcal{H}$ satisfying the Cauchy condition that

$$\|x_m - x_n\| \to 0$$

as m and n tend independently to infinity then there is a unique element $x \in \mathcal{H}$ such that $\|x_n - x\| \to 0$ as $n \to \infty$.

Let $B = \{x_n : n \in I\}$ be an orthonormal basis in a Hilbert space $\mathcal{H}$. I is the countable index set. Then

$$\begin{aligned}
&\langle x_n, x_m\rangle = \delta_{nm} \\
&x = \sum_{n\in I} \langle x, x_n\rangle\, x_n \quad \forall x \in \mathcal{H} \\
&\langle x, y\rangle = \sum_{n\in I} \overline{\langle x, x_n\rangle}\, \langle y, x_n\rangle \quad \forall x, y \in \mathcal{H} \\
&\Big(\langle x, x_n\rangle = 0 \quad \forall x_n \in B\Big) \Rightarrow x = 0 \\
&\|x\|^2 = \sum_{n\in I} |\,\langle x, x_n\rangle\,|^2 \quad \forall x \in \mathcal{H}
\end{aligned}$$

where the third equation is also known as *Parseval's relation*. We have the inequalities

$$|\,\langle x, y\rangle\,| \le \|x\| \cdot \|y\|$$

$$\|x+y\| \leq \|x\| + \|y\|$$

and the *parallelogram equality*

$$\|x+y\|^2 + \|x-y\|^2 = 2(\|x\|^2 + \|y\|^2) \; \forall \; x, y \; \in \; X.$$

Consider the following useful corollaries

$$\begin{aligned}
\langle \alpha x + \beta y, z \rangle &= \langle \alpha x, z \rangle + \langle \beta y, z \rangle = \alpha \langle x, z \rangle + \beta \langle y, z \rangle \\
\langle x, \alpha y \rangle &= \overline{\langle \alpha y, x \rangle} = \overline{\alpha} \overline{\langle y, x \rangle} = \overline{\alpha} \langle x, y \rangle \\
\langle x, \alpha y + \beta z \rangle &= \overline{\alpha} \langle x, y \rangle + \overline{\beta} \langle x, z \rangle .
\end{aligned}$$

A useful concept is that of orthogonality. An element x of an inner product space X is said to be *orthogonal* to an element $y \in X$ if

$$\langle x, y \rangle = 0.$$

We say x and y are orthogonal and we write $x \perp y$. Similarly for subsets $A, B \subset X$ we write $x \perp A$ if $x \perp a$ for all $a \in A$ and $A \perp B$ if $a \perp b$ for all $a \in A$ and all $b \in B$.

2.1.2 Applications

The Hilbert space $\mathbb{C}^n$

The n-dimensional vector space $\mathbb{C}^n$ is the space of all ordered n-tuples of complex numbers. An element $x \in \mathbb{C}^n$ is given by

$$x = (x_1, x_2, \ldots, x_n)^T \text{ with } x_j \; \in \; \mathbb{C} \text{ for } j = 1, \ldots, n.$$

We define the inner product between two elements $x, y \in \mathbb{C}^n$ by

$$\langle x, y \rangle = \sum_{j=1}^{n} x_j \overline{y_j}.$$

This is also commonly known as the *dot product*. The inner product induces the norm

$$\|x\| = \sqrt{\langle x, x \rangle} = \sqrt{\sum_{j=1}^{n} |x_j|^2}.$$

From this we find the metric

$$d(x, y) = \|x - y\| = \sqrt{\sum_{j=1}^{n} |x_j - y_j|^2}.$$

The *standard basis* in $\mathbb{C}^n$ is given by

$$\begin{pmatrix}1\\0\\0\\\vdots\\0\end{pmatrix}, \quad \begin{pmatrix}0\\1\\0\\\vdots\\0\end{pmatrix}, \quad \ldots, \quad \begin{pmatrix}0\\0\\0\\\vdots\\1\end{pmatrix}.$$

Consider $\mathbb{C}^2$. The standard basis is obviously

$$\left\{\begin{pmatrix}1\\0\end{pmatrix}, \quad \begin{pmatrix}0\\1\end{pmatrix}\right\}.$$

Another useful basis in $\mathbb{C}^2$ is

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

which is also known as the *Hadamard basis* and plays a large role in quantum computing. We are also able to find

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}$$

as an orthonormal basis in $\mathbb{C}^2$. This leads us to the useful concept of *mutually unbiased bases* (MUB).

In a finite n-dimensional Hilbert space two complete, orthonormal bases $\mathcal{B}_1$, $\mathcal{B}_2$ are said to be mutually unbiased if and only if

$$\forall\, |u\rangle, |v\rangle \in \mathcal{B}_1, \mathcal{B}_2, \qquad |\langle u|v\rangle| = \frac{1}{\sqrt{n}}$$

for $\mathcal{B}_1 \neq \mathcal{B}_2$. The physical meaning of this is that knowledge that a system is in a particular state in one basis implies complete ignorance of its state in the other basis (Revzen [99]). There can be at most $n+1$ MUB in an n-dimensional Hilbert space where one of the bases will always be the standard basis. An explicit formula for the remaining bases for $n = p \neq 2$ where p is prime is given by

$$|m, b\rangle := \frac{1}{\sqrt{n}} \sum_{j=0}^{n-1} \omega_n^{\frac{b}{2}j(j-1)-jm} |e_j\rangle \quad \text{with} \quad b, m = 0, 1, \ldots, d-1$$

where b denotes the basis, m labels the state within the base and $\omega_n := e^{i2\pi/n}$ is the n-th root of unity. Program 1 determining these MUB is provided in the Computer algebra implementation chapter.

Example. The bases found for $\mathbb{C}^3$ are given by

$$\left\{\begin{pmatrix}1\\0\\0\end{pmatrix}, \quad \begin{pmatrix}0\\1\\0\end{pmatrix}, \quad \begin{pmatrix}0\\0\\1\end{pmatrix}\right\}$$

$$\left\{ \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} \frac{1}{\sqrt{3}} \\ -\frac{2(3i+\sqrt{3})}{12} \\ \frac{2(3i-\sqrt{3})}{12} \end{pmatrix}, \quad \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{2(3i-\sqrt{3})}{12} \\ -\frac{2(3i+\sqrt{3})}{12} \end{pmatrix} \right\}$$

$$\left\{ \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ \frac{\sqrt{3}i-1}{2} \end{pmatrix}, \quad \begin{pmatrix} \frac{1}{\sqrt{3}} \\ -\frac{2(3i+\sqrt{3})}{12} \\ -\frac{2(3i+\sqrt{3})}{12} \end{pmatrix}, \quad \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{2(3i-\sqrt{3})}{12} \\ \frac{1}{\sqrt{3}} \end{pmatrix} \right\}$$

$$\left\{ \frac{1}{\sqrt{3}} \begin{pmatrix} 1 \\ 1 \\ -\frac{\sqrt{3}i+1}{2} \end{pmatrix}, \quad \begin{pmatrix} \frac{1}{\sqrt{3}} \\ -\frac{2(3i+\sqrt{3})}{12} \\ \frac{1}{\sqrt{3}} \end{pmatrix}, \quad \begin{pmatrix} \frac{1}{\sqrt{3}} \\ \frac{2(3i-\sqrt{3})}{12} \\ \frac{2(3i-\sqrt{3})}{12} \end{pmatrix} \right\}. \qquad \clubsuit$$

Example. Consider the Hilbert space $\mathbb{C}^4$. The vectors

$$\mathbf{v}_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad \mathbf{v}_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \quad \mathbf{v}_3 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}, \quad \mathbf{v}_4 = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}$$

are linearly independent and form an orthonormal basis in the Hilbert space $\mathbb{C}^4$. These vectors form the *Bell basis* and will be used extensively. We have

$$\begin{pmatrix} a \\ b \\ c \\ d \end{pmatrix} = \frac{1}{\sqrt{2}} \Big((a+d)\mathbf{v}_1 + (a-d)\mathbf{v}_2 + (b+c)\mathbf{v}_3 + (b-c)\mathbf{v}_4 \Big).$$

Thus any arbitrary element may be constructed from these vectors. $\clubsuit$

The Hilbert space of $n \times n$ matrices over $\mathbb{C}$

Define the Hilbert space $\mathcal{H}$ to consist of all $n \times n$ matrices over $\mathbb{C}$. We define the inner product between two elements $A, B \in \mathcal{H}$ by

$$\langle A, B \rangle := \mathrm{tr}(AB^*)$$

where * denotes the conjugate transpose of the matrix and tr is the trace of a matrix given by

$$\mathrm{tr}(A) := \sum_{j=1}^{n} e_j^T A e_j$$

where e_j is the j^{th} basis element. The inner product induces the norm

$$\|A\|_F \;=\; \sqrt{\langle A, A \rangle} \;=\; \sqrt{\mathrm{tr}(AA^*)}.$$

This is also known as the *Frobenius norm*. As with any other vector space multiple matrix norms may be defined. The *Euclidean norm* for matrices is defined by

$$\|A\|_2 := \sum_{j,k=1}^{n} |(A)_{j,k}|^2$$

and the *max norm* is defined by

$$\|A\|_{\max} := \max_{\|x\|=1} \|Ax\|.$$

It can be shown that the Frobenius norm and the Euclidean norm are equivalent

$$\begin{aligned}\|A\|_F^2 = \operatorname{tr}(A^*A) &= \sum_{j=1}^{n} e_j^* A^* A e_j = \sum_{j,k=1}^{n} e_j^* A^* e_k e_k^* A e_j \\ &= \sum_{j,k=1}^{n} (e_k^* A e_j)^* (e_k^* A e_j) = \sum_{j,k=1}^{n} \overline{(A)}_{k,j} (A)_{k,j} \\ &= \sum_{j,k=1}^{n} |(A)_{k,j}|^2 = \|A\|_2^2.\end{aligned}$$

In the Hilbert space of 2×2 matrices over $\mathbb{C}$ the *standard basis* is given by

$$\begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix}.$$

Another basis in this Hilbert space that is used extensively consists of the identity matrix I_2 and the *Pauli matrices*

$$I_2 = \sigma_0 = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

2.2 Kronecker and Tensor Products

Before introducing tensor products we introduce a new form of notation called *Dirac notation* (Dirac [27]) (or bra-ket notation). Column vectors are represented by kets $|\psi\rangle$ and the conjugate transpose (which will now be a row vector) is represented by a bra $\langle\psi|$. When writing the inner product (in the case of $\mathbb{C}^n$ the dot product) between $|\psi\rangle$ and $|\phi\rangle$ we write $\langle\psi|\phi\rangle$. Normal vector rules apply, for instance if we have $|\psi\rangle$ and $|\phi\rangle$ in $\mathbb{C}^n$ the product $|\psi\rangle\langle\phi|$ will provide us with an $n \times n$ matrix as expected. We are able to combine vector spaces using certain operations to form another vector space. Two such operations are the *direct sum* and the *tensor product*. Borisenko and Tarapov [17], Dass and Sharma [23], Dirac [27], Gottfried and Yan [44], Prugovečki [96], Steeb et al [123], [121], [122], [119], [124], Williams [154] amongst others have investigated properties of these operations.

2.2.1 Definitions

Let $\mathcal{H}_1$ and $\mathcal{H}_2$ be Hilbert spaces. We may define a third Hilbert space $\mathcal{H}$ in terms of $\mathcal{H}_1$ and $\mathcal{H}_2$. For each pair of vectors f_1, f_2 in $\mathcal{H}_1$,$\mathcal{H}_2$ there is a corresponding vector $f_1 \otimes f_2$ in $\mathcal{H}$ such that

$$\langle f_1 \otimes f_2 | g_1 \otimes g_2 \rangle = \langle f_1 | g_1 \rangle_{\mathcal{H}_1} \langle f_2 | g_2 \rangle_{\mathcal{H}_2} .$$

We term $\mathcal{H}$ the *tensor product* of $\mathcal{H}_1$ and $\mathcal{H}_2$ and denote it by $\mathcal{H}_1 \otimes \mathcal{H}_2$ (Prugovečki [96]). If $\widehat{A}_1$ and $\widehat{A}_2$ are linear operators in $\mathcal{H}_1$ and $\mathcal{H}_2$ then we define the operator $\widehat{A}_1 \otimes \widehat{A}_2$ in $\mathcal{H} = \mathcal{H}_1 \otimes \mathcal{H}_2$ by

$$(\widehat{A}_1 \otimes \widehat{A}_2)(f_1 \otimes f_2) = (\widehat{A}_1 f_1) \otimes (\widehat{A}_2 f_2).$$

We say $\widehat{A}_1 \otimes \widehat{A}_2$ is the tensor product of $\widehat{A}_1$ and $\widehat{A}_2$. We can define the tensor product of n Hilbert spaces.

In the finite dimensional Hilbert spaces $\mathbb{C}^n$ and $\mathbb{R}^n$ the tensor product reduces to the *Kronecker product* (Graham [45], Steeb and Hardy [122], van Loan [143]). Consider A an $m \times n$ matrix and B an $s \times t$ matrix. The Kronecker product given by $A \otimes B$ is the $(ms) \times (nt)$ matrix

$$\begin{pmatrix} a_{11}B & a_{12}B & \cdots & a_{1n}B \\ a_{21}B & a_{22}B & \cdots & a_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1}B & a_{m2}B & \cdots & a_{mn}B \end{pmatrix}.$$

Some properties of the Kronecker product are

(a) It is associative
$$A \otimes (B \otimes C) = (A \otimes B) \otimes C.$$

(b) The relation with ordinary matrix multiplication is
$$(A \otimes B)(C \otimes D) = (AC) \otimes (BD)$$
where we assume that the matrix products AC and BD exist.

(c) $\mathrm{tr}(X \otimes Y) = \mathrm{tr}(X)\mathrm{tr}(Y)$ where X and Y are square matrices.

(d) $\det(X \otimes Y) = (\det(X))^m (\det(Y))^n$ where X is $n \times n$ and Y is $m \times m$.

(e) $(X \otimes Y)^{-1} = X^{-1} \otimes Y^{-1}$ provided the inverses of X and Y exist.

(f) $(A \otimes B)^* = A^* \otimes B^*$.

(g) If $A\mathbf{u} = \lambda\mathbf{u}$ and $B\mathbf{v} = \mu\mathbf{v}$ are eigenvalue equations then
$$(A \otimes B)(\mathbf{u} \otimes \mathbf{v}) = \lambda\mu(\mathbf{u} \otimes \mathbf{v}).$$
i.e. $\mathbf{u}\otimes\mathbf{v}$ is an eigenvector of $A\otimes B$ with eigenvalue $\lambda\mu$. Similarly $A\otimes I + I\otimes B$ has the eigenvector $\mathbf{u} \otimes \mathbf{v}$ with eigenvalue $\lambda + \mu$.

Further useful relations to keep in mind are

(a) If A, B are *normal matrices* then $A \otimes B$ is also normal since

$$(A \otimes B)^*(A \otimes B) = (A^*A) \otimes (B^*B) = (AA^*) \otimes (BB^*) = (A \otimes B)(A \otimes B)^*.$$

(b) If U and V are *unitary matrices* then $U \otimes V$ is also unitary since

$$(U \otimes V)(U \otimes V)^* = (U \otimes V)(U^* \otimes V^*) = (UU^*) \otimes (VV^*) = I_{n^2}.$$

(c) If H and K are *Hermitian matrices* then $H \otimes K$ is also Hermitian since

$$(H \otimes K)^* = H^* \otimes K^* = H \otimes K.$$

(d) If Π_1 and Π_2 are *projection matrices* then $\Pi_1 \otimes \Pi_2$ is also a projection matrix since

$$(\Pi_1 \otimes \Pi_2)^* = \Pi_1 \otimes \Pi_2 \text{ from above and } (\Pi_1 \otimes \Pi_2)^2 = \Pi_1^2 \otimes \Pi_2^2 = \Pi_1 \otimes \Pi_2.$$

Consider A an $m \times n$ matrix and B an $s \times t$ matrix. The *direct sum* given by $A \oplus B$ is the $(m+s) \times (n+t)$ matrix

$$\begin{pmatrix} A & 0_{m\times t} \\ 0_{s\times n} & B \end{pmatrix}.$$

Formally

$$(A \oplus B)_{j,k} = \begin{cases} (A)_{j,k} & j \in \{1, \cdots, m\},\ k \in \{1, \cdots, n\} \\ (B)_{j-m,k-n} & j \in \{m+1, \cdots, m+s\},\ k \in \{n+1, \cdots, n+t\} \\ 0 & \text{otherwise} \end{cases}$$

If two matrices A and B have the same size we may define the direct sum between these matrices in terms of the Kronecker product

$$A \oplus B = \begin{pmatrix} 1\,0 \\ 0\,0 \end{pmatrix} \otimes A \ + \ \begin{pmatrix} 0\,0 \\ 0\,1 \end{pmatrix} \otimes B.$$

2.2.2 Applications

Example. Given an orthonormal basis in $\mathbb{C}^n$ and an orthonormal basis in $\mathbb{C}^m$ we can construct an orthonormal basis in $\mathbb{C}^{n\times m}$ by taking all possible Kronecker products between elements. Consider the Hadamard basis in $\mathbb{C}^2$

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

From the Hadamard basis we may construct an orthonormal basis in $\mathbb{C}^4$

$$\frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix}\otimes\begin{pmatrix}1\\1\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1\\1\\1\\1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\1\end{pmatrix}\otimes\begin{pmatrix}1\\-1\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1\\-1\\1\\-1\end{pmatrix},$$

$$\frac{1}{2}\begin{pmatrix}1\\-1\end{pmatrix}\otimes\begin{pmatrix}1\\1\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1\\1\\-1\\-1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\-1\end{pmatrix}\otimes\begin{pmatrix}1\\-1\end{pmatrix}=\frac{1}{2}\begin{pmatrix}1\\-1\\-1\\1\end{pmatrix}. \qquad \clubsuit$$

Example. We may extend the above concept to matrices. Consider the Hilbert space of all 2×2 matrices over $\mathbb{C}$ where a basis is given by the identity matrix $\sigma_0 = I_2$ and the Pauli matrices σ_1, σ_2, σ_3. Using this basis of 2×2 matrices over $\mathbb{C}$ we obtain a basis for 4×4 matrices over $\mathbb{C}$ from the 16 Kronecker products

$$\sigma_j\otimes\sigma_k \text{ with } j,k=0,1,2,3. \qquad \clubsuit$$

Example. Some vectors in the Hilbert space $\mathbb{C}^4$ can be written as the Kronecker product of two vectors in the Hilbert space $\mathbb{C}^2$. Then we say the state is *separable*. An example of a separable state is given by

$$\frac{1}{2}\begin{pmatrix}1\\-1\\1\\-1\end{pmatrix}=\frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}\otimes\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}.$$

However in almost all cases a vector in $\mathbb{C}^4$ cannot be written as a product and then we say the vector is *entangled*. Examples of entangled states are the Bell basis

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix},\quad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix},\quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix},\quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}. \qquad \clubsuit$$

Example. Consider the γ-matrices which are important for the Dirac equation

$$\gamma_1=\begin{pmatrix}0&0&0&-i\\0&0&-i&0\\0&i&0&0\\i&0&0&0\end{pmatrix},\quad \gamma_2=\begin{pmatrix}0&0&0&-1\\0&0&1&0\\0&1&0&0\\-1&0&0&0\end{pmatrix},$$

$$\gamma_3=\begin{pmatrix}0&0&-i&0\\0&0&0&i\\i&0&0&0\\0&-i&0&0\end{pmatrix},\quad \gamma_4=\begin{pmatrix}1&0&0&0\\0&1&0&0\\0&0&-1&0\\0&0&0&-1\end{pmatrix}.$$

We may write these matrices as Kronecker products of the Pauli spin matrices and I_2. We see that

$$\gamma_1 = \sigma_2 \otimes \sigma_1, \quad \gamma_2 = \sigma_2 \otimes \sigma_2, \quad \gamma_3 = \sigma_2 \otimes \sigma_3, \quad \gamma_4 = \sigma_3 \otimes \sigma_0.$$

We now find the anticommutators using properties of the Kronecker product

$$\begin{aligned}[\gamma_4, \gamma_1]_+ &= \gamma_4\gamma_1 + \gamma_1\gamma_4 \\ &= (\sigma_3 \otimes \sigma_0)(\sigma_2 \otimes \sigma_1) + (\sigma_2 \otimes \sigma_1)(\sigma_3 \otimes \sigma_0) \\ &= (\sigma_3\sigma_2) \otimes \sigma_1 + (\sigma_2\sigma_3) \otimes \sigma_1 \\ &= (\sigma_3\sigma_2 + \sigma_2\sigma_3) \otimes \sigma_1 = 0_4\end{aligned}$$

where 0_4 is the 4×4 zero matrix. Similarly we find $[\gamma_4, \gamma_2]_+ = [\gamma_4, \gamma_3]_+ = 0_4$. ♣

Example. We define the matrices

$$s_+ := \begin{pmatrix} 0\,1 \\ 0\,0 \end{pmatrix}, \quad s_- := \begin{pmatrix} 0\,0 \\ 1\,0 \end{pmatrix}$$

and

$$\begin{aligned}s_{j,+} &:= I_2 \otimes \ldots \otimes I_2 \otimes s_+ \otimes I_2 \otimes \ldots \otimes I_2 \\ s_{j,-} &:= I_2 \otimes \ldots \otimes I_2 \otimes s_- \otimes I_2 \otimes \ldots \otimes I_2\end{aligned}$$

where $s_\pm$ is at the j-th position and there are n Kronecker products. Let

$$P_j := s_{j,+}s_{j,-}.$$

We have

$$s_+s_- = \begin{pmatrix} 1\,0 \\ 0\,0 \end{pmatrix}$$

with $(s_+s_-)^2 = s_+s_-$ and $(s_+s_-)^* = s_+s_-$ so that s_+s_- is a projection matrix. Thus

$$P_j = I_2 \otimes \ldots \otimes I_2 \otimes \begin{pmatrix} 1\,0 \\ 0\,0 \end{pmatrix} \otimes I_2 \otimes \ldots \otimes I_2.$$

Since $I_2^2 = I_2^* = I_2$ it follows that $P_j^2 = P_j$ and $P_j^* = P_j$ so that P_j is a $2^n \times 2^n$ projection matrix. ♣

Example. Let σ_1, σ_2, σ_3 be the Pauli spin matrices. We define

$$R := \sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3.$$

Since $\mathrm{tr}(\sigma_1) = \mathrm{tr}(\sigma_2) = \mathrm{tr}(\sigma_3) = 0$ and $\mathrm{tr}(A \otimes B) = \mathrm{tr}(A)\mathrm{tr}(B)$ we see that $\mathrm{tr}(R) = 0$ so that $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 0$ where λ_j are the eigenvalues of R. We see that

$$R^2 = (\sigma_1 \otimes \sigma_1)^2 + (\sigma_2 \otimes \sigma_2)^2 + (\sigma_3 \otimes \sigma_3)^2 - 2(\sigma_1 \otimes \sigma_1 + \sigma_2 \otimes \sigma_2 + \sigma_3 \otimes \sigma_3) = 3I_4 - 2R.$$

We may use this to find the eigenvalues of R. From the eigenvalue equation we obtain

$$R^2\mathbf{u} = \lambda R\mathbf{u} = \lambda^2\mathbf{u}$$

so that

$$(3I_4 - 2R)\mathbf{u} = (3 - 2\lambda)\mathbf{u} = \lambda^2\mathbf{u}.$$

So $(\lambda^2 + 2\lambda - 3)\mathbf{u} = \mathbf{0}$. Thus $\lambda_+ = 1$ and $\lambda_- = -3$. Since $\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 = 0$ we see that $\lambda_{1,2,3} = 1$ and $\lambda_4 = -3$. ♣

Example. We find the vectors $\mathbf{u} \in \mathbb{C}^{16}$ such that

$$\begin{aligned}(I_2 \otimes \sigma_3 \otimes \sigma_1 \otimes \sigma_3)\mathbf{u} &= \mathbf{u}, \qquad (\sigma_3 \otimes \sigma_0 \otimes \sigma_3 \otimes \sigma_1)\mathbf{u} = \mathbf{u},\\ (\sigma_1 \otimes \sigma_3 \otimes \sigma_0 \otimes \sigma_3)\mathbf{u} &= \mathbf{u}, \qquad (\sigma_3 \otimes \sigma_1 \otimes \sigma_3 \otimes \sigma_0)\mathbf{u} = \mathbf{u}.\end{aligned}$$

The vector $\mathbf{u}$ that satisfies these conditions is

$$\mathbf{u} = [a\,(1\,1\,1\,{-1}\,1\,1\,{-1}\,1\,1\,{-1}\,1\,1\,{-1}\,1\,1\,1)]^T.$$ ♣

Example. Let σ_1, σ_2, σ_3 be the Pauli spin matrices. We define the 16×16 matrices

$$\begin{aligned}\gamma_1 &:= \sigma_2 \otimes \sigma_2 \otimes \sigma_2 \otimes \sigma_2, \quad \gamma_2 := \sigma_0 \otimes \sigma_1 \otimes \sigma_2 \otimes \sigma_2\\ \gamma_3 &:= \sigma_0 \otimes \sigma_3 \otimes \sigma_2 \otimes \sigma_2, \quad \gamma_4 := \sigma_1 \otimes \sigma_2 \otimes \sigma_0 \otimes \sigma_2\\ \gamma_5 &:= \sigma_3 \otimes \sigma_2 \otimes \sigma_0 \otimes \sigma_2, \quad \gamma_6 := \sigma_2 \otimes \sigma_0 \otimes \sigma_1 \otimes \sigma_2\\ \gamma_7 &:= \sigma_2 \otimes \sigma_0 \otimes \sigma_3 \otimes \sigma_2, \quad \gamma_8 := \sigma_0 \otimes \sigma_0 \otimes \sigma_0 \otimes \sigma_1\end{aligned}$$

and

$$c_j := \frac{1}{2}(\gamma_{2j} + i\gamma_{2j-1}), \quad c_j^\dagger := \frac{1}{2}(\gamma_{2j} - i\gamma_{2j-1})$$

for $j = 1, 2, 3, 4$. We find the anticommutators

$$[c_j, c_k]_+ = [c_j^\dagger, c_k^\dagger]_+ = 0_{16} \text{ and } [c_j, c_k^\dagger]_+ = \delta_{jk} I_{16}.$$

These satisfy the *Fermi anticommutation relations* (which will be discussed further in chapter 4.4) so that $c_j^\dagger$ and c_j are *Fermi creation* and *annihilation operators*. ♣

The *vec operator* converts any matrix into a column vector. Let A be a matrix with n columns, each represented by the column vector $\mathbf{a}_n$. I.e.

$$A = \begin{pmatrix}\mathbf{a}_1\,\mathbf{a}_2 \cdots \mathbf{a}_n\end{pmatrix}.$$

The vec operator forms a column vector by stacking each of the columns in A on top of each other. That is to say

$$\text{vec}(A) = \begin{pmatrix}\mathbf{a}_1\\ \mathbf{a}_2\\ \vdots\\ \mathbf{a}_n\end{pmatrix}.$$

A useful relationship is

$$\text{vec}(ABC) \;=\; (C^T \otimes A)\text{vec}(B).$$

From this it follows

$$\text{vec}(AB) \;=\; (I \otimes A)\text{vec}(B) \;=\; (B^T \otimes I)\text{vec}(A).$$

These are useful identities for solving matrix equations such as

$$AX + XB = C$$

where X is unknown. This problem becomes

$$\begin{aligned}\text{vec}(C) &= \text{vec}(AX) + \text{vec}(XB) \\ &= (I \otimes A)\text{vec}(X) + (B^T \otimes I)\text{vec}(X) \\ &= [I \otimes A + B^T \otimes I]\text{vec}(X)\end{aligned}$$

and now we can easily solve for X using elementary methods from linear algebra, converting back to matrix form at the end.

Example. Let A be an $n \times n$ matrix over C. We are able to find a matrix T_n such that

$$T_n\text{vec}(A) = \text{tr}(A)$$

is true, where $\text{tr}(A)$ is the trace of the matrix. We note that

$$\text{vec}(A) := \sum_{j=1}^{n} e_{j,n} \otimes (Ae_{j,n}) = (I_n \otimes A) \sum_{j=1}^{n} e_{j,n} \otimes e_{j,n}$$

and

$$\text{tr}(A) := \sum_{j=1}^{n} e_{j,n}^T A e_{j,n}$$

where $e_{j,n}$ denote the standard basis in $\mathbb{C}^n$. We find that $T_n = (\text{vec}(I_n))^T$. ♣

2.3 Group Theory

We discuss the mathematical field of group theory, starting with fundamental concepts and later introducing specific applications of group theory with focus on quantum theory and computing. Some authors who have studied group theory include Gallian [38], Ludwig and Falter [76], Miller [81], Milne [82], Nechaev et al [84], Planat and Jorrand [91], Steeb [120], Steeb and Hardy [124], Weyl [151], Wigner [153]. Group theory is the study of the mathematical entity known as a group.

2.3.1 Definitions

Consider a set G (not necessarily countable) together with a *binary operation* $\circ$ that assigns to each $a, b \in G$ an element $a \circ b \in G$. We say the set is closed under the operation. G is a *group* under the operation if the following axioms hold

1. $(a \circ b) \circ c \ = \ a \circ (b \circ c)$. (Associativity)
2. There exists an element $e \in G$ such that $a \circ e = e \circ a = a$ for all $a \in G$. This is known as the neutral or identity element of the group.
3. For every $a \in G$ there exists an element $a' \in G$ such that $aa' = a'a = e$. This is known as the inverse of a.

Depending on the binary operation given a group may be multiplicative or additive. We generalise the operation to multiplication and simplify discussion by denoting $a \circ b$ as ab, the additive case must however still be kept in mind. Some consequences of the axioms are that the identity element and inverse elements are unique. We indicate the unique inverse of an element a by a^{-1}. Another consequence is that the cancellation laws hold so that $ab = ac \Rightarrow b = c$ and $ba = ca \Rightarrow b = c$. For group elements $a, b \in G$ we have $(ab)^{-1} = b^{-1}a^{-1}$. We may summarise the interaction between elements in an operation table known as a *Cayley table*.

When $ab = ba$ we say the elements commute or are commutative. If $ab = ba$ for all elements in the group we say the group is commutative or *Abelian*. The Cayley table of an Abelian group is symmetrical about the diagonal. If G is a finite group such that the powers of one element generate the group ($G = \{a, a^2, \ldots, a^n = e\}$) we say the group is *cyclic* (denoted by $\langle a \rangle$) and it is generated by a. For an element $a \in G$ define

$$a^n = \begin{cases} aa \cdots a & n > 0 \ (n \text{ copies of } a) \\ e & n = 0 \\ a^{-1}a^{-1} \cdots a^{-1} & n < 0 \ (|n| \text{ copies of } a^{-1}) \end{cases}.$$

The *order of a group* is denoted by $|G|$ and is the number of elements in the group. The order of group may be finite or infinite. We also talk about the cardinality of the group. The *order of an element* $g \in G$ denoted by $|g|$ is the least number of times the element must be multiplied by itself to obtain the identity element. Symbolically $g^n = e$ implies that $|g| = n$.

A fundamental (non-Abelian) group that may be considered is the *general linear group* of $n \times n$ matrices over a field $\mathbb{F}$ where $\mathbb{F}$ is in general taken to be $\mathbb{C}$ or $\mathbb{R}$. We denote this by $GL(n, \mathbb{F})$ and this group consists of all $n \times n$ matrices over $\mathbb{F}$ with non-zero determinant where the group operation is matrix multiplication. Since the determinant of all matrices in the group is non-zero each element will have an inverse element and the identity element is the $n \times n$ identity matrix

denoted by I_n. Matrix groups are used extensively in this dissertation since we focus on the matrix mechanics formulation of quantum theory.

If a subset H of a group G is itself a group under the operation of G, we say H is a *subgroup* of G. A subgroup is said to be proper if it is not the entire group, in other words $H \neq G$ or $H \subset G$. The subgroup consisting only of the identity element is said to be the trivial subgroup. As an example the set consisting of all $n \times n$ matrices over $\mathbb{F}$ (where $\mathbb{F}$ is again taken to be $\mathbb{C}$ or $\mathbb{R}$ in general) with determinant equal to 1 is a subgroup of $GL(n, \mathbb{F})$. This subgroup is known as the *special linear group* of $n \times n$ matrices over $\mathbb{F}$ and is denoted by $SL(n, \mathbb{F})$.

Let G be a group and H a subgroup. We define the left and right *cosets* by

$$gH := \{gh : h \in H\}, \quad Hg := \{hg : h \in H\}.$$

If for all $g \in G$ the cosets are equal we say the subgroup H is a *normal* or *invariant* subgroup of G. This is denoted by $H \triangleleft G$.

The *center of a group* G denoted by $Z(G)$ is the subset of elements in G that commute with all other elements in G, i.e.

$$Z(G) := \{a \ \in \ G \mid ax = xa \ \forall \ x \ \in \ G\}.$$

It can be shown that the center of G is a subgroup of G.

Consider a fixed element g in a group G. The *centralizer* of g in G denoted by $C(g)$ is the set of all elements in G that commute with g, i.e.

$$C(g) := \{x \ \in \ G \mid xg = gx\}.$$

It can be shown that for each element g in a group G the centralizer of g is a subgroup of G.

A useful concept to consider is that of *permutations* where we may consider a permutation to be a mapping or function from a set A to itself. We may take this further and consider groups of permutations. Formally stated, given any set A and a collection G of bijections from A into itself that is closed under compositions and inverses. These bijections are known as permutations which simply put is a rearrangement of the objects in A. We say that G is a group of permutations acting on A.

An $n \times n$ binary matrix is called a *permutation matrix* if every row and column has exactly one 1 and 0s elsewhere. We may also see this as an $n \times n$ identity matrix where the rows have been permuted to create a new matrix. These matrices form a group under matrix multiplication. A permutation matrix is nonsingular with $\det(P_j) = \pm 1$ so that an inverse always exists. We see that $P_j P_j^T = I_n$ so that $P_j^{-1} = P_j^T$ where $j = 0, 1, \ldots, n! - 1$. For any n there are $n!$ permutations in the group. As an example for $n = 3$ there are the 6 permutation matrices

$$P_0 = \begin{pmatrix} 1\,0\,0 \\ 0\,1\,0 \\ 0\,0\,1 \end{pmatrix}, \quad P_1 = \begin{pmatrix} 1\,0\,0 \\ 0\,0\,1 \\ 0\,1\,0 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 0\,1\,0 \\ 1\,0\,0 \\ 0\,0\,1 \end{pmatrix},$$

$$P_3 = \begin{pmatrix} 0\,1\,0 \\ 0\,0\,1 \\ 1\,0\,0 \end{pmatrix}, \quad P_4 = \begin{pmatrix} 0\,0\,1 \\ 1\,0\,0 \\ 0\,1\,0 \end{pmatrix}, \quad P_5 = \begin{pmatrix} 0\,0\,1 \\ 0\,1\,0 \\ 1\,0\,0 \end{pmatrix}.$$

Program 2a in the Computer algebra implementation chapter generates permutation matrices for any given value of n.

It may be of interest to determine whether or not two elements in a group are *equivalent* to each other. Given a group G we say two elements $(a, b \in G)$ are equivalent if there exists $u \in G$ such that $u^{-1}au = b$. We denote this by $a \sim b$ This does satisfy an equivalence relation

1. Reflexivity:
   $a \sim a \; \forall \; a \in G$ where $u = e$.
2. Symmetry:
   $a \sim b$ then there exists $u \in G$ such that $u^{-1}au = b$
   $\Rightarrow a = ubu^{-1} = (u^{-1})^{-1}b(u^{-1}) = v^{-1}bv$ where $v = u^{-1} \in G$
   $\Rightarrow b \sim a$.
3. Transitivity:
   $a \sim b$ and $b \sim c$ then there exist $u, v \in G$ such that $u^{-1}au = b$ and $v^{-1}bv = c$
   $\Rightarrow (v^{-1}u^{-1})a(uv) = c$ or $(uv)^{-1}a(uv) = w^{-1}aw = c$ where $w = uv \in G$
   $\Rightarrow a \sim c$.

The subset of G consisting of elements which are equivalent to each other are called the *equivalence classes* of G. We achieve some simplification as a class may be treated as a single object. Distinction between members is trivial.

A *homomorphism* ϕ from a group $(G_1, \circ)$ to a group $(G_2, *)$ is a one-to-one mapping from G_1 to G_2 that preserves the group operation. Symbolically

$$\phi(a \circ b) = \phi(a) * \phi(b).$$

If the mapping is onto (invertible) we call it an *isomorphism* and say the groups are isomorphic. Symbolically we may write $G_1 \approx G_2$. In the case of an isomorphism we may conclude that the order of the groups is the same.

The *kernel* of a homomorphism ϕ from G_1 to a group with identity e_2 is the set

$$\text{Ker}(\phi) \; := \; \{x \; \in \; G_1 \mid \phi(x) = e_2\}.$$

In words the kernel of a homomorphism is the set of elements in G_1 that are mapped to the identity element in G_2.

Two useful group isomorphisms are *automorphisms* and *inner automorphisms* induced by a group element. Formally an isomorphism from a group G onto itself is called an automorphism of G. For $a \in G$ the function $\phi_a(x) = axa^{-1}$ for all $x \in G$ is the inner automorphism of G induced by a. The sets consisting of these isomorphisms are groups under function composition.

2.3.2 Applications

Pauli Group and Clifford Group

Two fundamental groups in quantum theory are the Pauli and Clifford groups and these have been studied by authors such as Dehaene and De Moor [26], Durt [28], Planat and Solé [92], Thas [142] amongst others. The *Pauli spin matrices* are given by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

These matrices are unitary and hermitian and may also be denoted by σ_x, σ_y, σ_z, respectively. They are elements of the Lie group $U(2)$. Sometimes the 2×2 identity matrix I_2 is included as a fourth Pauli matrix and may be referred to as σ_0. The Pauli matrices describe the *spin* of a system where this is a fundamental concept in quantum theory. The matrices $s_j := \sigma_j/2$ where $j = 1, 2, 3$ describe particles with spin $1/2$, i.e. the eigenvalues of the matrices s_j are $\pm 1/2$.

The *Pauli group* $\mathcal{P}_1$ is defined as

$$\mathcal{P}_1 := \{\pm I_2, \pm iI_2, \pm\sigma_1, \pm i\sigma_1, \pm\sigma_2, \pm i\sigma_2, \pm\sigma_3, \pm i\sigma_3\}$$

where the group operation is matrix multiplication. We say that this group operates on a single *qubit*. The group is not Abelian, the order is 16 and the identity element is obviously the identity matrix. A subgroup of $\mathcal{P}_1$ with 8 elements is given by

$$\{\pm I_2, \pm\sigma_1, \pm i\sigma_2, \pm\sigma_3\}.$$

We may extend the Pauli group to $2^n \times 2^n$ matrices acting on n-qubits. The group $\mathcal{P}_n$ of $2^n \times 2^n$ matrices is defined to consist of all n-fold tensor products of Pauli matrices and the multiplicative factors of $\pm 1, \pm i$ are included. Symbolically

$$\mathcal{P}_n \ := \ \{\ I_2,\ \sigma_1,\ \sigma_2,\ \sigma_3\}^{\otimes n} \ \otimes \ \{\ \pm 1,\ \pm i\}.$$

The order of the n-qubit Pauli group is $2^{2(n+1)}$ and it is generated by the Pauli matrices. Let S be a subgroup of the Pauli group $\mathcal{P}_n$ with $S = \{S_j\}$ and V_S the n-qubit subspace spanned by the states $\{|\psi_k\rangle\}$ such that

$$S_j\,|\psi_k\rangle = |\psi_k\rangle \ \text{ for all } j.$$

Then we say that S is the *stabilizer* of the subspace V_S and the states $|\psi_k\rangle$ are called *stabilizer states*.

The Clifford and Pauli groups are closely related. The n-qubit *Clifford group* $\mathcal{C}_n$ is the *normalizer* of the Pauli group. That is to say a $2^n \times 2^n$ unitary matrix U is an element of the Clifford group if and only if

$$UMU^* \in \mathcal{P}_n \text{ for each } M \in \mathcal{P}_n.$$

One may say that the Clifford group is the group of all matrices that leave the Pauli group invariant under conjugation. The Clifford group is the normalizer of the Pauli group in $U(2^n)$ where this is the group of all $2^n \times 2^n$ unitary matrices. $\mathcal{C}$ is defined by conjugation so that the overall phase of the unitary matrix is irrelevant. Both the Pauli and Clifford groups play a large role in error correction in quantum computing. Consider the matrix

$$U_H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = \frac{1}{\sqrt{2}}(\sigma_1 + \sigma_3) = U_H^*.$$

This is known as the *Hadamard gate* or the Walsh-Hadamard transform and plays a role in quantum computing. It is easily shown that this gate is an element of $\mathcal{C}_1$.

Finite Heisenberg Group

We now introduce the *finite Heisenberg group*, also known as the Heisenberg-Pauli group, where this has been studied by authors such as Kibler [63], Korbelář and Tolar [68], Vourdas [148] amongst others. This group plays an important role in quantum mechanics as the elements of this group provide some basic observables in finite dimensional Hilbert spaces. Let n be a positive integer. We define $\omega_n := e^{2i\pi/n} \in \mathbb{C}$ and we let Q_n and P_n denote the *generalized Pauli matrices*

$$Q_n := \text{diag}(1, \omega_n, \omega_n^2, \ldots, \omega_n^{n-1}) \ \in \ GL(n, \mathbb{C})$$
$$(P_n)_{j,k} := \delta_{j,k-1}, \quad j,k \in \mathbb{Z}_n, \qquad P_n \in GL(n, \mathbb{C}).$$

The subgroup of unitary matrices in the Lie group $GL(n, \mathbb{C})$ generated by Q_n and P_n defined by

$$\Pi_n := \left\{ \omega_n^j Q_n^k P_n^\ell \quad | \quad j,k,\ell \in \{0, 1, \ldots, n-1\} \right\}$$

is called the finite Heisenberg group. General properties of this group are

(a) The order of Π_n is n^3.

(b) The center of Π_n is given by

$$\left\{ \omega_n^j I_n \quad | \quad j \in \{0, 1, \ldots, n-1\} \right\}.$$

(c) $P_n Q_n = \omega_n Q_n P_n$.

Example. Let $n = 2$. We find the finite Heisenberg group

$$\Pi_2 = \left\{ \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}, \quad \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix}, \right.$$
$$\left. \begin{pmatrix} -1 & 0 \\ 0 & 1 \end{pmatrix}, \quad \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}, \quad \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \right\}.$$

Program 3 finding the finite dimensional Heisenberg group is provided in the Computer algebra implementation chapter. ♣

Braid Group

The braid group has been studied by authors such as Jacak et al [57], Kassel and Turaev [59], Georgiev [41], Manfredini et al [77], Nechaev et al [84], Rowell [104]. The braid group B_n of n strings has $n-1$ generators

$$\{\sigma_1, \sigma_2, \ldots, \sigma_{n-1}\}$$

with the relations

$$\begin{aligned}
&\sigma_i\sigma_{i+1}\sigma_i = \sigma_{i+1}\sigma_i\sigma_{i+1} \quad (1 \leq i < n-1)\\
&\sigma_i\sigma_j = \sigma_j\sigma_i \quad (|i-j| \geq 2)\\
&\sigma_i\sigma_i^{-1} = \sigma_i^{-1}\sigma_i = e
\end{aligned}$$

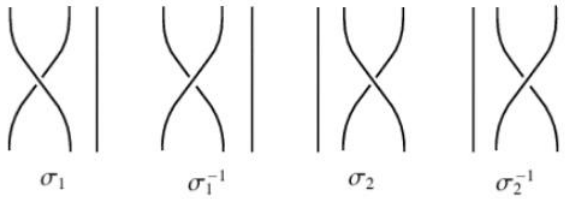

Figure 2.1: Graphical illustration of braids

Consider n strings oriented vertically from a lower to an upper bar. The least number of strings required to make a closed braid representation of a link n is called the *braid index*, where a link is a collection of knots which do not intersect but which may be linked together. Mathematically a knot is an embedding of a circle in 3-dimensional Euclidean space considered up to continuous isotopies. A general n-braid is constructed by iteratively applying the σ_i operator which switches the lower endpoints of the ith and $(i+1)$th strings keeping the upper endpoints fixed. The ith string is brought over the $(i+1)$th string. If the ith string passes below the $(i+1)$th string it is denoted by σ_i^{-1}. Any n-braid can be expressed as a *braid word*. As an example $\sigma_1\sigma_2\sigma_3\sigma_2^{-1}\sigma_1$ is a braid word in B_4.

Example. Consider the *braid relation*

$$(R \otimes I_2)(I_2 \otimes R)(R \otimes I_2) = (I_2 \otimes R)(R \otimes I_2)(I_2 \otimes R)$$

where R is a 4×4 matrix and I_2 is the 2×2 identity matrix. This is known as

the *Yang-Baxter equation*. We see that the *Bell matrix*

$$B := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \\ 0 & 1 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$$

satisfies this equality. Let

$$R := \begin{pmatrix} 0 & 0 & 0 & a \\ 0 & b & 0 & 0 \\ 0 & 0 & c & 0 \\ d & 0 & 0 & 0 \end{pmatrix}$$

the equality is satisfied when $b = c$. Program 4 which tests the equation is provided in the Computer algebra implementation chapter. ♣

2.4 Lie Groups and Lie Algebras

2.4.1 Definitions

Lie groups and Lie algebras have been studied by authors such as Belinfante and Kolman [7], de Azcárraga and Izquierdo[24], Fuchs [37], Pressley [94], Steeb and Hardy [124], Vilenkin and Klimyk [145]. An r parameter *Lie group* is an r dimensional smooth manifold that is also a group with smooth multiplication and inversion maps. An important example of a Lie group is the general linear group $GL(n, \mathbb{F})$ with $r = n^2$. Important Lie groups are

(a) Special linear group $SL(n, \mathbb{F}) \subset GL(n, \mathbb{F})$ with $\det A = 1$ and $r = n^2 - 1$.

(b) Orthogonal group $O(n) \subset GL(n, \mathbb{R})$ with $A^T A = I_n$ and $r = n(n-1)/2$.

(c) Unitary group $U(n) \subset GL(n, \mathbb{C})$ with $A^* A = I_n$ and $r = n^2$.

(d) Symplectic group $Sp(2n) \subset GL(2n, \mathbb{R})$ with

$$A^T J A = J = \begin{pmatrix} 0_n & -I_n \\ I_n & 0_n \end{pmatrix}$$

and $r = n(2n+1)$.

A real *Lie algebra* is a real vector space together with a bilinear map $[,] : L \times L \to L$ caled the *Lie bracket*. For the remainer of this dissertation we use the definition $[a, b] := ab - ba$. The following identities hold for all $a, b, c \in L$

(a) $[a, a] = 0$.

(b) $[a, [b, c]] + [b, [c, a]] + [c, [a, b]] = 0$ where this is the *Jacobi identity*.

(c) $[b,a] = -[a,b]$.

If $\mathcal{A}$ is an associative algebra over a field $\mathbb{F}$ with the definition

$$[a,b] := ab - ba, \qquad a,b \in \mathcal{A}$$

then $\mathcal{A}$ acquires the structure of a Lie algebra.

2.4.2 Applications

The $n \times n$ unitary matrices U form the compact Lie group $U(n)$ where unitary matrices are such that $U^*U = UU^* = I_n$ and so $U^* = U^{-1}$. Consider a quantum system that is described by a self-adjoint Hamilton operator $\widehat{H}$ acting on a Hilbert space $\mathcal{H}$. We consider the finite dimensional Hilbert space $\mathbb{C}^n$ and hermitian operators. It is of interest to us to find the $n \times n$ unitary matrices such that

$$U^*\widehat{H}U = \widehat{H}.$$

Note that if

$$U^*\widehat{H}U = \widehat{H} \quad \text{and} \quad V^*\widehat{H}V = \widehat{H}$$

then

$$(UV)^*\widehat{H}(UV) = \widehat{H}$$

and so we see that the set of unitary matrices that keep $\widehat{H}$ invariant form a group under matrix multiplication.

A finite subgroup of $U(n)$ are the $n \times n$ permutation matrices where there are $n!$ of these. For a given hermitian matrix $\widehat{H}$ we want to find all permutation matrices P such that $P^T\widehat{H}P = \widehat{H}$ where we note that $P^T = P^{-1}$. We are able to use the permutation matrices to construct projection matrices to decompose the Hilbert space into invariant sub-Hilbert spaces. If the permutation matrix P satisfies $P^2 = I_n$ then

$$\Pi_1 := \frac{1}{2}(I_n + P), \quad \Pi_2 := \frac{1}{2}(I_n - P)$$

are *projection matrices* which can be utilized to decompose the Hilbert space $\mathbb{C}^n$ into invariant subspaces.

Example. Let $c_j^\dagger$, c_j $(j = 1,2,3)$ be Fermi creation and annihilation operators (where these will be discussed in further detail in chapter 4.4). Consider the Hamilton operator

$$\widehat{H} = t(c_1^\dagger c_2 + c_1^\dagger c_3 + c_2^\dagger c_1 + c_2^\dagger c_3 + c_3^\dagger c_1 + c_3^\dagger c_2) + k_1 c_1^\dagger c_1 + k_2 c_2^\dagger c_2 + k_3 c_3^\dagger c_3$$

and the number operator

$$\widehat{N} := c_1^\dagger c_1 + c_2^\dagger c_2 + c_3^\dagger c_3.$$

Then $[H, \widehat{N}] = 0$. Given a basis with two Fermi particles

$$c_1^\dagger c_2^\dagger \left|0\right\rangle, \quad c_1^\dagger c_3^\dagger \left|0\right\rangle, c_2^\dagger c_3^\dagger \left|0\right\rangle.$$

We find the matrix representation of $\widehat{H}$

$$\widehat{H} = \begin{pmatrix} k_1 + k_2 & t & -t \\ t & k_1 + k_3 & t \\ -t & t & k_2 + k_3 \end{pmatrix}.$$

For the case $k_1 \neq k_2$, $k_1 \neq k_3$, $k_2 \neq k_3$ no symmetry is found. Similarly for $k_1 \neq k_2$, $k_1 \neq k_3$, $k_2 = k_3$ no symmetry is found. For $k = k_1 = k_2 - k_3$ the permutation matrix

$$P = \begin{pmatrix} 0\,0\,1 \\ 0\,1\,0 \\ 1\,0\,0 \end{pmatrix}$$

is obtained. Thus the projection matrices Π_1 and Π_2 defined above may be used to decompose the Hilbert space $\mathbb{C}^3$ into invariant subspaces. We find

$$\Pi_1 = \frac{1}{2}\begin{pmatrix} 1\,0\,1 \\ 0\,2\,0 \\ 1\,0\,1 \end{pmatrix}, \quad \Pi_2 = \frac{1}{2}\begin{pmatrix} 1 & 0 & -1 \\ 0 & 0 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

with

$$\Pi_1 \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} v_1 + v_3 \\ 2v_2 \\ v_1 + v_3 \end{pmatrix}, \quad \Pi_2 \begin{pmatrix} v_1 \\ v_2 \\ v_3 \end{pmatrix} = \frac{1}{2}\begin{pmatrix} v_1 - v_3 \\ 0 \\ -v_1 + v_3 \end{pmatrix}$$

where $\mathbf{v}$ is an arbitrary vector. So we see that Π_1 and Π_2 project into the subspaces spanned by the normalized vectors

$$\left\{ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \right\}$$

$$\left\{ \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ -1 \end{pmatrix} \right\}.$$

♣

Chapter 3

Quantum Theory

3.1 Postulates of Quantum Mechanics

We require a complete description of quantum theory and strive toward a theory that is consistent. There are two main formulations of quantum theory namely *matrix mechanics* that was developed by Heisenberg and his colleagues and *wave mechanics* that was developed by Schrödinger and his colleagues. The main difference between classical and quantum mechanics is that the quantum theory is a probabilistic description of nature. These differences between quantum and classical theory may be better understood when considering the *postulates* of quantum mechanics. These postulates may be formulated from different viewpoints (in specific we may consider them from a matrix mechanics view or from a wave function view) and with the focus placed on different aspects (for instance the focus will be different if we consider pure mechanics compared to if we considered the computing aspect of quantum theory). We are mostly interested in the matrix description of quantum theory. Many authors such as Dirac [27], Eisberg and Resnick [31], Flügge [34], Gasiorowicz [40], Glimm and Jaffe [43], Healey [48], Landau and Lifshitz [71], Messiah [80], Prugovečki [96], Schiff [107], Sewell [110], Shankar [112], Steeb [120], [123], Steeb and Hardy [124], ter Haar [140], von Neumann [146], Weyl [151], Wigner [153] have studied quantum theory. The standard postulates of quantum mechanics are given below.

Postulate 1: Let $\mathcal{S}$ denote a quantum system. The *pure states* of $\mathcal{S}$ may be described by normalized vectors $|\psi\rangle$ which are elements of some Hilbert space $\mathcal{H}$. We may visualize pure states as rays, in other words as unit vectors with arbitrary phase. This idea of representing a pure state by a ray leads to the probability interpretation of quantum mechanics. If we consider a physical system in state $|\psi\rangle$ then the probability of it being in the state $|\chi\rangle$ is given by

$$p = |\langle\psi|\chi\rangle|^2.$$

Since the states are normalized in $\mathcal{H}$ we know that $0 \leq p \leq 1$ as required from probability theory. The phase of $|\psi\rangle$ has no physical significance but the relative phase of vectors does have significance.

Example. Consider the Hilbert space $\mathcal{H} = \mathbb{C}^2$ and the normalized states

$$|\psi\rangle := \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi_1} \\ e^{i\phi_2} \end{pmatrix} \quad \text{and} \quad |\chi\rangle := \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

The probability p of the system to be in state $|\chi\rangle$ is given by

$$p(\phi_1, \phi_2) = |\langle\psi|\chi\rangle|^2 = \frac{1}{2}(1 + \cos(\phi_1 - \phi_2)).$$

p takes the maximum at 1 for $\phi_1 = \phi_2$ and the minimum at 0 for $\phi_1 - \phi_2 = \pi$. ♣

Postulate 2: Quantum states evolve in time according to the *Schrödinger equation*. We now introduce this equation for time independent $\widehat{H}$ as it is used in matrix mechanics

$$i\hbar \frac{\partial |\psi\rangle}{\partial t} = \widehat{H} |\psi\rangle .$$

$\widehat{H}$ is a self-adjoint operator that specifies the dynamics of the system. The solution to this partial differential equation is given by

$$|\psi(t)\rangle = \exp(-i\widehat{H}t/\hbar) |\psi(0)\rangle$$

where $|\psi(0)\rangle$ is the initial state of the system and is normalized so that $\langle\psi(0)|\psi(0)\rangle = 1$. We may simplify the expression to

$$|\psi(t)\rangle = \widehat{U}(t) |\psi(0)\rangle$$

where $\widehat{U}(t) = \exp(-i\widehat{H}t/\hbar)$ is a unitary operator.

Example. Consider the Hamilton operator

$$\widehat{H} := \hbar\omega\sigma_1 = \hbar\omega \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

where ω is the constant frequency. Then we find

$$\exp(-i\widehat{H}t/\hbar) = \begin{pmatrix} \cosh(-i\omega t) & \sinh(-i\omega t) \\ \sinh(-i\omega t) & \cosh(-i\omega t) \end{pmatrix} = \begin{pmatrix} \cos(\omega t) & -i\sin(\omega t) \\ -i\sin(\omega t) & \cos(\omega t) \end{pmatrix}.$$

Let

$$|\psi(0)\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

be the initial state. Then

$$|\psi(t)\rangle = \begin{pmatrix} -i\sin(\omega t) \\ \cos(\omega t) \end{pmatrix}$$

and the probability to find the state $|\psi(t)\rangle$ in the initial state $|\psi(0)\rangle$ is

$$p(t) = |\langle\psi(t)|\psi(0)\rangle|^2 = \cos^2(\omega t). \qquad \clubsuit$$

Example. Consider the Hamilton operator

$$\widehat{H} = \hbar\omega(\sigma_1 \otimes \sigma_3 \otimes \sigma_1)$$

in the Hilbert space $\mathbb{C}^8$ where σ_1 and σ_3 are Pauli spin operators and ω is the constant frequency. We find

$$\exp(-i\widehat{H}t/\hbar) = \cos(\omega t)I_8 - i\sin(\omega t)(\sigma_1 \otimes \sigma_3 \otimes \sigma_1).$$

Let

$$|\psi(0)\rangle = \begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix}$$

be the initial state. Then

$$|\psi(t)\rangle = \cos(\omega t)\begin{pmatrix}1\\0\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}1\\0\end{pmatrix} - i\sin(\omega t)\begin{pmatrix}0\\1\end{pmatrix} \otimes \begin{pmatrix}0\\-1\end{pmatrix} \otimes \begin{pmatrix}0\\1\end{pmatrix}.$$

The probability to find the state $|\psi(t)\rangle$ in the initial state $|\psi(0)\rangle$ is

$$p(t) = |\langle\psi(t)|\psi(0)\rangle|^2 = \cos^2(\omega t). \qquad \clubsuit$$

Postulate 3: Any quantity in a quantum system that can be measured or observed is known as an *observable*. Every observable a is associated with a self-adjoint operator $\widehat{A}$. For finite dimensional Hilbert spaces observables are represented by hermitian matrices. The only possible outcomes of a measurement on the observable a are the *eigenvalues* of $\widehat{A}$. Let λ_j represent the (real) eigenvalues of $\widehat{A}$ and $|\phi_j\rangle$ represent the corresponding normalized *eigenvectors*.

$$\widehat{A}\,|\phi_j\rangle = \lambda_j\,|\phi_j\rangle \text{ and } \langle\phi_j, \phi_k\rangle = \delta_{j,k}$$

must hold.

Example. Consider the linear hermitian operator

$$\widehat{A} = \frac{\hbar\omega}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix} = \omega S_x.$$

The possible outcomes of a measurement on this observable are $-\hbar\omega$, $\hbar\omega$, 0 with corresponding (normalized) eigenvectors

$$\frac{1}{2}\begin{pmatrix}1\\-\sqrt{2}\\1\end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix}1\\\sqrt{2}\\1\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\end{pmatrix}. \qquad \clubsuit$$

Postulate 4: Consider a quantum state described by the normalized vector $|\psi\rangle$. The measurement of observable a will yield an outcome λ_j with probability

$$p_j = |\langle\phi_j|\psi\rangle|^2$$

where $\langle\phi_j|\psi\rangle \in \mathbb{C}$ and $0 \leq p_j \leq 1$ must hold.

Example. Consider a quantum system described by the state

$$|\psi\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix}1\\1\\1\end{pmatrix}.$$

From the previous example the measurement of observable a will yield an outcome of $-\hbar\omega$ with probability $p_1 = \frac{3-2\sqrt{2}}{6}$, an outcome of $\hbar\omega$ with probability $p_2 = \frac{3+2\sqrt{2}}{6}$ and an outcome of 0 with probability $p_3 = 0$. $0 \leq p_j \leq 1$ and $\sum_{j=1}^{3} p_j = 1$ as required. ♣

Postulate 5: This is also known as the *projection postulate*. Immediately after measurement on a yields the value λ_j the state of the system is described by $|\psi_j\rangle$. The type of time evolution implied here is incompatible with postulate 2 and so we replace postulate 4 with the weaker postulate 4'.

Postulate 4': If a quantum system is described by the state $|\psi_j\rangle$ then a measurement on a will yield the outcome λ_j. This postulate eliminates the need for postulate 5.

Postulate 6: Observables in quantum mechanics are described by self-adjoint matrices (operators) that act on the Hilbert space $\mathcal{H}$. The *expected value* (average in a continuous system) of observable a with the corresponding operator A in the state $|\psi\rangle$ is given by

$$E_\psi(A) := \langle\psi, A\psi\rangle$$

where $\langle .,. \rangle$ is the *inner product* defined on $\mathcal{H}$.

When considering the Hilbert space of $n \times n$ matrices over $\mathbb{C}$ the inner product is defined by $\langle A, B\rangle := \mathrm{tr}(AB^*)$, where B^* is the conjugate transpose of B. We see that

$$E_\psi(\widehat{A}) = \langle\psi, \widehat{A}\psi\rangle = \mathrm{tr}(\psi(\widehat{A}\psi)^*) = \mathrm{tr}(\psi\psi^*\widehat{A}).$$

Example. Consider $\widehat{A} = \omega S_x$ from above and the state $|\psi\rangle = \frac{1}{\sqrt{3}}\begin{pmatrix}1&1&1\end{pmatrix}^T$. We see

$$E_\psi(\widehat{A}) = \frac{2\sqrt{2}\hbar\omega}{3}.$$ ♣

Postulate 7: This postulate relates to the evolution of a quantum system. There are two standard descriptions that may be considered namely the *Schrödinger picture* and the *Heisenberg picture*. This postulate ensures that the

probability of finding a system in a given state is independent of the time at which the experiment is performed. That is to say

$$|\langle\psi,\chi\rangle| = |\langle\psi(t),\chi(t)\rangle|.$$

In the Schrödinger picture the states $|\psi\rangle \in \mathcal{H}$ evolve in time according to the Schrödinger equation introduced previously and observables do not change with time. The expectation value is given by

$$E_{\psi(t)}(\widehat{A}) = \langle\psi(t), \widehat{A}\psi(t)\rangle$$

and $|\psi(t)\rangle$ is a time-dependent state. In the Heisenberg picture the states remain fixed in time and the observables evolve according to the *automorphism group*

$$\widehat{A} \to \widehat{A}(t) = \exp(it\widehat{H}/\hbar)\widehat{A}\exp(-it\widehat{H}/\hbar) = \widehat{U}(t)^*\widehat{A}\widehat{U}(t)$$

where we assume that the Hamilton operator $\widehat{H}$ does not depend explicitly on time. The *Heisenberg equation of motion* is given by the differential equation

$$-i\hbar\frac{d\widehat{A}(t)}{dt} = [\widehat{H}, \widehat{A}(t)].$$

The solution to this is given by

$$\widehat{A}(t) = \sum_{n=0}^{\infty}\frac{(it/\hbar)^n}{n!}[\widehat{H},[\widehat{H},\dots,[\widehat{H},\widehat{A}],\dots]] = \exp(it\widehat{H}/\hbar)\widehat{A}\exp(-it\widehat{H}/\hbar).$$

If $[\widehat{H},\widehat{A}] = 0$ then $\widehat{A}$ is called a constant of motion or a *conserved quantity*. The relation between the Heisenberg and Schrödinger pictures is given by

$$\langle\psi(t), \widehat{A}\psi(t)\rangle = \langle\psi, \widehat{A}(t)\psi\rangle$$

where $\psi = \psi(t=0)$.

Example. Let $\widehat{A}$, $\widehat{H}$ be $n \times n$ hermitian matrices, where $\widehat{H}$ plays the role of the Hamilton operator. Consider the Heisenberg equation of motion with $\widehat{A} = \widehat{A}(t=0) = \widehat{A}(0)$ and the solution of the initial value problem

$$\widehat{A}(t) = e^{i\widehat{H}t/\hbar}\widehat{A}e^{-i\widehat{H}t/\hbar}.$$

Let $E_j (j = 1, 2, \dots, n^2)$ be an orthonormal basis in the Hilbert space $\mathcal{H}$ of the $n \times n$ matrices with scalar product

$$\langle X, Y\rangle := \mathrm{tr}(XY^*), \text{ with } X, Y \in \mathcal{H}.$$

Now $\widehat{A}(t)$ can be expanded using the orthonormal basis

$$\widehat{A}(t) = \sum_{j=1}^{n^2} c_j(t)E_j$$

and $\widehat{H}$ can be expanded

$$\widehat{H} = \sum_{j=1}^{n^2} h_j E_j.$$

We wish to find the time evolution for the coefficients $c_j(t)$ where $j = 1, 2, \ldots, n^2$. We have

$$\frac{d\widehat{A}(t)}{dt} = \sum_{j=1}^{n^2} \frac{dc_j(t)}{dt} E_j.$$

Substituting we get

$$\sum_{j=1}^{n^2} \frac{dc_j(t)}{dt} E_j = \frac{i}{\hbar} \left[\sum_{k=1}^{n^2} h_k E_k, \sum_{j=1}^{n^2} c_j(t) E_j \right] = \frac{i}{\hbar} \sum_{k=1}^{n^2} \sum_{j=1}^{n^2} h_k c_j(t) [E_k, E_j].$$

We now take the scalar product on both sides of the equation with E_ℓ. This gives

$$\sum_{j=1}^{n^2} \frac{dc_j(t)}{dt} \mathrm{tr}(E_j E_\ell^*) = \frac{i}{\hbar} \sum_{k,j=1}^{n^2} h_k c_j(t) \mathrm{tr}([E_k, E_j] E_\ell^*)$$

where $\ell = 1, 2, \ldots, n^2$. Since $\mathrm{tr}(E_j E_\ell^*) = \delta_{j\ell}$ we obtain

$$\frac{dc_\ell(t)}{dt} = \frac{i}{\hbar} \sum_{k,j=1}^{n^2} h_k c_j(t) \mathrm{tr}([E_k, E_j] E_\ell^*) = \frac{i}{\hbar} \sum_{k,j=1}^{n^2} h_k c_j(t) \mathrm{tr}(E_k E_j E_j^* - E_j E_k E_\ell^*).$$

♣

Postulate 8: A quantum mechanical state is symmetric under the permutation of identical bosons and antisymmetric under the permutation of identical fermions. Fermi and Bose operators will be introduced in chapter 4.4.

3.2 Uncertainty Relation

Let $\widehat{A}$ and $\widehat{B}$ be self-adjoint operators in a Hilbert space $\mathcal{H}$ and let $|\psi\rangle$ be a normalized state in $\mathcal{H}$. The *uncertainty relation* (Robertson [101], Merzbacher [79], Lakshmibala [70]) is given by

$$(\Delta\widehat{A})(\Delta\widehat{B}) \geq \frac{1}{2} |\langle [\widehat{A}, \widehat{B}] \rangle|$$

where $\Delta\widehat{A}$ is the *standard deviation* of $\widehat{A}$ described by $|\psi\rangle$

$$\Delta\widehat{A} := \sqrt{\langle \widehat{A}^2 \rangle - \langle \widehat{A} \rangle^2}$$

with $\langle \widehat{A} \rangle := \langle \psi | \widehat{A} | \psi \rangle$ being the expected value of $\widehat{A}$. A stronger bound is given by

$$(\Delta \widehat{A})^2 (\Delta \widehat{B})^2 \geq \frac{1}{4} | \langle [\widehat{A}, \widehat{B}] \rangle | + \frac{1}{4} | \langle [\widehat{A} - \langle \widehat{A} \rangle I, \widehat{B} - \langle \widehat{B} \rangle I]_+ \rangle |^2$$

where $[\,,\,]_+$ denotes the anticommutator. When equality holds in the first inequality we say $|\psi\rangle$ is an *intelligent state* and when equality holds in the stronger inequality we say $|\psi\rangle$ is a generalized intelligent state. There is a connection between *stabilizer states* and intelligent states (Steeb [134]).

Example. Let $\widehat{A} = \sigma_1$ and $\widehat{B} = \sigma_3$ where σ_1 and σ_3 are the Pauli spin matrices. Consider

$$|\psi_1\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

where these vectors form the Hadamard basis and

$$|\psi_3\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ i \end{pmatrix}, \quad |\psi_4\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -i \end{pmatrix}.$$

We see that $|\psi_1\rangle$ and $|\psi_2\rangle$ are generalized intelligent states. We see that $|\psi_3\rangle$ and $|\psi_4\rangle$ are intelligent states with an equality in the weaker relation and inequality in the stronger relation. Program 5 is provided in the Computer algebra implementation chapter which evaluates these inequalities. ♣

Example. Consider the case where $\widehat{A} = \sigma_1 \otimes \sigma_1$ and $\widehat{B} = \sigma_3 \otimes \sigma_3$ where σ_1 and σ_3 are the Pauli spin matrices. We consider the states from the previous example with

$$|\psi\rangle := |\psi_i\rangle \otimes |\psi_j\rangle \qquad \text{with} \qquad i, j = 1, 2, 3, 4.$$

We see that $|\psi_1\rangle \otimes |\psi_1\rangle$, $|\psi_1\rangle \otimes |\psi_2\rangle$, $|\psi_2\rangle \otimes |\psi_1\rangle$, $|\psi_2\rangle \otimes |\psi_2\rangle$ are generalized intelligent states, $|\psi_3\rangle \otimes |\psi_3\rangle$, $|\psi_3\rangle \otimes |\psi_4\rangle$, $|\psi_4\rangle \otimes |\psi_3\rangle$, $|\psi_4\rangle \otimes |\psi_4\rangle$ are intelligent states and all other combinations of $|\psi\rangle$ satisfy both inequalities but neither equalities. ♣

Chapter 4

Matrix Properties

4.1 Introduction

The simplest quantum mechanical system known is the single *qubit* (quantum bit) which is a simple 2-state system. Physically this is a free particle of spin-1/2 where we introduce the concept of spin later in the dissertation. The formulation of quantum mechanics that we are interested in is the matrix formulation (or matrix mechanics) formulated by Heisenberg and his colleagues. As the name implies this formulation depends on matrices and as such we introduce some basic mathematical concepts before continuing with the discussion. We consider only finite dimensional Hilbert spaces. Thus the linear operators we consider presently are given by $n \times n$ matrices over $\mathbb{C}$.

4.2 Eigenvalue Problem

As we have seen we make extensive use of eigenvalues and eigenvectors in the study of quantum computing. To formally define the *eigenvalue problem* let A be an $n \times n$ matrix and λ a scalar. We say that λ is the *eigenvalue* of A if a nonzero vector $\mathbf{x}$ exists such that

$$A\mathbf{x} = \lambda\mathbf{x}.$$

$\mathbf{x}$ is the corresponding *eigenvector* to λ. This is equivalent to the system $A\mathbf{x} - \lambda\mathbf{x} = \mathbf{0}$ which may be written as

$$(A - \lambda I_n)\mathbf{x} = \mathbf{0}$$

where I_n is the $n \times n$ identity matrix. The system has nontrivial solutions if and only if

$$\det(A - \lambda I_n) = 0$$

holds. This is known as the *characteristic equation* of A and the resultant polynomial is known as the *characteristic polynomial*. The set of all eigenvalues of A is called the *spectrum* of A.

Example. Let n be odd and $n \geq 3$. Consider the matrices

$$A_3 = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} \\ 0 & 1 & 0 \\ \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}; \quad A_5 = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & 0 & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & 0 & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}$$

and the general case

$$A_n = \begin{pmatrix} \frac{1}{\sqrt{2}} & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & \frac{1}{\sqrt{2}} \\ 0 & \frac{1}{\sqrt{2}} & \cdots & 0 & 0 & 0 & \cdots & \frac{1}{\sqrt{2}} & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & 0 & \cdots & \frac{1}{\sqrt{2}} & 0 & \frac{1}{\sqrt{2}} & \cdots & 0 & 0 \\ 0 & 0 & \cdots & 0 & 1 & 0 & \cdots & 0 & 0 \\ 0 & 0 & \cdots & \frac{1}{\sqrt{2}} & 0 & -\frac{1}{\sqrt{2}} & \cdots & 0 & 0 \\ \vdots & \vdots & \cdots & \vdots & \vdots & \vdots & \cdots & \vdots & \vdots \\ 0 & \frac{1}{\sqrt{2}} & \cdots & 0 & 0 & 0 & \cdots & -\frac{1}{\sqrt{2}} & 0 \\ \frac{1}{\sqrt{2}} & 0 & \cdots & 0 & 0 & 0 & \cdots & 0 & -\frac{1}{\sqrt{2}} \end{pmatrix}.$$

We find the eigenvalues of A_3 to be 1 (with a multiplicity of 2) and -1 with corresponding (normalized) eigenvectors

$$1 : \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}, \quad \frac{1}{\sqrt{4-2\sqrt{2}}} \begin{pmatrix} 1 \\ 0 \\ \sqrt{2}-1 \end{pmatrix}$$

$$-1 : \frac{1}{\sqrt{4+2\sqrt{2}}} \begin{pmatrix} 1 \\ 0 \\ -\sqrt{2}-1 \end{pmatrix}.$$

We find the eigenvalues of A_5 to be 1 (with multiplicity of 3) and -1 (with multiplicity of 2) with corresponding (normalized) eigenvectors

$$1 : \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad \frac{1}{\sqrt{4-2\sqrt{2}}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \sqrt{2}-1 \end{pmatrix}, \quad \frac{1}{\sqrt{4-2\sqrt{2}}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ \sqrt{2}-1 \\ 0 \end{pmatrix}$$

$$-1 : \frac{1}{\sqrt{4+2\sqrt{2}}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ -\sqrt{2}-1 \end{pmatrix}, \quad \frac{1}{\sqrt{4+2\sqrt{2}}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ -\sqrt{2}-1 \\ 0 \end{pmatrix}.$$

For the general case A_n we find the eigenvalues 1 (with multiplicity $(n+1)/2$) and -1 (with multiplicity $(n-1)/2$) with corresponding (normalized) eigenvectors

$$1: \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}, \quad \frac{1}{\sqrt{4-2\sqrt{2}}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ \sqrt{2}-1 \end{pmatrix}, \quad \ldots, \quad \frac{1}{\sqrt{4-2\sqrt{2}}} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \sqrt{2}-1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

$$-1: \frac{1}{\sqrt{4+2\sqrt{2}}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \\ 0 \\ 0 \\ -\sqrt{2}-1 \end{pmatrix}, \quad \ldots, \quad \frac{1}{\sqrt{4+2\sqrt{2}}} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ -\sqrt{2}-1 \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \qquad \clubsuit$$

Some important properties of the eigenvalue problem that we use extensively are

(a) The eigenvalues of *hermitian matrices* are real.

(b) The eigenvalues of *unitary matrices* have an absolute value of 1 and may be written in the form $e^{i\phi}$.

(c) The spectral decomposition of a *normal matrix* A is given by

$$A = \sum_{j=1}^{n} \lambda_j \mathbf{x}_j \mathbf{x}_j^*$$

where the eigenvectors are normalized and pairwise orthogonal.

(d) The only possible eigenvalues of *projection matrices* are 0 and 1.

(e) The eigenvalues of *permutation matrices* lie on the complex unit circle and are evenly distributed. This is as expected since permutation matrices are a subgroup of the unitary matrices.

(f) The eigenvectors of two different eigenvalues are linearly independent.

Example. Consider the Hamilton operator given by the 4×4 diagonal matrix

$$\widehat{H} = \begin{pmatrix} 1\,0 & 0 & 0 \\ 0\,\epsilon & 0 & 0 \\ 0\,0 & -\epsilon & 0 \\ 0\,0 & 0 & -1 \end{pmatrix}$$

where $\epsilon \geq 0$. Thus the eigenvalues are ± 1, $\pm\epsilon$. For $\epsilon = 0$ the eigenvalue 0 is twice degenerate and the other eigenvalues are ± 1. Besides the identity matrix I_4 we find the permutation matrix

$$P = \begin{pmatrix} 1\,0\,0\,0 \\ 0\,0\,1\,0 \\ 0\,1\,0\,0 \\ 0\,0\,0\,1 \end{pmatrix}$$

such that $P^T \widehat{H} P = \widehat{H}$. Thus we have *level crossing* for $\epsilon = 0$. For $\epsilon = 1$ we have the eigenvalue $+1$ twice degenerate and the eigenvalue -1 twice degenerate, thus we have level crossing in both cases. We find three permutation matrices other than I_4 that satisfy $P^T \widehat{H} P = \widehat{H}$ namely

$$P_1 = \begin{pmatrix} 1\,0\,0\,0 \\ 0\,1\,0\,0 \\ 0\,0\,0\,1 \\ 0\,0\,1\,0 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 0\,1\,0\,0 \\ 1\,0\,0\,0 \\ 0\,0\,1\,0 \\ 0\,0\,0\,1 \end{pmatrix}, \quad P_3 = \begin{pmatrix} 0\,1\,0\,0 \\ 1\,0\,0\,0 \\ 0\,0\,0\,1 \\ 0\,0\,1\,0 \end{pmatrix}.$$

Figure 4.1 illustrates the eigenvalues as a function of ϵ

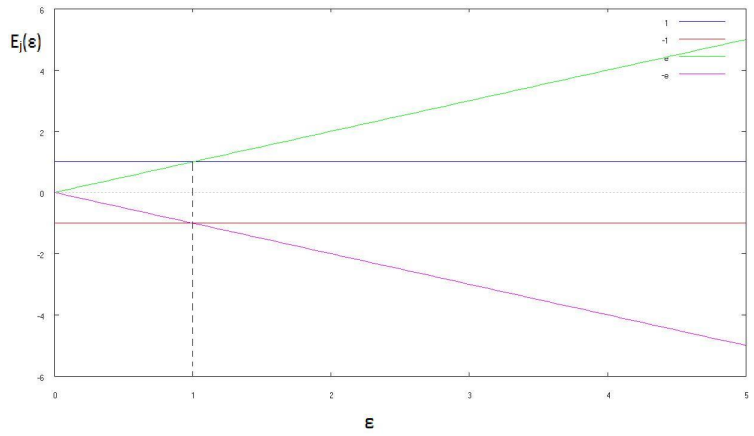

Figure 4.1: Eigenvalues of $\widehat{H}$

Here we see the crossing at $\epsilon = 0$ and $\epsilon = 1$. For all other ϵ there are no other permutation matrices with $P^T \widehat{H} P = \widehat{H}$ except the identity matrix. ♣

In 2005 Kirillov et al [64], [65] and Seyranian et al [111] studied the unfolding of eigenvalue surfaces of real symmetric and hermitian operators due to arbitrary perturbations near *diabolic points* and the coupling of eigenvalues of complex matrices at diabolic and *exceptional points*. In chapter 6 we discuss exceptional and diabolic points in great detail but we now introduce the concepts briefly and discuss the effect of these points on eigenvalues. At exceptional points both eigenvalues and eigenvectors merge forming a Jordan block. At diabolic points the eigenvalues coalesce while the corresponding eigenvectors remain linearly independent. Graphically we may see a diabolic point as the apex of a cone and an exceptional point as an inflection point. We may study these points for hermitian and non-hermitian Hamilton operators.

Considering the eigenvalue problem introduced above we assume the given matrix A has an eigenvalue λ_0 of multiplicity 2. This double eigenvalue can have one or two linearly independent eigenvectors which will determine the geometric multiplicity. Double eigenvalues appear at sets in parameter space whose codimensions depend on the matrix type and whether the degeneracy is an exceptional point (EP) or a diabolic point (DP). The following table lists these codimensions based on the results of von Neumann and Wigner [147] and Arnold [1]

Matrix type	Codimension of EP	Codimension of DP
real symmetric	DNE	2
real non-symmetric	1	3
hermitian	DNE	3
complex symmetric	2	4
complex non-symmetric	2	6

Table 4.1: Codimensions of eigenvalue degeneracies (Seyranian et al [111])

where DNE means that it is non-existent or does not exist.

4.3 Normal, Unitary and Hermitian Matrices

A matrix is said to be *normal* if $A^*A = AA^*$ is true. It can be shown that A is normal if and only if a unitary matrix U exists such that $A = UDU^*$ where D is a diagonal matrix. The entries of D are the eigenvalues of A and the column vectors of U are eigenvectors of A. *Hermitian*, *skew-hermitian* and *unitary* matrices are all normal.

If A is an $n \times n$ normal matrix with eigenvalues λ_j and orthonormal eigenvectors $\{|x_j\rangle\}$ then A can be decomposed as

$$A = \sum_{j=1}^{n} \lambda_j \, |x_j\rangle \, \langle x_j|.$$

This is the *spectral decomposition* of A.

We say a matrix is *hermitian* if $K^* = K$, a matrix is *skew-hermitian* if $K^* = -K$. A property of hermitian matrices is that their eigenvalues are always real and the eigenvectors of distinct eigenvalues are always orthogonal. A matrix is *unitary* if $UU^* = U^*U = I$ where I is the identity matrix. This means that the matrix U is always invertible with $U^{-1} = U^*$. If H is a hermitian matrix then iH is skew-hermitian and $\exp(iH)$ is a unitary matrix.

Let H be an $n \times n$ hermitian matrix with eigenvalues $\lambda_1 \ldots \lambda_n$ and corresponding pairwise orthogonal normalized eigenvectors $|x_1\rangle \ldots |x_n\rangle$. We can write the spectral decomposition

$$H = \sum_{j=1}^{n} \lambda_j |x_j\rangle \langle x_j|$$

as before. We define

$$P := I_n - |x_j\rangle \langle x_j| - |x_k\rangle \langle x_k| + |x_j\rangle \langle x_k| + |x_k\rangle \langle x_j| \quad \text{for} \quad j \neq k.$$

The condition on the eigenvalues of H so that $PHP^* = H$ holds is $\lambda_j = \lambda_k$ and we see that $P^2 = I_n$

Given an $n \times n$ hermitian matrix H we can form a unitary matrix V via the *Cayley transform* given by

$$V := (H - iI_n)(H + iI_n)^{-1}.$$

Program 6 is included in the Computer algebra implementation chapter to evaluate the Cayley transform of a given matrix.

Example. Let

$$\widehat{H} = \frac{1}{2} \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}.$$

We find

$$V = \begin{pmatrix} \frac{1}{2} - i & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} - i \end{pmatrix} \begin{pmatrix} \frac{1}{2} + i & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} + i \end{pmatrix}^{-1} = \begin{pmatrix} -\frac{1+i}{2} & \frac{1-i}{2} \\ \frac{1-i}{2} & -\frac{1+i}{2} \end{pmatrix}. \qquad \clubsuit$$

Let K be an $n \times n$ skew-hermitian matrix with the eigenvalues $\mu_1, \cdots, \mu_n$ and the corresponding normalized eigenvectors $|u_1\rangle, \cdots, |u_n\rangle$ where $\langle u_j | u_k \rangle = 0$ for $k \neq j$. We may write K as

$$K = \sum_{j=1}^{n} \mu_j |u_j\rangle \langle u_j|.$$

The matrices $|u_j\rangle \langle u_j|$ are projection matrices and the completeness relation

$$\sum_{j=1}^{n} |u_j\rangle \langle u_j| = I_n$$

holds. Every $n \times n$ unitary matrix can be written as $U = \exp(K)$ where K is skew-hermitian. Using the properties of K we find

$$U = \exp(K) = \exp\left(\sum_{j=1}^{n} \mu_j \left|u_j\right\rangle \left\langle u_j\right|\right) = \sum_{j=1}^{n} e^{\mu_j} \left|u_j\right\rangle \left\langle u_j\right|.$$

For a given unitary matrix U we may find a possible skew-hermitian matrix K

$$K = \sum_{j=1}^{n} \ln(\lambda_j) \left|u_j\right\rangle \left\langle u_j\right|$$

where λ_j are the eigenvalues of U and $|u_j\rangle$ are the corresponding normalized eigenvectors. The eigenvalues of U are of the form $e^{i\alpha}$ so that $\ln(e^{i\alpha}) = i\alpha$. Every hermitian matrix H can be written as $H = iK$ where K is skew-hermitian.

Example. Given the 2×2 unitary matrix

$$V(\theta, \phi) = \begin{pmatrix} \cos\theta & -e^{i\phi}\sin\theta \\ e^{-i\phi}\sin\theta & \cos\theta \end{pmatrix}$$

we find a possible K and H. The eigenvalues for $V(\theta, \phi)$ are $e^{-i\theta}$ and $e^{i\theta}$ with corresponding normalized eigenvectors

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ ie^{-i\phi} \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -ie^{-i\phi} \end{pmatrix}.$$

Then

$$\begin{aligned} K(\theta, \phi) &= \frac{-i\theta}{2} \begin{pmatrix} 1 \\ ie^{-i\phi} \end{pmatrix} \begin{pmatrix} 1 & ie^{-i\phi} \end{pmatrix} + \frac{i\theta}{2} \begin{pmatrix} 1 \\ -ie^{-i\phi} \end{pmatrix} \begin{pmatrix} 1 & -ie^{-i\phi} \end{pmatrix} \\ &= \begin{pmatrix} 0 & -\theta e^{i\phi} \\ \theta e^{-i\phi} & 0 \end{pmatrix} \end{aligned}$$

and

$$H(\theta, \phi) = iK(\theta, \phi) = \begin{pmatrix} 0 & -i\theta e^{i\phi} \\ i\theta e^{-i\phi} & 0 \end{pmatrix}. \qquad \clubsuit$$

Let $z \in \mathbb{C}$ and A, B be $n \times n$ matrices over $\mathbb{C}$. We say that B is *invariant* with respect to A if

$$e^{zA} B e^{-zA} = B$$

holds. If this condition is satisfied then $[A, B] = 0_n$ where $[,]$ denotes the commutator. If e^{zA} is unitary we have

$$UBU^* = B$$

where $U = e^{zA}$.

Example. Let $z \in \mathbb{C}$ and

$$A_1 = \begin{pmatrix} 0\,1 \\ 1\,0 \end{pmatrix}, \quad B_1 = \begin{pmatrix} b_{11}\,b_{12} \\ b_{12}\,b_{11} \end{pmatrix}.$$

$$A_2 = \begin{pmatrix} 0\,1 \\ 0\,0 \end{pmatrix}, \quad B_2 = \begin{pmatrix} b_{11}\,b_{12} \\ 0\;\;b_{11} \end{pmatrix}.$$

We find for A_1 and B_1

$$e^{zA_1} = \begin{pmatrix} \cosh(z)\,\sinh(z) \\ \sinh(z)\,\cosh(z) \end{pmatrix}, \quad e^{-zA_1} = \begin{pmatrix} \cosh(z) & -\sinh(z) \\ -\sinh(z) & \cosh(z) \end{pmatrix}.$$

We see that $e^{zA_1} B_1 e^{-zA_1} = B_1$ so that B_1 is invariant with respect to A_1. We find for A_2 and B_2

$$e^{zA_2} = \begin{pmatrix} 1\,z \\ 0\,1 \end{pmatrix}, \quad e^{-zA_2} = \begin{pmatrix} 1 & -z \\ 0 & 1 \end{pmatrix}.$$

Once again we see that $e^{zA_2} B_2 e^{-zA_2} = B_2$ and so B_2 is invariant with respect to A_2 and $[A_{1,2}, B_{1,2}] = 0_2$. ♣

Example. Let σ_1 and σ_3 be the Pauli spin matrices. We find unitary matrices U and V such that

$$U\sigma_1 U^* = \sigma_3 \text{ and } V(\sigma_1 \otimes \sigma_1)V^* = \sigma_3 \otimes \sigma_3.$$

We obtain

$$U = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} = U^* = U^{-1}$$

and we see that $V = U \otimes U$ since

$$(U \otimes U)(\sigma_1 \otimes \sigma_1)(U^* \otimes U^*) = (U\sigma_1 U^*) \otimes (U\sigma_1 U^*) = \sigma_3 \otimes \sigma_3. \qquad ♣$$

4.4 Matrix Decompositions

We are able to factorize a given matrix A into a product of factor matrices $F_1, F_2, \ldots, F_n$ and this is known as *matrix decomposition*. Some common decompositions used in quantum computing are

(a) Singular value decomposition (SVD).

(b) Cosine-sine decomposition.

(c) Polar decomposition.

(d) LU-decomposition.

(e) QR-decomposition.

Matrix decompositions help to simplify computations by breaking complicated matrices up into components that are easier to work with. Since we use matrices so extensively in quantum information theory these matrix reorderings are very useful. Among other things matrix decompositions (particularly SVD) allows us to obtain simple formulae for the composition of quantum channels and partial operations used in quantum information theory.

Let A be an arbitrary $m \times n$ matrix over $\mathbb{R}$. We may rewrite A as $A = U\Sigma V^T$ where U is an $m \times m$ orthogonal matrix, V is an $n \times n$ orthogonal matrix and Σ is an $m \times n$ diagonal matrix with nonnegative entries. This is a *singular value decomposition* and the steps used to obtain these factor matrices is given by

1. Find the eigenvalues λ_j of the matrix $A^T A$ and arrange them in descending order. The number of nonzero eigenvalues of this matrix is called r.

2. Find the corresponding orthonormal eigenvectors $\mathbf{v}_j$ of $A^T A$ and arrange them in the same order to form the column vectors of V (an $n \times n$ matrix).

3. Form the $m \times n$ diagonal matrix Σ by placing on the leading diagonal $\sigma_j = \sqrt{\lambda_j}$ of the matrix $A^T A$ found in the first step.

4. Find the first r column vectors of U (an $m \times m$ matrix) from

$$\mathbf{u}_j = \frac{1}{\sigma_j} A\mathbf{v}_j, \quad j = 1, 2, \ldots, r.$$

5. The remaining $m - r$ column vectors of U are obtained using the Gram-Schmidt orthogonalization process.

The SVD is in general not unique. Another useful application of the SVD is to find the Moore-Penrose pseudo-inverse of a matrix (Steeb [121]).

Example. A singular value decomposition of the density operator

$$\rho = \frac{1}{2} \begin{pmatrix} 1\,0\,0\,1 \\ 0\,0\,0\,0 \\ 0\,0\,0\,0 \\ 1\,0\,0\,1 \end{pmatrix}$$

is given by

$$\rho = \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & 0 & 0 & -1 \\ 0 & \sqrt{2} & 0 & 0 \\ 0 & 0 & \sqrt{2} & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1\,0\,0\,0 \\ 0\,0\,0\,0 \\ 0\,0\,0\,0 \\ 0\,0\,0\,0 \end{pmatrix} \frac{1}{\sqrt{2}} \begin{pmatrix} -1 & -1 & 0 & 0 \\ 0 & 0 & 0 & \sqrt{2} \\ 0 & 0 & \sqrt{2} & 0 \\ -1 & 1 & 0 & 0 \end{pmatrix}^T . \qquad \clubsuit$$

Any $2^n \times 2^n$ unitary matrix U can be decomposed as

$$U = \begin{pmatrix} U_1 & 0 \\ 0 & U_2 \end{pmatrix} \begin{pmatrix} C & S \\ -S & C \end{pmatrix} \begin{pmatrix} U_3 & 0 \\ 0 & U_4 \end{pmatrix}$$

where U_j are $2^{n-1} \times 2^{n-1}$ unitary matrices and

$$C = \mathrm{diag}(\cos\alpha_1, \cos\alpha_2, \ldots, \cos\alpha_{2^n/2})$$
$$S = \mathrm{diag}(\sin\alpha_1, \sin\alpha_2, \ldots, \sin\alpha_{2^n/2})$$

where $\alpha_j \in \mathbb{R}$. This is the *cosine-sine decomposition* (Steeb [121]).

Example. The cosine-sine decomposition of

$$A = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}$$

is given by

$$A = \frac{1}{2} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & -1 \\ 0 & 0 & -1 & -1 \end{pmatrix} \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 0 & -1 & 0 & 0 \end{pmatrix} \begin{pmatrix} 1 & 1 & 0 & 0 \\ 1 & -1 & 0 & 0 \\ 0 & 0 & -1 & 1 \\ 0 & 0 & 1 & 1 \end{pmatrix}. \qquad \clubsuit$$

For any $n \times n$ matrix A over $\mathbb{C}$ there exists a positive semi-definite matrix H and a unitary matrix U such that $A = HU$. This is known as *polar decomposition*. If A is nonsingular then H is positive definite and the decomposition is unique.

Example. The polar decomposition of

$$A = \begin{pmatrix} 1 & 0 & -4 \\ 0 & 5 & 4 \\ -4 & 4 & 3 \end{pmatrix}$$

is given by

$$A = \frac{1}{3} \begin{pmatrix} 11 & -4 & -4 \\ -4 & 17 & 8 \\ -4 & 8 & 17 \end{pmatrix} \frac{1}{9} \begin{pmatrix} 1 & 4 & -8 \\ 4 & 7 & 4 \\ -8 & 4 & 1 \end{pmatrix}.$$

Since $\det(A) \neq 0$ the matrix is nonsingular and the decomposition is unique. $\clubsuit$

4.5 Fourier Transform

4.5.1 The Quantum Fourier Transform

Consider the Hilbert space $\mathbb{C}^{2n}$ with the orthonormal basis

$$\{|0\rangle, |1\rangle, \cdots, |2^n - 1\rangle\}.$$

We define the *quantum Fourier transform* (QFT)

$$U_{QFT} := \frac{1}{\sqrt{2^n}} \sum_{j,k=0}^{2^n-1} e^{-i2\pi kj/2^n} |k\rangle \langle j|.$$

It may be shown that this is a unitary transform so that $U_{QFT}U_{QFT}^* = I_{2^n}$. This transform plays a large role in a number of *quantum algorithms* such as Shor's algorithm which is an algorithm for factorizing large integers.

Example. Let $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}$ denote an orthonormal basis in $\mathbb{C}^4$. We apply the quantum Fourier transform to the states

$$|\psi_1\rangle = \frac{1}{2}(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle + |2\rangle \otimes |0\rangle + |3\rangle \otimes |1\rangle)$$
$$|\psi_2\rangle = \frac{1}{2}(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle - |2\rangle \otimes |0\rangle - |3\rangle \otimes |1\rangle).$$

We find

$$(U_{QFT} \otimes I_4)|\psi_1\rangle = \frac{1}{\sqrt{2}}\left(|0\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) + |2\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle - |1\rangle)\right)$$
$$(U_{QFT} \otimes I_4)|\psi_1 2\rangle = \frac{1}{\sqrt{2}}\left(|1\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle) + |3\rangle \otimes \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)\right). \quad \clubsuit$$

4.5.2 The Discrete Fourier Transform

Let

$$\{|a_0\rangle, |a_1\rangle, \ldots, |a_{n-1}\rangle\}$$

be an orthonormal basis in the Hilbert space $\mathbb{C}^n$. We may define the *discrete Fourier transform* (DFT) as

$$|b_j\rangle := \frac{1}{\sqrt{n}} \sum_{k=0}^{n-1} \omega_n^{jk} |a_k\rangle, \quad j = 1, 2, \ldots, n$$

where $\omega_n := e^{2\pi i/n}$ is the n-th root of unity. The DFT is simply the inverse of the QFT under a change of basis with a non-power 2 dimension (however power 2 dimensions may still be considered). Applying this transform to a basis implies an inherent ordering where we require $a_0 < a_1 < \cdots < a_{n-1}$ to hold. Program 8 calculating the DFT for $\mathbb{C}^4$ is included in the Computer implementation section.

Example. Consider the standard basis in $\mathbb{C}^4$

$$|s_0\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad |s_1\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \end{pmatrix}, \quad |s_2\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |s_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

Applying the discrete Fourier transform we obtain

$$|f_{s0}\rangle = \frac{1}{2}\begin{pmatrix}1\\1\\1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix},$$

$$|f_{s1}\rangle = \frac{1}{2}\begin{pmatrix}1\\i\\-1\\-i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix},$$

$$|f_{s2}\rangle = \frac{1}{2}\begin{pmatrix}1\\-1\\1\\-1\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix},$$

$$|f_{s3}\rangle = \frac{1}{2}\begin{pmatrix}1\\-i\\-1\\i\end{pmatrix} = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}.$$

The standard basis is separable and we see that the new vectors obtained from the DFT are also separable and form an orthonormal basis. ♣

Example. Consider the Bell basis in $\mathbb{C}^4$

$$|b_0\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}, \quad |b_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix},$$

$$|b_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}, \quad |b_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}.$$

Applying the discrete Fourier transform we obtain

$$|f_{b0}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix} = \begin{pmatrix}1\\0\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \quad |f_{b1}\rangle = \frac{1}{2\sqrt{2}}\begin{pmatrix}1+i\\-1-i\\-1+i\\1-i\end{pmatrix},$$

$$|f_{b2}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\1\\1\end{pmatrix} = \begin{pmatrix}0\\1\end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}, \quad |f_{b1}\rangle = \frac{1}{2\sqrt{2}}\begin{pmatrix}1-i\\-1+i\\-1-i\\1+i\end{pmatrix}.$$

We see that even though all the original vectors in the Bell basis are entangled not all the vectors obtained from applying the DFT are entangled. The resultant vectors still form an orthonormal basis. ♣

We see that the discrete Fourier transform does not preserve the entangled state of the input vectors.

Chapter 5

Linear Operators

5.1 Introduction

After introducing useful mathematical principles in the previous chapter we are now able to introduce some linear operators that are of vital importance to us. We start by introducing the concept of observables and Hamilton operators which will be used extensively. Following this we introduce density operators which play a large role in quantum entanglement.

5.1.1 Observables and Hamilton Operators

When we speak of an *observable* we are talking about a quantity that is experimentally measurable either directly or indirectly. Based on the matrix formulation of quantum mechanics all physical observables are represented mathematically by matrices. Examples of observables are position, momentum and energy. The set of eigenvalues of an observable represent all possible outcomes when the observable is measured by means of experiment on the system. Since the outcomes of a real observable must be real we see that observables are represented by hermitian matrices. The corresponding eigenvector represents the state of the system immediately after measurement. We cannot know the precise state of the system before the measurement and the Copenhagen interpretation of quantum mechanics is only interested in the outcomes of measurement on a quantum system. In quantum mechanics we do not only consider a single 'copy' of the system but rather an ensemble of the system and the average of the results over the ensemble, denoted by $\langle \widehat{A} \rangle$ (where $\widehat{A}$ is the matrix observable), is the result that we are interested in. This is also known as the *expected value*.

In quantum mechanics the *Hamilton operator* denoted by $\widehat{H}$ is the operator that corresponds to the total energy of the system. Its spectrum is the set of possible

outcomes when the energy of the system is measured.

5.1.2 Density Operators

A *density operator* denoted by ρ is a positive semidefinite operator on a Hilbert space with unit trace. It is used in quantum theory to describe the statistical state of a quantum system. It is especially convenient for describing systems where the state is not completely known. A *pure state* $|\psi\rangle$ has a density matrix defined by

$$\rho := |\psi\rangle \langle\psi| .$$

For a pure state $\rho^2 = \rho$ holds. A *mixed state* has the density matrix

$$\rho := \sum_{j=1}^{n} p_j |\psi_j\rangle \langle\psi_j|$$

where $0 \leq p_j \leq 1$, $\sum_{j=1}^{n} p_j = 1$ and $\langle\psi_j|\psi_k\rangle = \delta_{jk}$. What this means is that we may have a system that is in state $|\psi_j\rangle$ with probability p_j. We call $\{p_j, |\psi_j\rangle\}$ an ensemble of pure states. The *expectation value* of an observable $\widehat{A}$ in the system is given by

$$\langle\widehat{A}\rangle := \mathrm{tr}(\widehat{A}\rho).$$

Let λ_j denote the eigenvalues of $\widehat{A}$ and $|x_j\rangle$ the corresponding eigenvectors. The probability of obtaining λ_j as outcome is given by

$$p_{\lambda_j} := \mathrm{tr}(|x_j\rangle \langle x_j| \rho).$$

Example. Let $r \geq 0$. We define

$$\rho := \frac{1}{2} \begin{pmatrix} 1 + r\cos(\theta) & r\sin(\theta)e^{-i\phi} \\ r\sin(\theta)e^{i\phi} & 1 - r\cos(\theta) \end{pmatrix}.$$

We require ρ to be a density matrix. $\mathrm{tr}(\rho) = 1$ as required and the matrix is hermitian (thus the eigenvalues are real). We find $\lambda_{1,2} = \frac{1}{2} \pm \frac{1}{2}r$. Thus $r \leq 1$ for ρ to be a density matrix. There is no condition on θ and ϕ. ♣

A useful application of the density operator is as a descriptive tool when considering subsystems of composite quantum systems. In this case we consider the *reduced density operator*. Consider the quantum system that is made up of the composite systems A and B. The density operator is defined by ρ_{AB}. The reduced density operator for system A is defined by

$$\rho_A := \mathrm{tr}_B(\rho_{AB})$$

where tr_B is the *partial trace* over system B defined by

$$\mathrm{tr}_B(\rho_{AB}) := \sum_{j=1}^{\dim(\mathcal{H}_B)} (I_A \otimes \langle\phi_j|)\rho_{AB}(I_A \otimes |\phi_j\rangle)$$

where $\mathcal{H}_B$ is the Hilbert space relevant to system B, $|\phi_j\rangle$ is an orthonormal basis for B ($j = 1, 2, \ldots, \dim(\mathcal{H}_B)$) and I_A is the identity operator in system A.

The *von Neumann equation* for a given density operator ρ and a given Hamilton operator $\widehat{H}$ is given by

$$i\hbar\frac{d\rho}{dt} = [\widehat{H}, \rho(t)]$$

with the solution

$$\rho(t) = e^{-i\widehat{H}t/\hbar}\rho(0)e^{i\widehat{H}t/\hbar}.$$

Example. Consider the state

$$|\psi\rangle = \begin{pmatrix} \cos\theta \\ e^{i\phi}\sin\theta \end{pmatrix}$$

and the density matrix

$$\rho = |\psi\rangle\langle\psi| = \begin{pmatrix} \cos^2\theta & e^{-i\phi}\cos\theta\sin\theta \\ e^{i\phi}\cos\theta\sin\theta & \sin^2\theta \end{pmatrix}.$$

Given the Hamilton operator

$$\widehat{H} = \hbar\omega\sigma_1.$$

We find

$$e^{-i\widehat{H}t/\hbar} = \begin{pmatrix} \cos(\omega t) & -i\sin(\omega t) \\ -i\sin(\omega t) & \cos(\omega t) \end{pmatrix}$$

and

$$e^{i\widehat{H}t/\hbar} = \begin{pmatrix} \cos(\omega t) & i\sin(\omega t) \\ i\sin(\omega t) & \cos(\omega t) \end{pmatrix}.$$

Solving the von Neumann equation we find

$$\rho_{11}(t) = \cos^2(\omega t)\cos^2(\theta) + \frac{ie^{-i\phi}}{4}(1 - e^{2i\phi})\sin(2\omega t)\sin(2\theta) + \sin^2(\omega t)\sin^2(\theta)$$

$$\rho_{12}(t) = \frac{i}{2}\sin(2\omega t)\cos(2\theta) + \frac{e^{-i\phi}}{2}\sin(2\theta)(\cos^2(\omega t) + e^{2i\phi}\sin^2(\omega t))$$

$$\rho_{21}(t) = -\frac{i}{2}\sin(2\omega t)\cos(2\theta) + \frac{e^{-i\phi}}{2}\sin(2\theta)(\sin^2(\omega t) + e^{2i\phi}\cos^2(\omega t))$$

$$\rho_{22}(t) = \cos^2(\omega t)\sin^2(\theta) - \frac{ie^{-i\phi}}{4}(1 - e^{2i\phi})\sin(2\omega t)\sin(2\theta) + \sin^2(\omega t)\cos^2(\theta).\clubsuit$$

5.2 Spin Hamilton Operators

5.2.1 Introduction

As understanding of quantum theory increased the experiments conducted became more involved and physicists developed a better intuition for what the

results should be based on developing quantum theory. In 1922 Stern and Gerlach conducted experiments where the outcomes were not consistent with the predicted outcomes based on the understanding of quantum theory up to that point [31]. The best way to explain the results obtained and the inconsistencies observed was to make the assumption that an electron has an intrinsic magnetic dipole moment due to the fact that it has an intrinsic angular momentum. We call this angular momentum the *spin* of the electron. With the introduction of this entity we see that any quantum state has a corresponding spin quantum number that describes the system. Some authors who have researched this topic include Auerbach [2], Bethe [13], Eisberg and Resnick [31], Heisenberg [50], Nielsen and Chuang [86], Onsager [88], Steeb et al [120], [122], [124], White [152].

Regarding the quantum spin numbers for different systems we have spin 0 for π mesons; spin 1/2 for electrons, muons, protons and neutrons; spin 1 for photons and higher spins for other particles or nuclei. Particles with integer spin are called *bosons* and particles with half-integer spin are called *fermions*.

5.2.2 Pauli Spin Operators

The simple spin-1/2 system may be described in terms of three operators that correspond to the Cartesian components of spin. These operators are known as *spin matrices*. These are given by the matrices

$$s_j := \frac{\sigma_j}{2} \quad \text{where} \quad j = 1, 2, 3$$

and σ_j are the *Pauli spin matrices* given by

$$\sigma_1 = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \sigma_2 = \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}, \quad \sigma_3 = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}.$$

Conventionally we also define the state vectors

$$|\uparrow\rangle := \begin{pmatrix} 1 & 0 \end{pmatrix}^T \text{ the spin-up vector}$$
$$|\downarrow\rangle := \begin{pmatrix} 0 & 1 \end{pmatrix}^T \text{ the spin-down vector.}$$

The eigenvalues of the Pauli spin matrices are +1 and -1 with the eigenvectors

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}; \quad \frac{1}{\sqrt{2}}\begin{pmatrix} -i \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix} i \\ 1 \end{pmatrix}; \quad \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

for σ_1, σ_2 and σ_3 respectively. When we consider the 4×4 hermitian matrices $\sigma_1 \otimes \sigma_1$, $\sigma_2 \otimes \sigma_2$, $\sigma_3 \otimes \sigma_3$ we again find the eigenvalues +1 (twice) and -1 (twice). Now the eigenvectors may be written as product (unentangled) states or as entangled states. Obviously the normalized eigenstates of $\sigma_1 \otimes \sigma_1$ are given by

$$\frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix},$$

$$\frac{1}{2}\begin{pmatrix}1\\-1\end{pmatrix}\otimes\begin{pmatrix}1\\1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}1\\-1\end{pmatrix}\otimes\begin{pmatrix}1\\-1\end{pmatrix}.$$

The eigenstates of $\sigma_2\otimes\sigma_2$ are given by

$$\frac{1}{2}\begin{pmatrix}i\\1\end{pmatrix}\otimes\begin{pmatrix}i\\1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}i\\1\end{pmatrix}\otimes\begin{pmatrix}-i\\1\end{pmatrix},$$

$$\frac{1}{2}\begin{pmatrix}-i\\1\end{pmatrix}\otimes\begin{pmatrix}i\\1\end{pmatrix},\quad \frac{1}{2}\begin{pmatrix}-i\\1\end{pmatrix}\otimes\begin{pmatrix}-i\\1\end{pmatrix}.$$

The eigenstates of $\sigma_3\otimes\sigma_3$ are given by

$$\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix},\quad \begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix},\quad \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}1\\0\end{pmatrix},\quad \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}.$$

All three matrices also admit the maximally entangled Bell basis as eigenstates.

The Pauli matrices together with I_2 form an orthogonal basis in the Hilbert space consisting of all 2×2 matrices over $\mathbb{C}$ with the inner product defined by $\langle A,B\rangle := \mathrm{tr}(AB^*)$ and we see that for an arbitrary matrix in this Hilbert space

$$A=\begin{pmatrix}a\,b\\c\,d\end{pmatrix}=\frac{a+d}{2}I_2+\frac{b+c}{2}\sigma_1+i\frac{b-c}{2}\sigma_2+\frac{a-d}{2}\sigma_3.$$

We are able to make this an orthonormal basis by multiplying each matrix by a factor $\frac{1}{\sqrt{2}}$. We find the following relationships

$$\sigma_1^2=\sigma_2^2=\sigma_3^2=I_2$$

where I_2 is the 2×2 identity matrix. In addition to this, the commutators are given by

$$[\sigma_1,\sigma_2]=2i\sigma_3,\quad [\sigma_2,\sigma_3]=2i\sigma_1,\quad [\sigma_3,\sigma_1]=2i\sigma_2$$

and the anticommutators are

$$[\sigma_1,\sigma_2]_+=[\sigma_2,\sigma_3]_+=[\sigma_3,\sigma_1]_+=0_2$$

where 0_2 is the 2×2 zero matrix. The trace for each of the Pauli matrices is zero. We may define the matrices

$$s_j:=\frac{\hbar}{2}\sigma_j \text{ where } j=1,2,3$$

$$\sigma_+:=\frac{1}{2}(\sigma_1+i\sigma_2),\quad \sigma_-:=\frac{1}{2}(\sigma_1-i\sigma_2)$$

$$\Lambda_+:=\frac{1}{2}(I_2+\sigma_3),\quad \Lambda_-:=\frac{1}{2}(I_2-\sigma_3)$$

where $\sigma_\pm$ are the spin-flip operators and $\Lambda_\pm$ are projection matrices. $\sigma_\pm$ and $\Lambda_\pm$ form another orthonormal basis in the Hilbert space consisting of 2×2 matrices

over $\mathbb{C}$. When we study the action of spin matrices on spin vectors we see that the following relations hold

$$\sigma_1 |\uparrow\rangle = |\downarrow\rangle, \quad \sigma_1 |\downarrow\rangle = |\uparrow\rangle, \quad \sigma_2 |\uparrow\rangle = i |\downarrow\rangle, \quad \sigma_2 |\downarrow\rangle = -i |\uparrow\rangle,$$
$$\sigma_3 |\uparrow\rangle = |\uparrow\rangle, \quad \sigma_3 |\downarrow\rangle = - |\downarrow\rangle.$$

Furthermore

$$\sigma_+ |\uparrow\rangle = \sigma_- |\downarrow\rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix}, \quad \sigma_+ |\downarrow\rangle = |\uparrow\rangle, \quad \sigma_- |\uparrow\rangle = |\downarrow\rangle$$

and

$$\Lambda_+ |\uparrow\rangle = |\uparrow\rangle, \quad \Lambda_- |\downarrow\rangle = |\downarrow\rangle, \quad \Lambda_+ |\downarrow\rangle = \Lambda_- |\uparrow\rangle = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Example. Consider the Pauli spin matrices σ_1, σ_2 and σ_3. We find the 2×2 hermitian matrices such that

$$\sigma_j H_2 \sigma_j = H_2 \text{ where } j = 1, 2, 3$$

and all 4×4 Hermitian matrices such that

$$(\sigma_j \otimes \sigma_j) H_4 (\sigma_j \otimes \sigma_j) = H_4 \text{ where } j = 1, 2, 3.$$

Let

$$H_2 = \begin{pmatrix} h_{11} & h_{12} \\ h_{21} & h_{22} \end{pmatrix}.$$

We see that for the above to hold $h_{11} = h_{22}$ and $h_{12} = h_{21} = 0$ must hold. So

$$H_2 = \begin{pmatrix} h & 0 \\ 0 & h \end{pmatrix}.$$

Let

$$H_4 = \begin{pmatrix} h_{11} & h_{12} & h_{13} & h_{14} \\ h_{21} & h_{22} & h_{23} & h_{24} \\ h_{31} & h_{32} & h_{33} & h_{34} \\ h_{41} & h_{42} & h_{43} & h_{44} \end{pmatrix}.$$

We see that for the above to hold H_4 must be in the form

$$H_4 = \begin{pmatrix} h_{11} & 0 & 0 & h_{14} \\ 0 & h_{22} & h_{23} & 0 \\ 0 & h_{23} & h_{22} & 0 \\ h_{14} & 0 & 0 & h_{11} \end{pmatrix}. \qquad \clubsuit$$

Example. Let σ_1, σ_2 and σ_3 be the Pauli spin matrices. We find 8×8 unitary matrices $U \in \mathcal{P}_3$ such that

$$U^* (\sigma_1 \otimes \sigma_2 \otimes \sigma_3) U = \sigma_1 \otimes \sigma_2 \otimes \sigma_3.$$

Obvious solutions are $I_2 \otimes I_2 \otimes I_2$ and $\sigma_1 \otimes \sigma_2 \otimes \sigma_3$ and we note that

$$P_1 := \frac{1}{2}(I_2 \otimes I_2 \otimes I_2 + \sigma_1 \otimes \sigma_2 \otimes \sigma_3)$$

$$P_2 := \frac{1}{2}(I_2 \otimes I_2 \otimes I_2 - \sigma_1 \otimes \sigma_2 \otimes \sigma_3)$$

are projection matrices with $P_1 P_2 = 0$. Other solutions for U are

$$I_2 \otimes \sigma_2 \otimes \sigma_3, \quad \sigma_1 \otimes I_2 \otimes I_2,$$

$$\sigma_1 \otimes I_2 \otimes \sigma_3, \quad I_2 \otimes \sigma_2 \otimes I_2,$$

$$\sigma_1 \otimes \sigma_2 \otimes I_2, \quad I_2 \otimes I_2 \otimes \sigma_3.$$

An additional factor of $\pm i$ or ± 1 may be multiplied with each of the terms. ♣

Example. Let σ_1, σ_2 and σ_3 denote the Pauli matrices. We define the spin matrices $S_1 := \frac{1}{2}\sigma_1$, $S_2 := \frac{1}{2}\sigma_2$ and $S_3 := \frac{1}{2}\sigma_3$. We define the Hamilton operator

$$\widehat{H} := 2J(S_1 \otimes S_1 + S_2 \otimes S_2 + S_3 \otimes S_3)$$

where $J \neq 0$ is a constant. We find

$$\widehat{H} = \frac{J}{2}\begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & -1 & 2 & 0 \\ 0 & 2 & -1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

with eigenvalues and corresponding normalized eigenvectors

$$-\frac{3J}{2} : \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}, \quad \frac{J}{2} : \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}.$$

Together with the identity matrix $I_4 = P_0$ we find the permutation matrices

$$P_1 = \begin{pmatrix} 1&0&0&0 \\ 0&0&1&0 \\ 0&1&0&0 \\ 0&0&0&1 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 0&0&0&1 \\ 0&1&0&0 \\ 0&0&1&0 \\ 1&0&0&0 \end{pmatrix}, \quad P_3 = \begin{pmatrix} 0&0&0&1 \\ 0&0&1&0 \\ 0&1&0&0 \\ 1&0&0&0 \end{pmatrix}$$

that satisfy $P^T \widehat{H} P = \widehat{H}$. ♣

Example. Let σ_1, σ_2 and σ_3 be the Pauli matrices and I_2 the 2×2 identity matrix. Consider the Hamilton operator

$$\widehat{H}_4 := B(\sigma_3 \otimes I_2 + I_2 \otimes \sigma_3) + J(\sigma_1 \otimes \sigma_1)$$

where $J > 0$ is constant and we consider different values of B. We find

$$\widehat{H}_4 = \begin{pmatrix} 2B & 0 & 0 & J \\ 0 & 0 & J & 0 \\ 0 & J & 0 & 0 \\ J & 0 & 0 & -2B \end{pmatrix}$$

with eigenvalues and normalized eigenvectors

$$-J : \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}, \quad J : \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix},$$

$$-\sqrt{\alpha} : \frac{J}{\sqrt{2\alpha + 4B\sqrt{\alpha}}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -\frac{\sqrt{\alpha}+2B}{J} \end{pmatrix}, \quad \sqrt{\alpha} : \frac{J}{\sqrt{2\alpha - 4B\sqrt{\alpha}}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ \frac{\sqrt{\alpha}-2B}{J} \end{pmatrix}$$

where $\alpha := J^2 + 4B^2$. When $B = 0$ the eigenvalues are $\pm J$ with multiplicity 2 and the normalized eigenvectors are the Bell basis and as such are entangled. When $B \neq 0$ the eigenvectors are still entangled but no degeneracy of eigenvalues exist.

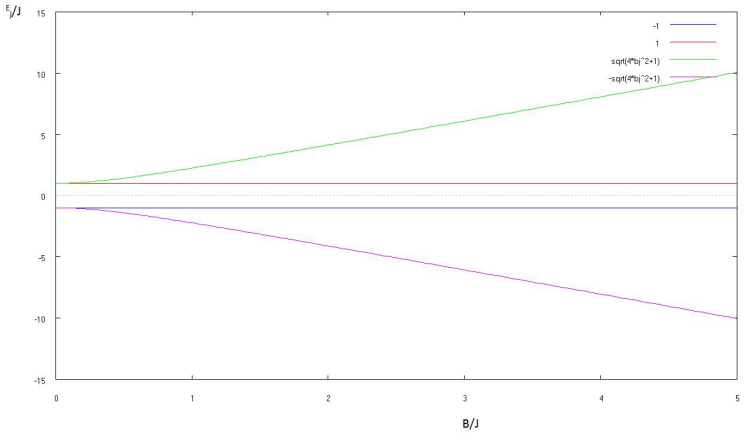

Figure 5.1: Energy levels of $\widehat{H}_4$

Figure 5.1 illustrates the eigenvalues as a function of B/J. So we see that level crossing only occurs when $B/J = 0$. We see that together with the identity matrix $I_4 = P_0$ the permutation matrix

$$P_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$$

satisfies $P^T \widehat{H} P = \widehat{H}$. Note that

$$[\sigma_1 \otimes \sigma_1, \sigma_3 \otimes I_2 + I_2 \otimes \sigma_3] = -2i(\sigma_1 \otimes \sigma_2 + \sigma_2 \otimes \sigma_1) \neq 0_4. \qquad \clubsuit$$

Example. Let σ_1, σ_2 and σ_3 be the Pauli matrices and I_2 the 2×2 identity matrix. Consider the Hamilton operator with the triple spin interaction

$$\widehat{H}_8 := B(\sigma_3 \otimes I_2 \otimes I_2 + I_2 \otimes \sigma_3 \otimes I_2 + I_2 \otimes I_2 \otimes \sigma_3) + J(\sigma_1 \otimes \sigma_2 \otimes \sigma_3).$$

$J > 0$ is constant as before and we consider different values of B. We find

$$\widehat{H}_8 = \begin{pmatrix} 3B & 0 & 0 & 0 & 0 & 0 & -iJ & 0 \\ 0 & B & 0 & 0 & 0 & 0 & 0 & iJ \\ 0 & 0 & B & 0 & iJ & 0 & 0 & 0 \\ 0 & 0 & 0 & -B & 0 & -iJ & 0 & 0 \\ 0 & 0 & -iJ & 0 & B & 0 & 0 & 0 \\ 0 & 0 & 0 & iJ & 0 & -B & 0 & 0 \\ iJ & 0 & 0 & 0 & 0 & 0 & -B & 0 \\ 0 & -iJ & 0 & 0 & 0 & 0 & 0 & -3B \end{pmatrix}.$$

We find the eigenvalues and normalized eigenvectors

$$B \pm \sqrt{\alpha} : \frac{J}{\sqrt{2\alpha \mp 4B\sqrt{\alpha}}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \pm\frac{i\sqrt{\alpha} \mp 2iB}{J} \\ 0 \end{pmatrix},$$

$$-B \pm \sqrt{\alpha} : \frac{J}{\sqrt{2\alpha \mp 4B\sqrt{\alpha}}} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \mp\frac{i\sqrt{\alpha} \mp 2iB}{J} \end{pmatrix},$$

$$B \pm J : \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \\ \mp i \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad -B \pm J : \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ \pm i \\ 0 \\ 0 \end{pmatrix}$$

where $\alpha := J^2 + 4B^2$ as before. When $B = 0$ the eigenvalues are $\pm J$ each with multiplicity 4 and the normalized eigenvectors are

$$J : \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\0\\0\\0\\i\\0\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\0\\0\\0\\0\\0\\-i\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\1\\0\\-i\\0\\0\\0\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\0\\1\\0\\i\\0\\0\end{pmatrix},$$

$$-J : \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\0\\0\\0\\-i\\0\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\0\\0\\0\\0\\0\\i\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\1\\0\\i\\0\\0\\0\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\0\\1\\0\\-i\\0\\0\end{pmatrix}.$$

We see that the eigenvectors are entangled.

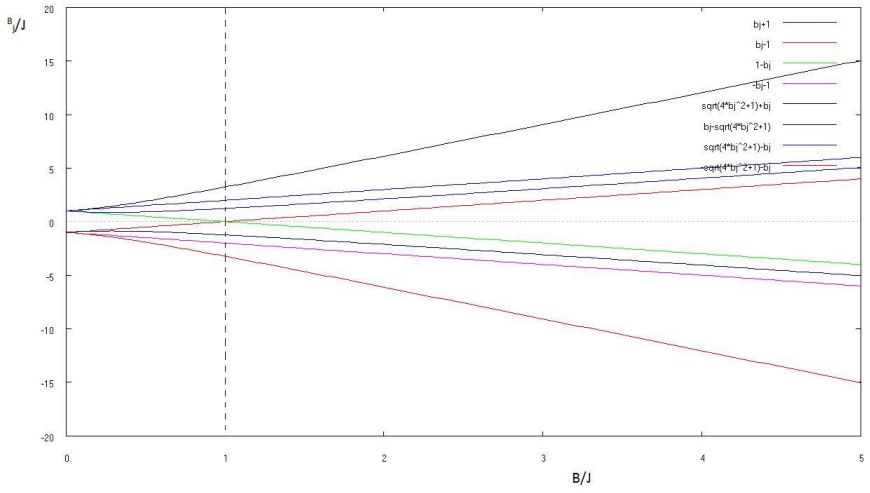

Figure 5.2: Energy levels of $\widehat{H}_8$

Figure 5.2 illustrates the eigenvalues as a function of B/J. We see that level crossing occurs when $B/J = 0$ and when $B/J = 1$. Note that

$$[\sigma_3 \otimes I_2 \otimes I_2 + I_2 \otimes \sigma_3 \otimes I_2 + I_2 \otimes I_2 \otimes \sigma_3, \sigma_1 \otimes \sigma_2 \otimes \sigma_3] \neq 0_8. \qquad \clubsuit$$

Example. Let $\mathcal{H}_1$, $\mathcal{H}_2$ be Hilbert spaces and $\mathcal{H}_1 \otimes \mathcal{H}_2$ be the product space. We may often write a self-adjoint Hamilton operator acting on the product space $\mathcal{H}_1 \otimes \mathcal{H}_2$ as

$$\widehat{H} := \widehat{H}_1 \otimes I_2 + I_1 \otimes \widehat{H}_2 + \epsilon \widehat{V}$$

where $\widehat{H}_1$ acts on $\mathcal{H}_1$, $\widehat{H}_2$ acts on $\mathcal{H}_2$, I_1 is the identity operator acting on $\mathcal{H}_1$ and I_2 is the identity operator acting on $\mathcal{H}_2$. We now consider specific cases of this (Steeb et al [137]). Consider the Hamilton operators

$$\widehat{H} := \alpha A \otimes I_n + I_n \otimes \beta B + \epsilon (A \otimes B)$$

$$\widehat{K} := \alpha A \otimes I_n + I_n \otimes \beta B + \epsilon (B \otimes A)$$

where we let $\alpha := \hbar\omega_1$, $\beta := \hbar\omega_2$ and $A := \sigma_3$, $B := \sigma_1$. We find

$$\widehat{H} = \begin{pmatrix} \hbar\omega_1 & \hbar\omega_2 + \epsilon & 0 & 0 \\ \hbar\omega_2 + \epsilon & \hbar\omega_1 & 0 & 0 \\ 0 & 0 & -\hbar\omega_1 & \hbar\omega_2 - \epsilon \\ 0 & 0 & \hbar\omega_2 - \epsilon & -\hbar\omega_1 \end{pmatrix}$$

$$\widehat{K} = \begin{pmatrix} \hbar\omega_1 & \hbar\omega_2 & \epsilon & 0 \\ \hbar\omega_2 & \hbar\omega_1 & 0 & -\epsilon \\ \epsilon & 0 & -\hbar\omega_1 & \hbar\omega_2 \\ 0 & -\epsilon & \hbar\omega_2 & -\hbar\omega_1 \end{pmatrix}.$$

The eigenvalues for $\widehat{H}$ are

$$E_1 = \hbar\omega_1 + \hbar\omega_2 + \epsilon, \quad E_2 = \hbar\omega_1 - \hbar\omega_2 - \epsilon,$$

$$E_3 = -\hbar\omega_1 + \hbar\omega_2 - \epsilon, \quad E_4 = -\hbar\omega_1 - \hbar\omega_2 + \epsilon$$

with the following corresponding eigenvectors

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix},$$

$$\frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

We see that these may be written as product states and as such are not entangled. The eigenvalues for $\widehat{K}$ are

$$\widetilde{E}_1 = -\sqrt{\hbar^2(\omega_1 + \omega_2)^2 + \epsilon^2}, \quad \widetilde{E}_2 = \sqrt{\hbar^2(\omega_1 + \omega_2)^2 + \epsilon^2},$$

$$\widetilde{E}_3 = -\sqrt{\hbar^2(\omega_1 - \omega_2)^2 + \epsilon^2}, \quad \widetilde{E}_4 = \sqrt{\hbar^2(\omega_1 - \omega_2)^2 + \epsilon^2}$$

with corresponding (unnormalized) eigenvectors

$$\begin{pmatrix} \epsilon \\ \epsilon \\ \widetilde{E}_1 - \hbar(\omega_1 + \omega_2) \\ \widetilde{E}_2 + \hbar(\omega_1 + \omega_2) \end{pmatrix}, \quad \begin{pmatrix} \epsilon \\ \epsilon \\ \widetilde{E}_2 - \hbar(\omega_1 + \omega_2) \\ \widetilde{E}_1 + \hbar(\omega_1 + \omega_2) \end{pmatrix},$$

$$\begin{pmatrix} \epsilon \\ -\epsilon \\ \widetilde{E}_3 - \hbar(\omega_1 - \omega_2) \\ \widetilde{E}_3 - \hbar(\omega_1 - \omega_2) \end{pmatrix}, \quad \begin{pmatrix} \epsilon \\ -\epsilon \\ \widetilde{E}_4 - \hbar(\omega_1 - \omega_2) \\ \widetilde{E}_4 - \hbar(\omega_1 - \omega_2) \end{pmatrix}.$$

We see that these are entangled and cannot be written as product states. Due to the discrete symmetry of $\widehat{H}$ there is energy level crossing. The permutation matrices P with $P\widehat{H}P^T = \widehat{H}$ are given by $P_0 = I_4$, $P_1 = I_2 \oplus \sigma_1$, $P_2 = \sigma_1 \oplus I_2$, $P_3 = \sigma_1 \oplus \sigma_1$. The Hamilton operator $\widehat{K}$ has no energy level crossing for $\epsilon > 0$ since only $P_0 = I_4$ is admitted as a discrete symmetry and we say the symmetry is broken. ♣

We introduce the following theorem (Steeb and Hardy [122]). Let A_1, A_2, A_3 be $n \times n$ matrices over $\mathbb{C}$ and I_n be the $n \times n$ identity matrix. Consider the matrix

$$\begin{aligned} M = & c_1(A_1 \otimes I_n \otimes I_n + I_n \otimes A_2 \otimes I_n + I_n \otimes I_n \otimes A_3) \\ & + c_2(A_1 \otimes A_2 \otimes I_n + A_1 \otimes I_n \otimes A_3 + I_n \otimes A_2 \otimes A_3) \\ & + c_3(A_1 \otimes A_2 \otimes A_3) \end{aligned}$$

where c_1, c_2, c_3 are constants. Since the terms in M are pairwise commutative we can write $\exp(M)$ as

$$\begin{aligned} e^M = & e^{c_1(A_1 \otimes I_n \otimes I_n)} e^{c_1(I_n \otimes A_2 \otimes I_n)} e^{c_1(I_n \otimes I_n \otimes A_3)} e^{c_2(A_1 \otimes A_2 \otimes I_n)} e^{c_2(A_1 \otimes I_n \otimes A_3)} \\ & \times e^{c_2(I_n \otimes A_2 \otimes A_3)} e^{c_3(A_1 \otimes A_2 \otimes A_3)}. \end{aligned}$$

Example. Consider the operator with triple spin interaction of spin-$\frac{1}{2}$

$$\begin{aligned} \widehat{H}_{1/2} = & J_1(\sigma_1 \otimes I_2 \otimes I_2 + I_2 \otimes \sigma_2 \otimes I_2 + I_2 \otimes I_2 \otimes \sigma_3) \\ & + J_2(\sigma_1 \otimes \sigma_2 \otimes I_2 + \sigma_1 \otimes I_2 \otimes \sigma_3 + I_2 \otimes \sigma_2 \otimes \sigma_3) \\ & + J_3(\sigma_1 \otimes \sigma_2 \otimes \sigma_3) \end{aligned}$$

where σ_1, σ_2, σ_3 are the Pauli spin matrices and I_2 the identity matrix. This operator acts in $\mathbb{C}^8$. We define the unitary operator

$$U_{1/2}(t) := e^{-i\widehat{H}_{1/2}\cdot}$$

Using the theorem introduced above we find

$$\begin{aligned}
U_{1/2}(t) = &\left(I_8\cos\left(\frac{tJ_1}{\hbar}\right) - i\sigma_1\otimes I_2\otimes I_2\sin\left(\frac{tJ_1}{\hbar}\right)\right)\\
&\times\left(I_8\cos\left(\frac{tJ_1}{\hbar}\right) - iI_2\otimes\sigma_2\otimes I_2\sin\left(\frac{tJ_1}{\hbar}\right)\right)\\
&\times\left(I_8\cos\left(\frac{tJ_1}{\hbar}\right) - iI_2\otimes I_2\otimes\sigma_3\sin\left(\frac{tJ_1}{\hbar}\right)\right)\\
&\times\left(I_8\cos\left(\frac{tJ_2}{\hbar}\right) - i\sigma_1\otimes\sigma_2\otimes I_2\sin\left(\frac{tJ_2}{\hbar}\right)\right)\\
&\times\left(I_8\cos\left(\frac{tJ_2}{\hbar}\right) - i\sigma_1\otimes I_2\otimes\sigma_3\sin\left(\frac{tJ_2}{\hbar}\right)\right)\\
&\times\left(I_8\cos\left(\frac{tJ_2}{\hbar}\right) - iI_2\otimes\sigma_2\otimes\sigma_3\sin\left(\frac{tJ_2}{\hbar}\right)\right)\\
&\times\left(I_8\cos\left(\frac{tJ_3}{\hbar}\right) - i\sigma_1\otimes\sigma_2\otimes\sigma_3\sin\left(\frac{tJ_3}{\hbar}\right)\right).
\end{aligned}$$

We may apply this unitary operator to entangled and unentangled states. The resultant states may in turn be entangled or unentangled depending on the chosen parameters. ♣

Example. Consider the operator with triple spin interaction of spin-1

$$\begin{aligned}
\widehat{H}_1 = &J_1(s_1\otimes I_3\otimes I_3 + I_3\otimes s_2\otimes I_3 + I_3\otimes I_3\otimes s_3)\\
&+J_2(s_1\otimes s_2\otimes I_3 + s_1\otimes I_3\otimes s_3 + I_3\otimes s_2\otimes s_3)\\
&+J_3(s_1\otimes s_2\otimes s_3)
\end{aligned}$$

where s_1, s_2 and s_3 are the trace-less hermitian matrices

$$s_1 := \frac{1}{\sqrt{2}}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix},\quad s_2 := \frac{1}{\sqrt{2}}\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}, s_3 := \begin{pmatrix}1&0&0\\0&0&0\\0&0&-1\end{pmatrix}.$$

This operator acts in the Hilbert space $\mathbb{C}^{27}$. We define the unitary operator

$$U_1(t) := e^{-i\widehat{H}_1 t/\hbar}.$$

Using the theorem introduced above we find

$$\begin{aligned}
U_1(t) = &\left(I_{27} - is_1 \otimes I_3 \otimes I_3 \sin\left(\frac{tJ_1}{\hbar}\right) + s_1^2 \otimes I_3 \otimes I_3 \left(\cos\left(\frac{tJ_1}{\hbar}\right) - 1\right)\right) \\
&\times \left(I_{27} - iI_3 \otimes s_2 \otimes I_3 \sin\left(\frac{tJ_1}{\hbar}\right) + I_3 \otimes s_2^2 \otimes I_3 \left(\cos\left(\frac{tJ_1}{\hbar}\right) - 1\right)\right) \\
&\times \left(I_{27} - iI_3 \otimes I_3 \otimes s_3 \sin\left(\frac{tJ_1}{\hbar}\right) + I_3 \otimes I_3 \otimes s_3^2 \left(\cos\left(\frac{tJ_1}{\hbar}\right) - 1\right)\right) \\
&\times \left(I_{27} - is_1 \otimes s_2 \otimes I_3 \sin\left(\frac{tJ_2}{\hbar}\right) + s_1^2 \otimes s_2^2 \otimes I_3 \left(\cos\left(\frac{tJ_2}{\hbar}\right) - 1\right)\right) \\
&\times \left(I_{27} - is_1 \otimes I_3 \otimes s_3 \sin\left(\frac{tJ_2}{\hbar}\right) + s_1^2 \otimes I_3 \otimes s_3^2 \left(\cos\left(\frac{tJ_2}{\hbar}\right) - 1\right)\right) \\
&\times \left(I_{27} - iI_3 \otimes s_2 \otimes s_3 \sin\left(\frac{tJ_2}{\hbar}\right) + I_3 \otimes s_2^2 \otimes s_3^2 \left(\cos\left(\frac{tJ_2}{\hbar}\right) - 1\right)\right) \\
&\times \left(I_{27} - is_1 \otimes s_2 \otimes s_3 \sin\left(\frac{tJ_3}{\hbar}\right) + s_1^2 \otimes s_2^2 \otimes s_3^2 \left(\cos\left(\frac{tJ_3}{\hbar}\right) - 1\right)\right).
\end{aligned}$$

We may apply this unitary operator to entangled and unentangled states. The resultant states may in turn be entangled or unentangled depending on the chosen parameters. ♣

5.3 Fermi Operators

We introduce new operators namely *creation* and *annihilation operators* which may be used in systems with multiple particles, quantum harmonic oscillators and fields of quantum computing where continuous variables are applied such as quantum teleportation and quantum cryptography. When creation and annihilation operators are used instead of wavefunctions we call this second quantization. These operators adhere to commutation (bosons) and anticommutation (fermions) rules to form Hilbert spaces in which we work and their function is to change the number of fixed quanta of energy in the system. The creation operator is the Hermitian adjoint of the annihilation operator. Authors who have studied this include Auerbach [2], Berezin [9], Khomskii [62], Nolting and Ramakanth [87], Prigogine and Rice [95], Sarkar [106], Smit [117], Steeb et al [123], [122], [124].

Fermions are particles with half-integer spin and they obey Fermi-Dirac statistics as well as the *Pauli exclusion principle*. This principle states that no two quanta of the same type may occupy the same quantum state. We may consider Fermi operators with or without spin. We introduce the spinless Fermi operators first. Fermi operators play a large role in solid state physics. Consider a family of linear operators c_j, $c_j^\dagger$ with $j = 1, 2, \ldots, n$ defined on a finite

dimensional Hilbert space $\mathcal{H}$ satisfying the *anticommutation relations*

$$[c_j, c_k]_+ = [c_j^\dagger, c_k^\dagger]_+ = 0 \text{ and } [c_j, c_k^\dagger]_+ = \delta_{j,k} I$$

where I is the identity operator and 0 is the zero operator of the Hilbert space, $\delta_{j,k}$ denotes the Kronecker delta. The indices are the quantum number (e.g. spin, angular momentum, etc.) of the operator. $c_j^\dagger$ is called a Fermi creation operator and c_j is a Fermi annihilation operator. A direct consequence of the anticommutation relations is

$$c_j^\dagger c_j^\dagger = c_j c_j = 0$$

which illustrates the Pauli exclusion principle as required. We define the normalized *vacuum state* $|0\rangle$ with the property

$$c_j |0\rangle = 0 \quad \text{and} \quad \langle 0| c_j^\dagger = 0$$

where $j = 1, 2, \ldots, n$. This is the quantum state with the lowest possible energy and contains no quanta. New states may be constructed from the vacuum state and the creation operators. It is useful to determine the commutation relationship between creation and annihilation operators

$$[c_i^\dagger, c_j] = c_i^\dagger c_j - c_j c_i^\dagger = c_i^\dagger c_j + c_j c_i^\dagger - c_j c_i^\dagger - c_j c_i^\dagger = \delta_{ij} I - 2 c_j c_i^\dagger.$$

When $n = 1$ we find a matrix representation of the operators $c^\dagger$, c and $\widehat{N}$ where we define $\widehat{N} := c^\dagger c$ to be the *number operator*. We find

$$c^\dagger = \begin{pmatrix} 0\,1 \\ 0\,0 \end{pmatrix} = \frac{1}{2}(\sigma_1 + i\sigma_2) = \frac{1}{2}\sigma_+$$

$$c = \begin{pmatrix} 0\,0 \\ 1\,0 \end{pmatrix} = \frac{1}{2}(\sigma_1 - i\sigma_2) = \frac{1}{2}\sigma_-$$

and the matrix representations for $|0\rangle$ and $c^\dagger |0\rangle$ are given by

$$|0\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}, \quad c^\dagger |0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

For arbitrary n we have

$$c_k^\dagger = \sigma_3 \otimes \cdots \otimes \sigma_3 \otimes \left(\frac{1}{2}\sigma_+\right) \otimes I_2 \otimes \cdots \otimes I_2$$

$$c_k = \sigma_3 \otimes \cdots \otimes \sigma_3 \otimes \left(\frac{1}{2}\sigma_-\right) \otimes I_2 \otimes \cdots \otimes I_2$$

where there are n terms in total and $\frac{1}{2}\sigma_\pm$ is in the kth position (Steeb [123]).

Example. Let $c_1^\dagger$, $c_2^\dagger$ be Fermi creation operators. Consider the hermitian Hamilton operator

$$\widehat{H} := t(c_1^\dagger c_2^\dagger + c_2 c_1).$$

Let $\widehat{N} := c_1^\dagger c_1 + c_2^\dagger c_2$ be the number operator. Furthermore consider the basis

$$|s_0\rangle = |0\rangle\,, \quad |s_1\rangle = c_1^\dagger\,|0\rangle\,, \quad |s_2\rangle = c_2^\dagger\,|0\rangle\,, \quad |s_3\rangle = c_1^\dagger c_2^\dagger\,|0\rangle\,.$$

We find the commutator

$$[\widehat{H}, \widehat{N}] = 2t(c_2^\dagger c_1^\dagger - c_2 c_1).$$

Using the given basis we find

$$\widehat{H}\,|s_0\rangle = t\,|s_3\rangle\,, \quad \widehat{H}\,|s_1\rangle = 0, \quad \widehat{H}\,|s_2\rangle = 0, \quad \widehat{H}\,|s_3\rangle = t\,|s_0\rangle$$

which gives us the matrix representation of $\widehat{H}$

$$\widehat{H} = \begin{pmatrix} 0\,0\,0\,t \\ 0\,0\,0\,0 \\ 0\,0\,0\,0 \\ t\,0\,0\,0 \end{pmatrix}. \qquad \clubsuit$$

5.3.1 Hubbard Model

We now study Fermi operators with spin as well as introducing the *Hubbard model*. The Hubbard model is a simplified approximate model for electrons in a solid which interact with each other through Coulomb interaction. This model takes into account the quantum mechanical motion of electrons in a solid and the nonlinear repulsive interaction between electrons. Despite being too simple to describe actual solids faithfully it is a very important model in theoretical physics and exhibits various interesting phenomena. The Hubbard model plays an important role in the modeling of magnetism, charge density waves and high-T_c superconductivity. An interesting phenomena that has been studied is that the 1 dimensional Hubbard Hamilton operator for the benzene molecule appears to violate the *non-crossing rule* (Yuzbashyan et al [160]). This will be expanded upon in a later section.

We consider a family of linear operators $c_{js}, c_{js}^\dagger$ with $j = 1, 2, \ldots, n$ defined on a finite dimensional Hilbert space $\mathcal{H}$ satisfying the anticommutation relations

$$[c_{js}, c_{ks'}]_+ = [c_{js}^\dagger, c_{ks'}^\dagger]_+ = 0 \text{ and } [c_{js}, c_{ks'}^\dagger]_+ = \delta_{jk}\delta_{ss'} I$$

where I is the identity operator, 0 is the zero operator, $j, k = 1, 2, \ldots, n$ and $s, s' \in \{\uparrow, \downarrow\}$. As before these operators are annihilation and creation operators for fermions and now we have included spin with the quantum number. The normalized *vacuum state* $|0\rangle$ is defined with the property $c_{js}\,|0\rangle = 0$. Other states may now be constructed from the vacuum state and the creation operators. From above it follows that the operators obey the Pauli exclusion principle as expected. In other words $(c_{js}^\dagger)^2 = (c_{js})^2 = 0$. We introduce a convention to order the operators, both with respect to spin as well as the quantum number.

All spin up operators are placed on the left and we set the Fermi operators with the lower quantum number on the left hand side.

We may define the spin $\mathbf{S}_i$ and quasispin $\mathbf{R}_i$ operators by

$$\widehat{S}_{ix} = \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\downarrow} + c_{i\downarrow}^\dagger c_{i\uparrow}), \quad \widehat{S}_{iy} = \frac{1}{2i}(c_{i\uparrow}^\dagger c_{i\downarrow} - c_{i\downarrow}^\dagger c_{i\uparrow}), \quad \widehat{S}_{iz} = \frac{1}{2}(n_{i\uparrow} - n_{i\downarrow}),$$

$$\widehat{R}_{ix} = \frac{1}{2}(c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger + c_{i\downarrow} c_{i\uparrow}), \quad \widehat{R}_{iy} = \frac{1}{2i}(c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger - c_{i\uparrow} c_{i\downarrow}), \quad \widehat{R}_{iz} = \frac{1}{2}(n_{i\uparrow} + n_{i\downarrow} - 1).$$

where $n_{is} := c_{is}^\dagger c_{is}$. Both of these operators form a Lie algebra under the commutator (Steeb et al [127], [130], [129]).

Example. In Wannier representation the two-point Hubbard model with cyclic boundary conditions is given by

$$\widehat{H} = t(c_{1\uparrow}^\dagger c_{2\uparrow} + c_{1\downarrow}^\dagger c_{2\downarrow} + c_{2\uparrow}^\dagger c_{1\uparrow} + c_{2\downarrow}^\dagger c_{1\downarrow}) + U(n_{1\uparrow} n_{1\downarrow} + n_{2\uparrow} n_{2\downarrow})$$

where $n_{js} := c_{js}^\dagger c_{js}$ with the parameters $t > 0$ and $U > 0$ (Steeb et al [133]). The Fermi operators obey the anticommutation relations. The total number operator $\widehat{N}$ and the total spin operator $\widehat{S}_z$ in the z direction are defined by

$$\widehat{N} := \sum_{j=1}^{2} (c_{j\uparrow}^\dagger c_{j\uparrow} + c_{j\downarrow}^\dagger c_{j\downarrow}), \quad \widehat{S}_z := \frac{1}{2} \sum_{j=1}^{2} (c_{j\uparrow}^\dagger c_{j\uparrow} - c_{j\downarrow}^\dagger c_{j\downarrow})$$

and $[\widehat{H}, \widehat{N}] = [\widehat{H}, \widehat{S}_z] = 0$. We consider the subspace with 2 electrons $N = 2$ and $S_z = 0$. A basis for this system is

$$|s_1\rangle := c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle, \quad |s_2\rangle := c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle, \quad |s_3\rangle := c_{2\uparrow}^\dagger c_{1\downarrow}^\dagger |0\rangle, \quad |s_4\rangle := c_{2\uparrow}^\dagger c_{2\downarrow}^\dagger |0\rangle.$$

Another basis that may be considered is

$$|b_1\rangle := \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger + c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger) |0\rangle, \quad |b_2\rangle := \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger + c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger) |0\rangle,$$

$$|b_3\rangle := \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger - c_{2\downarrow}^\dagger c_{1\uparrow}^\dagger) |0\rangle, \quad |b_4\rangle := \frac{1}{\sqrt{2}}(c_{1\downarrow}^\dagger c_{1\uparrow}^\dagger - c_{2\downarrow}^\dagger c_{2\uparrow}^\dagger) |0\rangle.$$

These states may be considered as the Bell states. We find the matrix representations of $\widehat{H}$ in these bases (Steeb and Hardy [122]). Applying $\widehat{H}$ to the given bases gives us

$$\widehat{H} |s_1\rangle = U |s_1\rangle + t |s_2\rangle + t |s_3\rangle, \quad \widehat{H} |s_2\rangle = t |s_1\rangle + t |s_4\rangle,$$

$$\widehat{H} |s_3\rangle = t |s_1\rangle + t |s_4\rangle, \quad \widehat{H} |s_4\rangle = t |s_2\rangle + t |s_3\rangle + U |s_4\rangle.$$

This yields the matrix representation

$$\widehat{H}_s = \begin{pmatrix} U & t & t & 0 \\ t & 0 & 0 & t \\ t & 0 & 0 & t \\ 0 & t & t & U \end{pmatrix}.$$

This matrix representation admits symmetries given by the permutation matrices

$$P_0 = I_4, \quad P_1 = \begin{pmatrix} 1\,0\,0\,0 \\ 0\,0\,1\,0 \\ 0\,1\,0\,0 \\ 0\,0\,0\,1 \end{pmatrix}, \quad P_2 = \begin{pmatrix} 0\,0\,0\,1 \\ 0\,1\,0\,0 \\ 0\,0\,1\,0 \\ 1\,0\,0\,0 \end{pmatrix}, \quad P_3 = \begin{pmatrix} 0\,0\,0\,1 \\ 0\,0\,1\,0 \\ 0\,1\,0\,0 \\ 1\,0\,0\,0 \end{pmatrix}$$

where $P_j^T \widehat{H}_s P_j = \widehat{H}_s$. We see $P_1P_2 = P_3$, $P_1P_3 = P_2$, $P_2P_3 = P_1$ and $P_1^2 = P_2^2 = P_3^2 = I_4$. Thus we can form the projection matrices

$$\Pi_{1_+} = \frac{1}{2}(I_4 + P_1), \quad \Pi_{2_+} = \frac{1}{2}(I_4 + P_2), \quad \Pi_{3_+} = \frac{1}{2}(I_4 + P_3),$$

$$\Pi_{1_-} = \frac{1}{2}(I_4 - P_1), \quad \Pi_{2_-} = \frac{1}{2}(I_4 - P_2), \quad \Pi_{3_-} = \frac{1}{2}(I_4 - P_3).$$

Consider $\Pi_{3_\pm}$. We have

$$\Pi_{3_+} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} v_1 + v_4 \\ v_2 + v_3 \\ v_2 + v_3 \\ v_1 + v_4 \end{pmatrix}, \quad \Pi_{3_-} \begin{pmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{pmatrix} = \frac{1}{2} \begin{pmatrix} v_1 - v_4 \\ v_2 - v_3 \\ -v_2 + v_3 \\ -v_1 + v_4 \end{pmatrix}$$

where $\mathbf{v}$ is an arbitrary vector. So we see that $\Pi_{3_\pm}$ projects into the subspaces spanned by the normalized vectors

$$\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} \right\},$$

$$\left\{ \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \quad \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix} \right\}.$$

We see that these are the Bell states. Considering the second basis we find

$$\widehat{H}\,|b_1\rangle = U\,|s_1\rangle + 2t\,|s_2\rangle\,, \quad \widehat{H}\,|b_2\rangle = 2t\,|s_1\rangle\,, \quad \widehat{H}\,|b_3\rangle = 0, \quad \widehat{H}\,|b_4\rangle = U\,|s_4\rangle$$

yielding the matrix representation

$$\widehat{H}_b = \begin{pmatrix} U & 2t & 0 & 0 \\ 2t & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & U \end{pmatrix} = \begin{pmatrix} U & 2t \\ 2t & 0 \end{pmatrix} \oplus \begin{pmatrix} 0 & 0 \\ 0 & U \end{pmatrix}$$

where $\oplus$ denotes the *direct sum*. Only the identity matrix $P_0 = I_4$ satisfies $P_j^T \widehat{H}_s P_j = \widehat{H}_s$. ♣

Chapter 6

Entanglement

6.1 Introduction

Historically quantum entanglement has been studied by physicists such as Einstein [29], Bohr [14], Weyl [151], Einstein et al [30], Schrödinger [108], [109] and Bell [6]. More recently this phenomenon and its applications has been studied by authors such as Raimond and Dalibard [97], Knight [67], Cleve and Buhrman [20], Bruß [15], S-J. Gu et al [46], Horodecki et al [55], Bruß and Macchiavello [16].

Entanglement is a type of quantum correlation that is one of the most striking features of quantum mechanics and sets it apart from classical mechanics. This resource enforces a departure from classical thought. Entanglement occurs when a pair of particles interact physically and then become separated with the interaction being such that each resulting member of the pair is described by the same state. When a measurement is made on one member of the entangled pair and it takes on a specific value (for example spin up), then the other member of the pair will take on a correlated value (for example spin down). This correlation is instantaneous and is observed even though the entangled pair may be separated by arbitrarily large distances. This correlation is what makes quantum entanglement a powerful tool in transmitting information. Entangled quantum states are an important component of quantum computing techniques such as quantum error-correction, dense coding and quantum teleportation.

Consider a quantum state $|\psi\rangle$ in the composite Hilbert space $\mathcal{H}^{AB} = \mathcal{H}^A \otimes \mathcal{H}^B$. We may ask ourselves whether or not this state can be decomposed into the Kronecker product of two states in the component Hilbert spaces $\mathcal{H}^A$ and $\mathcal{H}^B$. If this is possible we say the state is unentangled and if this is not possible then the state is entangled.

Example. Consider the normalized state

$$|\psi\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}.$$

Then $|\psi\rangle$ can be written as

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

We say that $|\psi\rangle$ is *separable* or a *product state*. A state that cannot be written as a product state is said to be *entangled*. ♣

Example. Consider the normalized vector

$$|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\phi} \\ 0 \\ 0 \\ 1 \end{pmatrix} \in \mathbb{C}^4.$$

We assume there exists the states $|u\rangle = (u_1, u_2)^T$ and $|v\rangle = (v_1, v_2)^T$ in the Hilbert space $\mathbb{C}^2$ such that $|\psi\rangle = |u\rangle \otimes |v\rangle$ is true. From this assumption we obtain the equations

$$u_1 v_1 = e^{i\phi}/\sqrt{2}, \quad u_1 v_2 = 0, \quad u_2 v_1 = 0, \quad u_2 v_2 = 1/\sqrt{2}.$$

These equations cannot be satisfied simultaneously and our initial assumption was incorrect. $|\psi\rangle$ cannot be written as a Kronecker product of two vectors and is thus entangled. ♣

We introduce the states

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix},$$

$$|\psi_3\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 0 \\ -1 \end{pmatrix}, \quad |\psi_4\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}.$$

These states form the *Bell basis* in $\mathbb{C}^4$ and are maximally entangled.

Consider the Hilbert space $\mathcal{H} = \mathbb{C}^n$ and the product space $\mathcal{H} \otimes \mathcal{H}$. Let A be an arbitrary $n \times n$ matrix over $\mathbb{C}$. A normalized state $|\psi\rangle \in \mathcal{H} \otimes \mathcal{H}$ is called *maximally entangled* if

$$\langle\psi| (A \otimes I_n) |\psi\rangle = \dim(\mathcal{H})^{-1} \mathrm{tr}(A)$$

holds.

Example. Consider the normalized states in $\mathbb{C}^4$

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad |\psi_3\rangle = \frac{1}{2}\begin{pmatrix} 1 \\ 1 \\ -1 \\ 1 \end{pmatrix}.$$

In all three cases we have $\dim(\mathcal{H}) = \dim(\mathbb{C}^2) = 2$. Let

$$A = \begin{pmatrix} a_{11}\, a_{12} \\ a_{21}\, a_{22} \end{pmatrix}$$

so that $\mathrm{tr}(A) = a_{11} + a_{22}$. Then

$$A \otimes I_2 = \begin{pmatrix} a_{11} & 0 & a_{12} & 0 \\ 0 & a_{11} & 0 & a_{12} \\ a_{21} & 0 & a_{22} & 0 \\ 0 & a_{21} & 0 & a_{22} \end{pmatrix}.$$

For the left-hand side of the equation to determine if a state is maximally entangled we find

$$\begin{aligned} \langle\psi_1| (A \otimes I_2) |\psi_1\rangle &= \frac{1}{2}(a_{11} + a_{22}) \\ \langle\psi_2| (A \otimes I_2) |\psi_2\rangle &= \frac{1}{2}(a_{11} + a_{12} + a_{21} + a_{22}) \neq \frac{1}{2}(a_{11} + a_{22}) \\ \langle\psi_3| (A \otimes I_2) |\psi_3\rangle &= \frac{1}{2}(a_{11} + a_{22}). \end{aligned}$$

Thereby showing that $|\psi_1\rangle$ and $|\psi_3\rangle$ are maximally entangled. For $|\psi_2\rangle$ we have

$$|\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix}.$$

Program 9 is provided in the Computer algebra implementation chapter that determines if a given vector is maximally entangled. ♣

Let $|\psi\rangle$ be a given state in the Hilbert space $\mathbb{C}^n$ and let X, Y be two $n \times n$ hermitian matrices. We define the *correlation* for a given state as

$$C_{XY}(|\psi\rangle) := \langle\psi|XY|\psi\rangle - \langle\psi|X|\psi\rangle \langle\psi|Y|\psi\rangle .$$

Example. Consider the Hilbert space $\mathbb{C}^4$ and let

$$X = \begin{pmatrix} 0\,0\,0\,1 \\ 0\,0\,1\,0 \\ 0\,1\,0\,0 \\ 1\,0\,0\,0 \end{pmatrix}, \quad Y = \begin{pmatrix} 1\,0\,0\,0 \\ 0\,0\,0\,1 \\ 0\,0\,1\,0 \\ 0\,1\,0\,0 \end{pmatrix}.$$

Consider the normalized states

$$|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}, \quad |\phi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\\0\\0\end{pmatrix}$$

where $|\psi\rangle$ is one of the (entangled) Bell states and $|\phi\rangle$ is a separable state. We find

$$C_{XY}(|\psi\rangle) = 0, \quad C_{XY}(|\phi\rangle) = \frac{1}{2}. \qquad \clubsuit$$

It has been shown that a completely entangled state belonging to a finite dimensional Hilbert space is equivalent to a simultaneous eigenstate of two unitary operators (Ban [4]). Suppose that

$$\{|a_0\rangle, |a_1\rangle, \ldots, |a_{n-1}\rangle\}$$

is a complete orthonormal basis of a Hilbert space $\mathcal{H}_n$. We then perform the *discrete Fourier transform* introduced in chapter 4.1 to obtain a new orthonormal basis

$$\{|b_0\rangle, |b_1\rangle, \ldots, |b_{n-1}\rangle\}.$$

Using these two sets we introduce the hermitian operators $\widehat{A}$ and $\widehat{B}$ which are *complementary* with each other

$$\widehat{A} := \sum_{k=0}^{n-1} k\,|a_k\rangle\langle a_k|, \quad \widehat{B} := \sum_{k=0}^{n-1} k\,|b_k\rangle\langle b_k|.$$

We further introduce four new hermitian operators defined on the Hilbert space $\mathcal{H}_n \otimes \mathcal{H}_n$ by the relations

$$\widehat{A}_1 := \widehat{A} \otimes I_4, \quad \widehat{A}_2 := I_4 \otimes \widehat{A}, \quad \widehat{B}_1 := \widehat{B} \otimes I_4, \quad \widehat{B}_2 := I_4 \otimes \widehat{B}$$

and from these we define the unitary matrices

$$\widehat{M}_- := \exp((2\pi i/n)m(\widehat{A}_1 - \widehat{A}_2)), \quad \widehat{M}_+ := \exp((2\pi i/n)q(\widehat{B}_1 + \widehat{B}_2))$$

for any integers m and q. We introduce the fully entangled states

$$\begin{aligned}|\Psi_{jk}\rangle &= \frac{1}{\sqrt{n}}\sum_{\ell=0}^{n-1} |a_{\ell+j \bmod n}\rangle \otimes |a_\ell\rangle\, e^{(2\pi i/n)k\ell} \\ &= \frac{1}{\sqrt{n}}\sum_{\ell=0}^{n-1} |b_\ell\rangle \otimes |b_{k-\ell \bmod n}\rangle\, e^{-(2\pi i/n)j\ell}\end{aligned}$$

where $j, k = 0, 1, \ldots, n-1$. It may be seen that $|\Psi_{jk}\rangle$ are simultaneous eigenstates of $\widehat{M}_-$ and $\widehat{M}_+$ such that

$$\widehat{M}_- |\Psi_{jk}\rangle = \omega^{jm} |\Psi_{jk}\rangle, \quad \widehat{M}_+ |\Psi_{jk}\rangle = \omega^{kq} |\Psi_{jk}\rangle.$$

So it has been shown that a completely entangled state belonging to the Hilbert space $\mathcal{H}_n \otimes \mathcal{H}_n$ is a simultaneous eigenstate of two unitary operators $\widehat{M}_{\mp}$ where the hermitian matrices $\widehat{A}$ and $\widehat{B}$ are complementary with each other.

Entanglement plays a large role in quantum information theory and enables us to achieve tasks that would otherwise be impossible. Interference impairs the ability to transport states over long distances and introduces the need for error correcting. A way that we overcome the problem of noise is to distribute the quantum states over the 'noisy' channel that is available and use high quality quantum processes (known as local operations - LO) in the respective laboratories. These LO are independent and occur in a controlled environment. Classical communication (CC) is used to coordinate the quantum actions. Such a process is known as *local operations and classical communication* ($LOCC$). The term entanglement is used to describe any quantum correlation that cannot be created by LOCC alone. Quantum entanglement may be exploited to perform tasks that are inefficient or even impossible in the classical realm and plays a large role in quantum communication science. An example of how entanglement may be harnessed is in teleportation where classical communication is combined with entanglement to transmit quantum states and data. Some basic properties of entanglement are

(a) Separable states contain no entanglement.

(b) All non-separable states are entangled (cannot be reproduced by LOCC alone) meaning that such states possess an additional useful resource not present in separable states.

(c) Entanglement of states does not change under LOCC transformations or local unitary operations.

(d) We may quantify the amount of entanglement and see that states may be maximally entangled. It can be seen that in a two party system consisting of two fixed d-dimensional subsystems (qudits) any *pure state* equivalent to

$$|\psi_d^+\rangle = \frac{|00\rangle + |11\rangle + \cdots + |(d-1)(d-1)\rangle}{\sqrt{d}}$$

is maximally entangled. Here $|jj\rangle \equiv |j\rangle \otimes |j\rangle$ (Plenio and Virmani [93]).

Example. Consider the Pauli spin matrix σ_2. The eigenvalues for this matrix are 1 and -1. The corresponding normalized eigenvectors are

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\ i\end{pmatrix} \text{ and } \frac{1}{\sqrt{2}}\begin{pmatrix}1\\ -i\end{pmatrix}.$$

It is easy to show that

$$A = \sigma_2 \otimes \sigma_2 = \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} \otimes \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} = \begin{pmatrix}0 & 0 & 0 & -1\\ 0 & 0 & 1 & 0\\ 0 & 1 & 0 & 0\\ -1 & 0 & 0 & 0\end{pmatrix}$$

with eigenvalues 1 (multiplicity 2) and -1 (multiplicity 2). The four product eigenstates are given by

$$|\phi_1\rangle = \frac{1}{2}\begin{pmatrix}1\\ i\end{pmatrix}\otimes\begin{pmatrix}1\\ i\end{pmatrix}, \quad |\phi_2\rangle = \frac{1}{2}\begin{pmatrix}1\\ i\end{pmatrix}\otimes\begin{pmatrix}1\\ -i\end{pmatrix},$$

$$|\phi_3\rangle = \frac{1}{2}\begin{pmatrix}1\\ -i\end{pmatrix}\otimes\begin{pmatrix}1\\ i\end{pmatrix}, \quad |\phi_4\rangle = \frac{1}{2}\begin{pmatrix}1\\ -i\end{pmatrix}\otimes\begin{pmatrix}1\\ -i\end{pmatrix}.$$

These vectors are eigenvectors of the above matrix $\sigma_2 \otimes \sigma_2$

$$A|\phi_1\rangle = |\phi_1\rangle, \quad A|\phi_2\rangle = -|\phi_2\rangle, \quad A|\phi_3\rangle = -|\phi_3\rangle, \quad A|\phi_4\rangle = |\phi_4\rangle.$$

We can show two examples of sets of entangled states in this (composite) Hilbert space, the first being the Bell states

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}.$$

These are eigenvectors of A. Another set of fully entangled states are

$$\frac{1}{2}\begin{pmatrix}-1\\-1\\-1\\1\end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix}-1\\1\\1\\1\end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix}1\\-1\\1\\1\end{pmatrix}, \quad \frac{1}{2}\begin{pmatrix}1\\1\\-1\\1\end{pmatrix}.$$

Once again these are eigenvectors of A. This example has useful applications in physics. ♣

Example. Consider the Hilbert space $\mathbb{C}^4$ and the Hamilton operator

$$\widehat{H} = \hbar\omega(\sigma_3 \otimes \sigma_3) + \Delta(\sigma_1 \otimes \sigma_1)$$

where $\omega, \Delta > 0$. We investigate this operator as well as the unitary operator $U(t) = \exp(-i\widehat{H}t/\hbar)$ (Steeb [135]). We find the 4×4 matrix

$$\widehat{H} = \begin{pmatrix}\hbar\omega & 0 & 0 & \Delta\\ 0 & -\hbar\omega & \Delta & 0\\ 0 & \Delta & -\hbar\omega & 0\\ \Delta & 0 & 0 & \hbar\omega\end{pmatrix}$$

with the eigenvalues

$$\hbar\omega + \Delta, \quad -\hbar\omega - \Delta, \quad -\hbar\omega + \Delta, \quad \hbar\omega - \Delta$$

and corresponding normalized eigenvectors

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}.$$

We see that these states do not depend on ω or Δ and are fully entangled since they are the Bell states. We consider the unitary operator $U(t)$

$$\begin{aligned} U(t) &= \exp(-i\widehat{H}t/\hbar) = e^{-i\omega t(\sigma_3\otimes\sigma_3)}e^{-i\Delta t(\sigma_1\otimes\sigma_1)/\hbar} \\ &= I_4\cos(\omega t)\cos(\Delta t/\hbar) + i(\sigma_3\otimes\sigma_3)\sin(\omega t)\cos(\Delta t/\hbar) \\ &\quad + i(\sigma_1\otimes\sigma_1)\cos(\omega t)\sin(\Delta t/\hbar) - (\sigma_3\sigma_1)\otimes(\sigma_3\sigma_1)\sin(\omega t)\sin(\Delta t/\hbar). \end{aligned}$$

When we apply $U(t)$ to an unentangled state, depending on the choice of parameters we may obtain an entangled state. For example

$$U(t)\begin{pmatrix}1\\0\\0\\0\end{pmatrix} = \begin{pmatrix}\cos(\omega t)\cos(\Delta t/\hbar) + i\sin(\omega t)\cos(\Delta t/\hbar)\\0\\0\\-\sin(\omega t)\sin(\Delta t/\hbar) + i\cos(\omega t)\sin(\Delta t/\hbar)\end{pmatrix}.$$

For the case where $\hbar\omega = \Delta$ energy *level crossing* occurs. This Hamilton operator may be extended to N factors and this will be discussed in chapter 6.3. ♣

6.2 Measures of Entanglement

It is clear that to be able to exploit this resource we require a quantitative measure of the entanglement of states. Measures of entanglement have been studied by various authors. In 1997 Vedral et al [144] discussed various requirements of measures of entanglement together with introducing different entanglement measures. Some of these measures have practical applications whereas some of them are of theoretic interest only. In 1998 Bennett et al [8] discussed quantum nonlocality without entanglement. They showed that even if a pair of separated observers performed a sequence of local operations and classical communication (LOCC) on an orthogonal set of product states presented to them they could not reliably distinguish between the states. In 1999 Coffman et al [21] studied distributed entanglement between three qubits. They showed that if three quantum states A, B and C were entangled with each other then there is a trade-off between As entanglement with B and its entanglement with C. They discussed the entanglement measure known as the tangle and intoduced a relationship between τ_{AB}, τ_{AC} and τ_{BC}. In 2002 Bruß [15] produced a tutorial describing different ways of quantifying entanglement using appropriate measures, how to characterize entanglement and how to classify entangled states based on their usefulness. In 2007 Plenio and Virmani [93] discussed various entanglement measures focusing on the finite dimensional bipartite case. In 2009 Horodecki et al [55] investigated entanglement and different entanglement measures. They investigated the role of entanglement in quantum communication and how one may exploit entanglement in quantum cryptography. In 2011 Sperling and Vogel [118] investigated quantifying entanglement, focusing on universal entanglement measures that are invariant under local invertible operations. They identified that the Schmidt number is a universal measure

of entanglement. In 2011 Streltsov et al [138] discussed an easy implementable algorithm for the geometric measure of entanglement. They introduced an algorithm for approximating the entanglement of any mixed multipartite state (where multipartite entanglement is discussed at the end of the chapter) reducing the problem to an eigenvalue problem and a singular value decomposition. In 2011 Bruß and Macchiavello [16] investigated the multipartite entanglement of states used in quantum algorithms and showed that many quantum algorithms exploit multipartite entanglement.

Bell's theorem enables us to verify experimentally the effects of quantum mechanics and provide a way to quantify quantum correlations. In 1991 Ekert [32] investigated quantum cryptography based on Bell's theorem. Bell's inequalities provided some of the first measures of entanglement however it was found that in some cases these inequalities do not provide a sufficient measure for quantum correlations. Today there are several more measures of entanglement such as the entropy of entanglement, the entanglement of formation, the tangle (which is the squared concurrence of the state) and the Schmidt number to name a few. Some of these measures have physical relevance whereas others are merely of academic interest. An entanglement measure is a mathematical quantity that captures the essential features associated with entanglement and some of the desired properties of such a measure are

(i) A bipartite measure of entanglement $E(\rho)$ is a mapping $\rho \rightarrow E(\rho) \in \mathbb{R}^+$ where ρ is the *density matrix* associated with the state. When we consider the maximally entangled pure state $|\psi_d^+\rangle$ introduced previously we require $E(|\psi_d^+\rangle \langle\psi_d^+|) = \log(d)$.

(ii) $E(\rho) = 0$ if ρ represents a separable state.

(iii) E does not increase under LOCC.

(iv) For a pure state $|\psi\rangle \langle\psi|$ the measure reduces to the entropy of entanglement.

6.2.1 Entropy of Entanglement

Entropy is a measure of how much uncertainty there is in the state of a physical system and plays a role in both classical and quantum information theory. In classical information theory we consider the *Shannon entropy* where probability distributions play a role. In quantum information theory we use the *von Neumann entropy* where density operators replace the probability distributions. We define the von Neumann entropy

$$S(\rho) := -\text{tr}(\rho \log_2 \rho).$$

Let λ_j be the eigenvalues of ρ. Then

$$S(\rho) = -\sum_j \lambda_j \log_2 \lambda_j.$$

One defines $0\log_2 0 \equiv 0$.

Consider two Hilbert spaces $\mathcal{H}_A$ and $\mathcal{H}_B$ with identity operators I_A, I_B and orthonormal bases $|\psi_j\rangle$ $(j = 1, 2, \ldots, \dim(\mathcal{H}_A))$ and $|\phi_j\rangle$ $(j = 1, 2, \ldots, \dim(\mathcal{H}_B))$ respectively. Then we define the *partial trace* of ρ over subsystems A and B as follows

$$\rho_B := \mathrm{tr}_A(\rho) = \sum_{j=1}^{\dim(\mathcal{H}_A)} (\langle\psi_j| \otimes I_B)\rho(|\psi_j\rangle \otimes I_B)$$

and

$$\rho_A := \mathrm{tr}_B(\rho) = \sum_{j=1}^{\dim(\mathcal{H}_B)} (I_A \otimes \langle\phi_j|)\rho(I_A \otimes |\phi_j\rangle).$$

The *entropy of entanglement* for a pure state $|\psi\rangle$ is defined as

$$E(|\psi\rangle\langle\psi|) := S(\mathrm{tr}_A |\psi\rangle\langle\psi|) = S(\mathrm{tr}_B |\psi\rangle\langle\psi|).$$

Example. We consider the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ where $\mathcal{H}_A = \mathcal{H}_B = \mathbb{C}^2$ and the standard basis is used. Consider the states

$$|\psi_1\rangle := \frac{1}{2}\begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix}, \quad |\psi_2\rangle := \frac{1}{\sqrt{2}}\begin{pmatrix} e^{i\phi} \\ 0 \\ 0 \\ 1 \end{pmatrix}$$

where $|\psi_1\rangle$ is a disentangled state and $|\psi_2\rangle$ is an entangled state. We find

$$\rho_1 = \frac{1}{4}\begin{pmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{pmatrix}, \quad \rho_{1,A} = \frac{1}{2}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}, \quad \rho_{1,B} = \frac{1}{2}\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix}$$

with the eigenvalues for both of these being 0 and 1.

$$E(\rho_1) = S(\rho_{1,A}) = 0.$$

Similarly

$$\rho_2 = \frac{1}{2}\begin{pmatrix} 1 & 0 & 0 & e^{i\phi} \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ e^{-i\phi} & 0 & 0 & 1 \end{pmatrix}, \quad \rho_{2,A} = \frac{1}{2}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = \rho_{2,B}$$

with the eigenvalue being $\frac{1}{2}$ with multiplicity 2.

$$E(\rho_2) = S(\rho_{2,A}) = 1. \qquad \clubsuit$$

Example. Consider the state in $\mathbb{C}^4$

$$|\psi\rangle = \frac{1}{2}(U_1 \otimes U_2)\begin{pmatrix} 1 \\ -1 \\ -1 \\ 1 \end{pmatrix} = (U_1 \otimes U_2)\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

where $U_1, U_2 \in U(2)$. We choose the basis

$$\left\{ U_2 \begin{pmatrix} 1 \\ 0 \end{pmatrix}, U_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} \right\}$$

to calculate the partial trace. We find

$$\rho = \frac{1}{4} (U_1 \otimes U_2) \left(\begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} \right) (U_1^* \otimes U_2^*),$$

$$\rho_A = \frac{1}{2} U_1 \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} U_1^*, \quad \rho_B = \frac{1}{2} U_2 \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} U_2^*.$$

We find $E(\rho) = 0$ which is to be expected since we see that $|\psi\rangle$ can be written as a product state and is thus separable. ♣

6.2.2 Tangle

Let ρ denote the density operator for a pair of qubits A, B in the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$ where $\mathcal{H}_A = \mathcal{H}_B = \mathbb{C}^2$. This density operator may be pure or mixed. We define the *spin-flipped density operator*

$$\widetilde{\rho} := (\sigma_2 \otimes \sigma_2) \rho^* (\sigma_2 \otimes \sigma_2)$$

where σ_2 is the Pauli spin matrix in the y direction. We define the *tangle* of the density operator ρ as

$$\tau_{AB} := [\max\{\mu_1 - \mu_2 - \mu_3 - \mu_4, 0\}]^2$$

where μ_j are the square root of the eigenvalues of $\rho\widetilde{\rho}$ ordered in decreasing order. For the special case where we are working with a *pure state* we see that the tangle reduces to

$$\tau_{AB} = 4 \det \rho_A.$$

Another measure that may be introduced is the *concurrence* $\mathcal{C}$ which is the square root of the tangle.

Example. Consider the following states in the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$

$$|\psi_1\rangle = \frac{1}{2} \begin{pmatrix} 1 \\ -1 \\ 1 \\ -1 \end{pmatrix} = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix} \otimes \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$|\psi_2\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix} = \frac{1}{\sqrt{2}} \left(\begin{pmatrix} 1 \\ 0 \end{pmatrix} \otimes \begin{pmatrix} 0 \\ 1 \end{pmatrix} + \begin{pmatrix} 0 \\ 1 \end{pmatrix} \otimes \begin{pmatrix} 1 \\ 0 \end{pmatrix} \right).$$

Clearly $|\psi_1\rangle$ is separable and $|\psi_2\rangle$ is entangled. We find

$$\rho_1 = \frac{1}{4}\begin{pmatrix} 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & -1 & 1 \end{pmatrix}, \quad \widetilde{\rho_1} = \frac{1}{4}\begin{pmatrix} 1 & 1 & -1 & -1 \\ 1 & 1 & -1 & -1 \\ -1 & -1 & 1 & 1 \\ -1 & -1 & 1 & 1 \end{pmatrix}$$

so that $\tau_{AB,1} = 0$. Similarly

$$\rho_2 = \frac{1}{2}\begin{pmatrix} 0\,0\,0\,0 \\ 0\,1\,1\,0 \\ 0\,1\,1\,0 \\ 0\,0\,0\,0 \end{pmatrix}, \quad \widetilde{\rho_2} = \rho_2$$

so that $\tau_{AB,2} = 1$. We see that for a separable state $\tau_{AB} = 0$ and for an entangled state $\tau_{AB} > 0$. The Bell states are maximally entangled and we see that $0 < \tau_{AB} \leq 1$ for entangled states. ♣

Example. Consider the density matrix of the *Werner state* (Werner [150]) in $\mathbb{C}^4$

$$\rho_W := r\,|\phi^+\rangle\,\langle\phi^+| + \frac{1-r}{4} I_4$$

where $|\phi^+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1\,0\,0\,1 \end{pmatrix}^T$ is a Bell state and $0 \leq r \leq 1$. We determine the concurrence. We have

$$\rho_W = \begin{pmatrix} \frac{1+r}{4} & 0 & 0 & \frac{1}{2} \\ 0 & \frac{1-r}{4} & 0 & 0 \\ 0 & 0 & \frac{1-r}{4} & 0 \\ \frac{r}{2} & 0 & 0 & \frac{1+r}{4} \end{pmatrix}$$

with the eigenvalues $\frac{1+3r}{4}$ and $\frac{1-r}{4}$ (with multiplicity 3). Now

$$\mathcal{C}(\rho_W) = \max\{\lambda_1 - \lambda_2 - \lambda_3 - \lambda_4, 0\} = \max\left\{\frac{3r-1}{2}, 0\right\}.$$

If $r = 0$ we have $\mathcal{C}(\rho_W) = 0$, if $r = 1$ we have $\mathcal{C}(\rho_W) = 1$ and if $r = \frac{2}{3}$ we have $\mathcal{C}(\rho_W) = \frac{1}{2}$. ♣

6.2.3 Entanglement of Formation

Let ρ be a density operator over the Hilbert space $\mathbb{C}^2 \otimes \mathbb{C}^2$. We define the entanglement of formation

$$E_f(\rho) := \{p_k, |\psi_k\rangle\}_{\min} \sum_{j=0}^{|\{p_k,|\psi_k\rangle\}|} p_j S(\mathrm{tr}_{\mathbb{C}^2}(|\psi_j\rangle\,\langle\psi_j|))$$

where $\{p_k, |\psi_k\rangle\}_{\min}$ indicates that the minimum is taken over all mixtures which realize ρ and $S(\rho)$ is the *von Neumann entropy* introduced previously. We calculate $E_f(\rho)$ from

$$E_f(\rho) = h\left(\frac{1+\sqrt{1-\tau}}{2}\right)$$

where τ is the *tangle* and $h(p)$ is the *Shannon entropy* defined as

$$h(p) := -p\log_2 p - (1-p)\log_2(1-p).$$

Example. Consider the following two states where one is separable and the other is entangled

$$|\psi_1\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\-1\\0\end{pmatrix}, \quad |\psi_2\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}.$$

The state $|\psi_2\rangle$ is one of the Bell states and is thus maximally entangled. We find $\tau_1 = 0$ as expected since $|\psi_1\rangle$ is separable and so

$$E_f(\rho_1) = h(1) = 0.$$

Similarly $\tau_2 = 1$ as expected since $|\psi_2\rangle$ is maximally entangled and so

$$E_f(\rho_2) = h\left(\frac{1}{2}\right) = 1.$$

We see that $0 \leq E_f(\rho) \leq 1$ where $E_f(\rho) = 0$ indicates a separable state and $E_f(\rho) = 1$ indicates a maximally entangled state. ♣

Example. We introduce the Werner state (Werner [150]) with

$$\begin{aligned}\rho_W &= \frac{5}{8}|\phi^+\rangle\langle\phi^+| + \frac{1}{8}(|\phi^-\rangle\langle\phi^-| + |\psi^+\rangle\langle\psi^+| + |\psi^-\rangle\langle\psi^-|)\\ &= \frac{1}{2}|\phi^+\rangle\langle\phi^+| + \frac{1}{8}I_4\\ &= \frac{1}{8}\begin{pmatrix}3&0&0&2\\0&1&0&0\\0&0&1&0\\2&0&0&3\end{pmatrix}.\end{aligned}$$

We find $\tau = \frac{1}{16}$ and so

$$E_f(\rho_W) = h\left(\frac{4-\sqrt{15}}{8}\right) = 0.11762.$$ ♣

6.2.4 Schmidt Number

Suppose $|\psi\rangle$ is a pure state of a composite system $\mathcal{H}_A \otimes \mathcal{H}_B$. Then there exist orthonormal states $|j\rangle_A \in \mathcal{H}_A$ and orthonormal states $|j\rangle_B \in \mathcal{H}_B$ such that

$$|\psi\rangle = \sum_{j=1}^{\min(\dim(\mathcal{H}_A),\dim(\mathcal{H}_B))} \lambda_j |j\rangle_A \otimes |j\rangle_B$$

is the *Schmidt decomposition* of $|\psi\rangle$ where the λ_j are known as *Schmidt coefficients*.

Let $\mathcal{H}_A$ and $\mathcal{H}_B$ be finite-dimensional Hilbert spaces over $\mathbb{C}$. Let $|\psi\rangle$ denote a pure state in the Hilbert space $\mathcal{H}_A \otimes \mathcal{H}_B$. The *Schmidt number* (or rank) of $|\psi\rangle$ is the smallest non-negative integer $\mathrm{Sch}(|\psi\rangle, \mathcal{H}_A, \mathcal{H}_B)$ such that $|\psi\rangle$ can be written as

$$|\psi\rangle = \sum_{j=1}^{\mathrm{Sch}(|\psi\rangle,\mathcal{H}_A,\mathcal{H}_B)} |\psi_j\rangle_A \otimes |\psi_j\rangle_B$$

where $|\psi_j\rangle_A \in \mathcal{H}_A$ and $|\psi_j\rangle_B \in \mathcal{H}_B$. Consider the Schmidt decomposition of $|\psi\rangle$ as defined above. The Schmidt number is then the number of non-zero λ_j where λ_j^2 are the eigenvalues of the matrix $\rho_A = \mathrm{tr}_B \rho$ for $\rho = |\psi\rangle\langle\psi|$. A separable state has a Schmidt number 1 and an entangled state has a Schmidt number greater than 1 (Sperling and Vogel [118]).

Example. Consider the quantum state

$$|\psi\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} e^{i\phi} \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

We calculate the Schmidt number. From before we know that

$$\rho_A = \frac{1}{2} I_2$$

where I_2 is the 2×2 identity matrix. The eigenvalue is $\frac{1}{2}$ with multiplicity 2 so that $\mathrm{Sch}(|\psi\rangle, \mathbb{C}^2, \mathbb{C}^2) = 2$. This is as expected as we know that the state is entangled. ♣

Example. Let $f : \{0,1\}^2 \to \{0,1\}$ be a boolean function. We may define

$$|\psi_f\rangle := \frac{1}{2} \sum_{a,b \in \{0,1\}} (-1)^{f(a,b)} |a\rangle \otimes |b\rangle.$$

We determine and compare the Schmidt numbers of $|\psi_{OR}\rangle$ and $|\psi_{XOR}\rangle$ over $\mathbb{C}^2 \otimes \mathbb{C}^2$ where the standard basis $\{|0\rangle := (0\ 1)^T, |1\rangle := (1\ 0)^T\}$ is considered

(Steeb and Hardy [122]). We obtain

$$\begin{aligned}|\psi_{OR}\rangle &= \frac{1}{2}(|0\rangle\otimes|0\rangle - |0\rangle\otimes|1\rangle - |1\rangle\otimes|0\rangle - |1\rangle\otimes|1\rangle)\\ &= \frac{1}{2}\left(-1\,-1\,-1\,1\right)^T\end{aligned}$$

$$\begin{aligned}|\psi_{XOR}\rangle &= \frac{1}{2}(|0\rangle\otimes|0\rangle - |0\rangle\otimes|1\rangle - |1\rangle\otimes|0\rangle + |1\rangle\otimes|1\rangle)\\ &= \frac{1}{2}\left(1\,-1\,-1\,1\right)^T.\end{aligned}$$

We obtain

$$\begin{aligned}\rho_{OR,A} &= (I_2\otimes\langle 0|)\rho_{OR}(I_2\otimes|0\rangle) + (I_2\otimes\langle 1|)\rho_{OR}(I_2\otimes|1\rangle)\\ &= \frac{1}{2}\begin{pmatrix}1&0\\0&1\end{pmatrix}\end{aligned}$$

with eigenvalue $\frac{1}{2}$ with multiplicity 2 so that $\mathrm{Sch}(|\psi_{OR}\rangle, \mathbb{C}^2, \mathbb{C}^2) = 2$.

$$\begin{aligned}\rho_{XOR,A} &= (I_2\otimes\langle 0|)\rho_{XOR}(I_2\otimes|0\rangle) + (I_2\otimes\langle 1|)\rho_{XOR}(I_2\otimes|1\rangle)\\ &= \frac{1}{2}\begin{pmatrix}1&-1\\-1&1\end{pmatrix}\end{aligned}$$

with eigenvalues 0 and 1 so that $\mathrm{Sch}(|\psi_{XOR}\rangle, \mathbb{C}^2, \mathbb{C}^2) = 1$. We see that

$$|\psi_{XOR}\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}\otimes\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-1\end{pmatrix}$$

showing that it is a separable state in the Hilbert space. ♣

Example. Consider the following state in the Hilbert space $\mathbb{C}^4\otimes\mathbb{C}^2$

$$|\psi\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}i\\0\\0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}.$$

In this case $\mathcal{H}_A$ is $\mathbb{C}^4$. We determine the Schmidt number for this state. We find

$$\rho_A = \frac{1}{2}\begin{pmatrix}1&0&0&i\\0&0&0&0\\0&0&0&0\\-i&0&0&1\end{pmatrix}$$

with eigenvalues 0 (with multiplicity 3) and 1 so that $\mathrm{Sch}(|\psi\rangle, \mathbb{C}^4, \mathbb{C}^2) = 1$. This state is separable in the given Hilbert space. However we may also write the state as

$$\left(\begin{pmatrix}1\\0\end{pmatrix}\otimes\begin{pmatrix}i\\0\end{pmatrix} + \begin{pmatrix}0\\1\end{pmatrix}\otimes\begin{pmatrix}0\\1\end{pmatrix}\right)\otimes\begin{pmatrix}0\\1\end{pmatrix}$$

in the Hilbert space $(\mathbb{C}^2 \otimes \mathbb{C}^2) \otimes \mathbb{C}^2$ in which case the state is entangled. ♣

In the following section we introduce *multipartite entanglement* where the systems are composed of $N > 2$ subsystems. This leads to the concept of the *generalized Schmidt decomposition*. Suppose $|\psi\rangle$ is a pure state of a composite system $\mathcal{H}_{A_1} \otimes \mathcal{H}_{A_2} \otimes \cdots \otimes \mathcal{H}_{A_N}$. Then there exist orthonormal states $|j\rangle_{A_\ell} \in \mathcal{H}_{A_\ell}$ for $\ell = 1, 2, \ldots, N$ such that

$$|\psi\rangle = \sum_{j=1}^{\min(\dim(\mathcal{H}_{A_1}),\ldots,\dim(\mathcal{H}_{A_N}))} \lambda_j |j\rangle_{A_1} \otimes |j\rangle_{A_2} \otimes \cdots \otimes |j\rangle_{A_N}$$

is the generalized Schmidt decomposition of $|\psi\rangle$ where the λ_j are known as Schmidt coefficients as before.

6.3 Multipartite Entanglement

Up to now we have considered bipartite entanglement where we consider the entanglement shared between two systems. We now consider systems that are composed of more than two subsystems. The entanglement shared by these systems is now referred to as multipartite entanglement. Before we considered states that were fully entangled (or fully separable) now with the introduction of more subsystems we may consider the concept of *partial separability*. Many of the entanglement measures introduced for bipartite systems may be extended to cover the multipartite case however more parameters are needed to calculate the entanglement. The extension to higher dimensional Hilbert spaces have recently been studied by many authors such as Ban [4], Friedland and Gour [36], Hong and Gao [54], Li et al [73], Sheikholeslam and Gulliver [116], Steeb and Hardy [124], Wong and Christensen [155], Wu et al [156].

A pure N-partite state is separable if and only if all the reduced density matrices of the elementary subsystems describe pure states. In a bipartite case separability can be determined by calculating the Schmidt decomposition of the state. Unfortunately this concept cannot straightforwardly be generalized to the case of N separate subsystems (A. Peres [90], Thapliyal [141]). In addition to these methods a separability condition based on comparing the amplitudes and phases of the components of the state has been presented by Matsueda and Cohen [78]. For other ways to detect the separability of pure states one may see Yu and Song [158], [159] and Brassard and Mor [18].

A comprehensive measure for multipartite entanglement is the *N-tangle* which is related to the tangle in bipartite systems introduced earlier. We consider the finite-dimensional Hilbert space $\mathcal{H} = \mathbb{C}^{2^N}$ with $N = 3$ or N even. We consider the normalized states

$$|\psi\rangle = \sum_{j_1, j_2, \ldots, j_N = 0}^{1} c_{j_1, j_2, \ldots, j_N} |j_1\rangle \otimes |j_2\rangle \otimes \cdots \otimes |j_N\rangle$$

in the Hilbert space where $|0\rangle$, $|1\rangle$ denote the standard basis in $\mathbb{C}^2$. We introduce ϵ_{jk} $(j,k=0,1)$ and define $\epsilon_{00}=\epsilon_{11}=0$, $\epsilon_{01}=1$ and $\epsilon_{10}=-1$. The N-tangle is then defined by

$$\tau_{1\ldots N} := 2\Big| \sum_{\substack{\alpha_1,\ldots,\alpha_N=0 \\ \ldots \\ \delta_1,\ldots,\delta_N=0}}^{1} c_{\alpha_1\ldots\alpha_N} c_{\beta_1\ldots\beta_N} c_{\gamma_1\ldots\gamma_N} c_{\delta_1\ldots\delta_N} \times \epsilon_{\alpha_1\beta_1}\epsilon_{\alpha_2\beta_2}\ldots\epsilon_{\alpha_{N-1}\beta_{N-1}}\epsilon_{\gamma_1\delta_1}\epsilon_{\gamma_2\delta_2}\ldots\epsilon_{\gamma_{N-1}\delta_{N-1}}\epsilon_{\alpha_N\gamma_N}\epsilon_{\beta_N\delta_N}\Big|.$$

We see that this measurement for entanglement in a multipartite system is considerably more complicated than the bipartite equivalent introduced previously with many more additional variables. The more subsystems we deal with, the more variables are introduced. In the Computer algebra implementation section we include program 10 for calculating the 3-tangle.

Example. Consider the GHZ-state

$$|GHZ\rangle = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

Here $N=3$ and we find $\tau_{123}=1$ so that the state is maximally entangled under this measure. ♣

Example. Consider the *Werner state* (Werner [150])

$$|W\rangle = \frac{1}{\sqrt{3}} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}.$$

$N=3$ and $\tau_{123}=0$. This means that under the measure that we are considering (the N-tangle) the state $|W\rangle$ is not entangled. However the state is clearly not separable since the state cannot be written as a product state. This state is non-separable and also not entangled under this measure. ♣

Example. Let $N=4$ and consider the state where

$$c_{0000}=c_{1111}=\frac{1}{\sqrt{2}}$$

and all other coefficients are 0. We find $\tau_{1234} = 1$ and as such see that the state is fully entangled under this measure. ♣

Chapter 7

Exceptional and Diabolic Points

7.1 Introduction

A significant property of quantum mechanics is that the *energy spectrum* of a given quantum system is quantized. That is, the system can possess only a discrete number of energies. The energy of the system is given by the eigenvalues of the *Hamilton operator* $\widehat{H}$ of the system. We call the fixed amount of energy that the system can have the *energy levels* of the system. When more than one state is at the same energy we say the energy levels are degenerate. We may consider discrete and continuous spectra.

We consider Hamilton operators $\widehat{H}$ acting on a finite dimensional Hilbert space $\mathcal{H}$ ensuring that the energy spectrum is discrete. We also assume it is bounded from below. In many cases this operator depends on a real parameter and the question arises whether or not energy levels can cross by changing this parameter. This leads us to the *non-crossing rule* which was formulated by von Neumann and Wigner in 1929 [147], proving the theorem put forward by Hund [56]. This theorem shows that the real symmetric matrices (respectively hermitian matrices) with a multiple eigenvalue form a real algebraic variety of codimension 2 (respectively 3) in the space of all real symmetric matrices(all hermitian matrices). This implies the non-crossing rule which states that a generic one parameter family of real symmetric matrices (two parameter family of hermitian matrices) contains no matrix with a multiple eigenvalue (Friedland et al [35], Steeb et al [125], [126], [135]). Simply put the potential energy curves corresponding to states of the same symmetry cannot cross. A Hamilton operator may depend on other real parameters that may give rise to certain degeneracies. When the Hamilton operator depends on a single real parameter

we refer to this as a *coupling*. Two types of degeneracies may occur. A *permanent degeneracy* implies that energy levels remain degenerate for all values of the parameter and the existence of such a degeneracy suggests the existence of non-commuting symmetry operators. The second type of degeneracy is a crossing of energy levels that occurs at a particular value of the parameter. Energy level crossing is closely related to the symmetries of a system. In the absence of symmetries energy levels repel or equivalently the energy levels do not cross. Multiple level crossings at a certain point indicate a higher degree of symmetry at this point than at others (Yuzbashyan et al [160]). We may also consider the question of entanglement together with the question of energy level crossing.

At *exceptional points* and *diabolic points* width bifurcations occur and they are physically meaningful as they influence the dynamics of both open as well as closed quantum systems. The geometric phase that arises from encircling exceptional points differ from the phase that arises from encircling diabolic points. These phenomena are worth investigating.

Exceptional points may be studied for both hermitian and non-hermitian operators as have been investigated historically by Kato in 1984 [60] and by numerous authors since. In 1991 Heiss and Steeb [51] discussed the Riemann sheet structure of the energy levels of an N-dimensional symmetric matrix problem. They showed that singularities of the energy levels are related to avoided level crossings. These singularities are exceptional points. In 1993 Steeb and Heiss [128] investigated the exceptional points for a three level Hamilton system. In 2002 Yuzbashyan et al [160] investigated the degeneracies of the energy spectrum of finite quantum systems using the Hamilton operator of the Hubbard model as example. They studied the various symmetries that arose and investigated the existence of an additional parameter independent symmetry in the model. In 2004 Harney and Heiss [47] studied the eigenvectors of decaying quantum systems at exceptional points of the Hamilton operator. They paid special attention to the properties of the system under time reversal symmetry breaking at the exceptional points. In 2005 Rotter [102] investigated avoided level crossings and singular points. She discussed the influence of branch points on the dynamics of both open and closed quantum systems as well as highlighting some differences between exceptional and diabolic points. In 2010 Rotter [103] discussed the role of exceptional points in quantum systems. She discussed the basic mathematical properties of exceptional points and considered their role in the description of real physical quantum systems. In 2011 Elsen et al [33] discussed exceptional points in bichromatic Wannier-Stark systems. They localized these degeneracies of the spectum in parameter space. In 2012 Liertzer et al [75] studied the affects of exceptional points on lasers and they found that the above-threshold behaviour of a laser is strongly affected by exceptional points which are induced by pumping the laser nonuniformly. They saw that in the vicinity of these singularities the laser may turn off even when the overall pump power deposited in the system was increased. In 2012 Ramezani et al [98] studied exceptional point dynamics in photonic honeycomb lattices with PT (parity

and time) symmetry.

In 2004 Heiss [53] investigated the specific characteristics of exceptional points of non-hermitian operators for real-parameter values. He studied theses results by considering a classical problem that lead to exceptional points of a non-hermitian matrix. In 2007 Geyer et al [42] studied various properties of non-hermitian operators and the physical implications of such operators. They investigated the metric associated with these operators and the points at which it is undefined, which are the exceptional points of the system. In 2009 Cartaris et al [19] investigated exceptional points in spectra of the hydrogen atom. They introduced a procedure to systematically search for these exceptional points and they introduced a simple example for a non-hermitian operator. In 2012 Ryu et al [105] investigated multiple exceptional points, or degeneracies, of non-hermitian Hamilton operators where there were three eigenmodes interacting with each other. They verified their expectations using numerical methods for an open quantum system.

Exceptional points are also known as inflection points and occur at singularities of eigenvalues and eigenvectors. An exceptional point is a point where both eigenvalues and eigenvectors merge to form a Jordan block. At these singular points at least two eigenvalues of an operator coalesce. There are only a finite number of these exceptional points and each level repulsion is associated with an exceptional point. The closer two levels approach each other for real values of coupling strength the nearer these exceptional points are to the real axis (Steeb et al [126]).

Diabolic points arise at a point of double eigenvalue with two linearly independent eigenvectors and bifurcations occur at these points. Authors who have studied diabolic points historically include Teller [139], Berry [10], Berry and Wilkinson [12]. In 2000 Park and Garg [89] studied the degeneracies (diabolic points) in magnetic molecules that have a four-fold symmetry axis. In 2005 Kirillov et al [64] presented a new theory of unfolding of eigenvalue surfaces of real symmetric and Hermitian matrices due to an arbitrary complex perturbation near a diabolic point. As a physical application they studied singularities of the surfaces of refractive indices in crystal optics. In 2005 Seyranian et al [111] presented a paper describing a general theory for coupling of eigenvalues of complex matrices at diabolic and exceptional points. Two physical examples were discussed illustrating the accuracy of the presented theory. This has been discussed in chapter 4.2 when we introduced the *eigenvalue problem*. In 2006 Nesterov and de la Cruz [85] studied complex magnetic monopoles and geometric phases around diabolic and exceptional points. In 2006 Kirillov and Guenther [66] studied the Krein space related perturbation theory for MHD alpha-2-dynamos and the resonant unfolding of diabolical points. In 2010 Steeb [136] investigated diabolic points and entanglement for a hierarchy of spin Hamilton operators acting in the finite-dimensional Hilbert space $\mathbb{C}^{2^N}$. Diabolic points play a role in superconducting circuits and in 2012 Monjou and Leone [83] studied a merging of diabolic points in the context of superconducting circuits. They studied

a solvable four-level model and applied it to a circuit whose diabolic points are already known. This circuit was the Cooper pairs pump studied by Leone and Monjou in 2011 [72]. The diabolic points of the Fe_8 molecular magnet were investigated in 2000 by Garg [39], 2001 by Keçecioğlu and Garg [61] and in 2011 by Li and Garg [74]. This is of interest as this magnetic molecule is rich in degeneracies and these have been identified as diabolic points. In the 2001 paper the authors introduced an exactly solvable model.

We say that the eigenvalues coalesce while the corresponding eigenvectors remain different. In addition to considering these types of points or eigenvalues it is also useful to consider the level of entanglement of the corresponding eigenvectors. The two energies near a diabolic point would vary locally as

$$E(\alpha, \beta) = E_d \pm \sqrt{\alpha^2 + \beta^2}$$

where α, β are real parameters.

7.2 Exceptional Points

7.2.1 Real Symmetric Case (Hermitian operators)

Consider a closed quantum system where the system is isolated from the environment. First consider the Hamilton operator

$$\widehat{H}_B = \begin{pmatrix} \epsilon_1 & \omega \\ \omega & \epsilon_2 \end{pmatrix}.$$

The eigenvalues are

$$E_{1,2} = \frac{1}{2}\left(\epsilon_1 + \epsilon_2 \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4\omega^2}\right).$$

We see that the energies of the system are discrete and will never cross since

$$\sqrt{(\epsilon_1 - \epsilon_2)^2 + 4\omega^2} > 0$$

implies that E_1 and E_2 will be different. When $E_1 = E_2$ we say this is an *exceptional point*.

Mathematically consider a hermitian Hamilton operator $\widehat{H}$ of the form

$$\widehat{H}(\epsilon) = \widehat{H}_0 + \epsilon \widehat{H}_1$$

where $\widehat{H}_0$ and $\widehat{H}_1$ are real symmetric $n \times n$ matrices with $\widehat{H}_0$ being a diagonal matrix. In perturbation theory for linear operators we say that $\widehat{H}_0$ is the unperturbed operator and $\epsilon\widehat{H}_1$ is the perturbation. The eigenvalues are obtained by solving the characteristic polynomial

$$\det\left(\widehat{H}(\epsilon) - EI_n\right) = 0.$$

The number of eigenvalues of $\widehat{H}(\epsilon)$ is independent of ϵ with the exception of the exceptional points where the eigenvalues coalesce. The exceptional points in the complex ϵ plane are defined by the solution of the characteristic polynomial together with

$$\frac{d}{dE}\left(\det\left(\widehat{H}(\epsilon)-EI_n\right)\right)=0.$$

Example. Consider the two level system

$$\widehat{H}(\epsilon)=\begin{pmatrix}0&0\\0&1\end{pmatrix}+\epsilon\begin{pmatrix}0&1\\1&0\end{pmatrix}.$$

We obtain

$$E^2-E-\epsilon^2=0,\quad 2E-1=0.$$

We find the exceptional points $\epsilon_{1,2}=\pm i/2$. Now consider the 2×2 matrix

$$\widehat{H}(\epsilon_1=i/2)=\begin{pmatrix}0&\frac{i}{2}\\\frac{i}{2}&1\end{pmatrix}$$

with the single eigenvalue $E=\frac{1}{2}$ and only one linearly independent eigenvector

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\-i\end{pmatrix}.$$

Consider now the 2×2 matrix

$$\widehat{H}(\epsilon_2=-i/2)=\begin{pmatrix}0&\frac{-i}{2}\\\frac{-i}{2}&1\end{pmatrix}$$

with the single eigenvalue $E=\frac{1}{2}$ and only one linearly independent eigenvector

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\i\end{pmatrix}.$$

The eigenvectors for $\widehat{H}(\epsilon_1)$ and $\widehat{H}(\epsilon_2)$ are orthonormal to each other. ♣

Example. Consider the three level system (Steeb and Heiss [128])

$$\widehat{H}(\epsilon)=\begin{pmatrix}0&0&0\\0&1&0\\0&0&2\end{pmatrix}+\epsilon\begin{pmatrix}0&1&0\\1&0&c\\0&c&0\end{pmatrix}$$

where $c\in\mathbb{R}$. We find

$$E^3-3E^2-E(c^2\epsilon^2+\epsilon^2-2)+2\epsilon^2=0,\quad E^2-2E-\frac{1}{3}(c^2\epsilon^2+\epsilon^2-2)=0.$$

Solving the second equation with respect to E gives

$$E_{1,2}=1\pm\frac{1}{3}\sqrt{3(c^2\epsilon^2+\epsilon^2+1)}=1\pm\frac{1}{3}\sqrt{U}.$$

Substituting $E_{1,2}$ into the first equation gives

$$\pm 2\sqrt{U}(c^2\epsilon^2+\epsilon^2+1)+9c^2\epsilon^2-9\epsilon^2=0.$$

We introduce the abbreviations

$$\begin{aligned}
A &:= -c^3+c^2+c-1\\
B_1 &:= 3c^5+15c^4-18c^3-18c^2+15c+3\\
B_2 &:= 10c^4-52c^2+10\\
B_3 &:= 3c^3-15c^2-15c+3.
\end{aligned}$$

We find the exceptional points

$$\begin{aligned}
\epsilon_1(c) &= \frac{\left(A^{\frac{1}{3}}B_3(-i\sqrt{3}-1)+B_2-3A^{\frac{2}{3}}(c^2+6c+1)(i\sqrt{3}-1)\right)^{\frac{1}{2}}}{2(c^2+1)^{\frac{3}{2}}}\\
\epsilon_2(c) &= -\epsilon_1(c), \quad \epsilon_3(c)=\epsilon_1^*(c), \quad \epsilon_4(c)=-\epsilon_1^*(c)\\
\epsilon_5(c) &= \frac{\left(A^{\frac{1}{3}}B_3+\frac{B_2}{2}-3A^{\frac{2}{3}}(c^2+6c+1)\right)^{\frac{1}{2}}}{2(c^2+1)^{\frac{3}{2}}}\\
\epsilon_6(c) &= \epsilon_5^*(c).
\end{aligned}$$

Consider the special case where $c\to 1$. We find $A\to 0$ which causes a confluence of exceptional points

$$\epsilon_1\to\frac{i}{\sqrt{2}}, \quad \epsilon_4\to\frac{i}{\sqrt{2}}, \quad \epsilon_5\to\frac{i}{\sqrt{2}}$$

and

$$\epsilon_2\to-\frac{i}{\sqrt{2}}, \quad \epsilon_3\to-\frac{i}{\sqrt{2}}, \quad \epsilon_6\to-\frac{i}{\sqrt{2}}.$$

This confluence simplifies the analytic structure in that two branch points cancel one another. The eigenvalues in this case are given by

$$E_\pm(\epsilon)=1\pm\sqrt{2\epsilon^2+1}, \quad E_2=1. \qquad \clubsuit$$

7.2.2 Non-Hermitian Operators

In physics we may also consider non-hermitian systems to study exceptional points. Some authors who have looked at this case are Kato [60], Heiss [53] and Rotter [102], [103]. Here we call them *crossing points* of eigenvalue trajectories or *branch points*. We now consider the situation where the quantum system interacts with an environment (an open quantum system). We consider when the quantum system is opened by embedding it into an environment where there is a continuum of scattering wave functions. Consider the Hamilton operator

$$\widehat{H}_{eff}=\widehat{H}_B+V_{BC}\frac{1}{E^+-\widehat{H}_C}V_{CB}.$$

$\widehat{H}_C$ is the Hamilton operator providing the scattering of wave functions of the environment and V_{BC}, V_{CB} are the coupling matrix elements. The second term of $\widehat{H}_{eff}$ takes into account the coupling of eigenstates of the closed system $\widehat{H}_B$ with the environment via the incoming and outgoing waves when the system is opened. Since $\widehat{H}_{eff}$ describes a subsystem that is embedded into another subsystem it is non-hermitian. When the system is weakly opened (the coupling term is small) the states avoid crossing in a similar manner to discrete states. Considering non-hermitian operators allows us to consider the system's embedding into an environment.

Consider the 2×2 Hamilton operator introduced previously

$$\widehat{H}(\omega) := \begin{pmatrix} \epsilon_1 & \omega \\ \omega & \epsilon_2 \end{pmatrix}$$

where $\epsilon_{1,2}$ are the unperturbed energies of the system and ω is the interaction between the two levels. The interaction ω contains exclusively the coupling of the states via the environment and allows us to study environmentally induced effects in an open quantum system. The eigenvalues of $\widehat{H}(\omega)$ are

$$E_{1,2} = \frac{1}{2}\left(\epsilon_1 + \epsilon_2 \pm \sqrt{(\epsilon_1 - \epsilon_2)^2 + 4\omega^2}\right)$$

as before. The eigenvalues coalesce when

$$\frac{\epsilon_1 - \epsilon_2}{2\omega} = \pm i$$

and we call these crossing points the exceptional points.

Example. Consider the Hamilton operator

$$\widehat{H}_1 := \sigma_3 + i\sigma_1$$

where σ_1 and σ_3 represent the Pauli spin matrices for describing a spin-$\frac{1}{2}$ system. We find

$$\widehat{H}_1 = \begin{pmatrix} 1 & i \\ i & -1 \end{pmatrix}.$$

The matrix is not normal and thus not hermitian. We find the eigenvalue 0 with multiplicity 2 and the normalized eigenvector

$$\frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ i \end{pmatrix}. \qquad \clubsuit$$

Example. Consider the Hamilton operator

$$\widehat{H}_2 := s_3 + is_1$$

where s_1 and s_3 represent the Pauli spin matrices for describing a spin-1 system. We find

$$\widehat{H}_2 = \frac{1}{\sqrt{2}}\begin{pmatrix} \sqrt{2}\, i & 0 & \\ i & 0 & i \\ 0 & i & -\sqrt{2} \end{pmatrix}.$$

The matrix is not normal and thus not hermitian. We find the eigenvalue 0 with multiplicity 3 and the normalized eigenvector

$$\frac{1}{2}\begin{pmatrix}1\\ \sqrt{2}i\\ -1\end{pmatrix}. \qquad \clubsuit$$

Exceptional points have many applications mathematically as well as in physics. Amongst other things one may investigate the relation between exceptional points and the phenomenon of resonance trapping and dynamical phase transitions.

7.3 Diabolic Points in Spin Systems

We consider diabolic points for some spin-systems (Steeb [136]). Let σ_1, σ_2 and σ_3 be the Pauli spin matrices. We consider the diabolic points and entanglement for the eigenvectors of the following Hamilton operators

$$\widehat{H}_2 := \hbar\omega(\sigma_3 \otimes \sigma_3) + \Delta_1(\sigma_1 \otimes \sigma_1) + \Delta_2(\sigma_2 \otimes \sigma_2)$$
$$\widehat{H}_3 := \hbar\omega(\sigma_3 \otimes \sigma_3 \otimes \sigma_3) + \Delta_1(\sigma_1 \otimes \sigma_1 \otimes \sigma_1) + \Delta_2(\sigma_2 \otimes \sigma_2 \otimes \sigma_2)$$

where $\omega > 0$ and $\Delta_1, \Delta_2 \geq 0$. We then extend this to an arbitrary Hamilton operator $\widehat{H}_N$ with N factors where $N > 2$.

Note that $\widehat{H}_2$ is similar to the Hamilton operator investigated in chapter 5.1. We find

$$\widehat{H}_2 = \begin{pmatrix} \hbar\omega & 0 & 0 & \Delta_1 - \Delta_2 \\ 0 & -\hbar\omega & \Delta_1 + \Delta_2 & 0 \\ 0 & \Delta_1 + \Delta_2 & -\hbar\omega & 0 \\ \Delta_1 - \Delta_2 & 0 & 0 & \hbar\omega \end{pmatrix}$$

with the eigenvalues

$$\hbar\omega + \Delta_1 - \Delta_2, \quad \hbar\omega - \Delta_1 + \Delta_2, \quad -\hbar\omega + \Delta_1 + \Delta_2, \quad -\hbar\omega - \Delta_1 - \Delta_2$$

and corresponding normalized eigenvectors

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\1\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\-1\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\1\\0\end{pmatrix}, \quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\-1\\0\end{pmatrix}.$$

We see the eigenvectors do not depend on $\hbar\omega$, $\Delta_{1,2}$ and are in fact the Bell states and as such are fully entangled.

We find

$$\widehat{H}_3 = \begin{pmatrix} \hbar\omega & 0 & 0 & 0 & 0 & 0 & 0 & i\Delta_2 + \Delta_1 \\ 0 & -\hbar\omega & 0 & 0 & 0 & 0 & \Delta_1 - i\Delta_2 & 0 \\ 0 & 0 & -\hbar\omega & 0 & 0 & \Delta_1 - i\Delta_2 & 0 & 0 \\ 0 & 0 & 0 & \hbar\omega & i\Delta_2 + \Delta_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & \Delta_1 - i\Delta_2 & -\hbar\omega & 0 & 0 & 0 \\ 0 & 0 & i\Delta_2 + \Delta_1 & 0 & 0 & \hbar\omega & 0 & 0 \\ 0 & i\Delta_2 + \Delta_1 & 0 & 0 & 0 & 0 & \hbar\omega & 0 \\ \Delta_1 - i\Delta_2 & 0 & 0 & 0 & 0 & 0 & 0 & -\hbar\omega \end{pmatrix}$$

with the eigenvalues

$$\sqrt{\hbar^2\omega^2 + \Delta_1^2 + \Delta_2^2}, \quad -\sqrt{\hbar^2\omega^2 + \Delta_1^2 + \Delta_2^2}.$$

We let $E \equiv \sqrt{\hbar^2\omega^2 + \Delta_1^2 + \Delta_2^2}$. We find corresponding eigenvectors

$$\begin{pmatrix} E + \hbar\omega \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ \Delta_1 - i\Delta_2 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ E + \hbar\omega \\ 0 \\ 0 \\ 0 \\ 0 \\ \Delta_1 - i\Delta_2 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ E + \hbar\omega \\ 0 \\ 0 \\ \Delta_1 - i\Delta_2 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ E + \hbar\omega \\ \Delta_1 - i\Delta_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

with the normalization factor

$$\frac{1}{\sqrt{(E + \hbar\omega)^2 + \Delta_1^2 + \Delta_2^2}}$$

and

$$\begin{pmatrix} E - \hbar\omega \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ 0 \\ -\Delta_1 + i\Delta_2 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ E - \hbar\omega \\ 0 \\ 0 \\ 0 \\ 0 \\ -\Delta_1 + i\Delta_2 \\ 0 \end{pmatrix},$$

$$\begin{pmatrix} 0 \\ 0 \\ E - \hbar\omega \\ 0 \\ 0 \\ -\Delta_1 + i\Delta_2 \\ 0 \\ 0 \end{pmatrix}, \quad \begin{pmatrix} 0 \\ 0 \\ 0 \\ E - \hbar\omega \\ -\Delta_1 + i\Delta_2 \\ 0 \\ 0 \\ 0 \end{pmatrix}$$

with the normalization factor

$$\frac{1}{\sqrt{(E-\hbar\omega)^2+\Delta_1^2+\Delta_2^2}}.$$

These may be entangled depending on the parameters ω and $\Delta_{1,2}$. Considering the (normalized) first eigenvector

$$\frac{1}{\sqrt{(E-\hbar\omega)^2+\Delta_1^2+\Delta_2^2}}\left(E+\hbar\omega\,0\,0\,0\,0\,0\,0\,\Delta_1-i\Delta_2\right)^T$$

we find the 3-tangle

$$\tau_{123}=\left(\frac{2(E+\hbar\omega)(-\Delta_1+i\Delta_2)}{(E+\hbar\omega)^2+\Delta_1^2+\Delta_2^2}\right)^2.$$

For this eigenvector to be maximally entangled we require $\tau_{123}=1$ to hold. For this to be true

$$\Delta_1^2+\Delta_2^2=0 \quad \text{or} \quad \omega^2=\frac{-2\Delta_2(\Delta_2+i\Delta_1)}{\hbar^2}.$$

The 3-tangle may be determined similarly for the other eigenstates.

We now consider the general case where $N>2$ with

$$\widehat{H}_N=\hbar\omega(\sigma_3\otimes\cdots\otimes\sigma_3)+\Delta_1(\sigma_1\otimes\cdots\otimes\sigma_1)+\Delta_2(\sigma_2\otimes\cdots\otimes\sigma_2)$$

where there are N factors. We consider even and odd values of N separately. For N even we consider even and odd multiples of 2 (in other words $N=2n$ with n even or odd). When n is even the eigenvalues are

$$E_1=\hbar\omega+\Delta_1+\Delta_2, \quad E_2=\hbar\omega-\Delta_1-\Delta_2,$$

$$E_3=-\hbar\omega+\Delta_1-\Delta_2, \quad E_4=-\hbar\omega-\Delta_1+\Delta_2.$$

When n is odd the eigenvalues are

$$E_1=\hbar\omega+\Delta_1-\Delta_2, \quad E_2=\hbar\omega-\Delta_1+\Delta_2,$$

$$E_3=-\hbar\omega+\Delta_1+\Delta_2, \quad E_4=-\hbar\omega-\Delta_1-\Delta_2.$$

In both cases the eigenvalues have multiplicity 2^{N-2}. We see for N even there are no diabolic points however there is energy level crossing. The corresponding 2^N normalized eigenvectors are the same for the two cases of n and do not

depend on $\Delta_{1,2}$ or $\hbar\omega$. They are given by

$$\frac{1}{\sqrt{2}}\begin{pmatrix}1\\0\\0\\0\\0\\\vdots\\0\\0\\0\\0\\\pm1\end{pmatrix},\quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\0\\1\\0\\\vdots\\0\\\pm1\\0\\0\\0\end{pmatrix},\quad \cdots,\quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\\vdots\\0\\1\\0\\0\\\pm1\\0\\\vdots\\0\end{pmatrix}$$

and

$$\frac{1}{\sqrt{2}}\begin{pmatrix}0\\1\\0\\0\\\vdots\\0\\0\\\pm1\\0\\\end{pmatrix},\quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\0\\1\\0\\\vdots\\0\\\pm1\\0\\0\end{pmatrix},\quad \cdots,\quad \frac{1}{\sqrt{2}}\begin{pmatrix}0\\\vdots\\0\\1\\\pm1\\0\\\vdots\\0\end{pmatrix}$$

respectively. These eigenvectors form an orthonormal basis in the Hilbert space $\mathbb{C}^{2^N}$ and are fully entangled.

For N odd we find the two eigenvalues $\pm E$ from before with the eigenvectors

$$\begin{pmatrix}E\pm\hbar\omega\\0\\0\\\vdots\\0\\0\\\pm(\Delta_1-(-i)^N\Delta_2)\end{pmatrix},\quad \begin{pmatrix}0\\E\pm\hbar\omega\\0\\\vdots\\0\\\pm(\Delta_1-(-i)^N\Delta_2)\\0\end{pmatrix},\quad \cdots,$$

$$\begin{pmatrix}0\\\vdots\\0\\E\pm\hbar\omega\\\pm(\Delta_1-(-i)^N\Delta_2)\\0\\\vdots\\0\end{pmatrix}.$$

So we see that for N even the Hamilton operator provides a fully entangled basis. When N is odd we may vary the given parameters to move between entangled and unentangled states.

Once again we recall from a mathematical point of view that at diabolic points the eigenvalues coalesce and that the eigenvectors remain linearly independent. At exceptional points both eigenvalues and eigenvectors merge (Kirillov et al [64], [65], Seyranian et al [111]). We have discussed this in chapter 4.2 as well.

7.4 Conservation Laws, Level Crossing and Symmetries

It can happen in a quantum mechanical system that there are energy level crossings of the same parameter independent symmetry. This seems to be a violation of the non-crossing rule introduced earlier. This however indicates that higher invariants (*conserved quantities*) may exist. Typical examples that may be studied are the four point Hubbard model (Steeb et al [127], [129]) and the six point Hubbard model (Yuzbashyan et al [160]).

Consider first the four point Hubbard model. The Wannier representation is given by

$$\widehat{H} := t\sum_{j=1}^{4}\sum_{s\in\{\uparrow,\downarrow\}}(c_{j+1s}^{\dagger}c_{js}+c_{js}^{\dagger}c_{j+1s})+U\sum_{j=1}^{4}n_{j\uparrow}n_{j\downarrow}$$

with the cyclic boundary condition $5\equiv 1$ and $n_{js}:=c_{js}^{\dagger}c_{js}$. The total number operator $\widehat{N}_e$ and the total spin operator in z direction $\widehat{S}_z$ are given by

$$\widehat{N}_e := \sum_{j=1}^{4}\sum_{s\in\{\uparrow,\downarrow\}} n_{js}, \quad \widehat{S}_z := \frac{1}{2}\sum_{j=1}^{4}(n_{j\uparrow}-n_{j\downarrow}).$$

Since the Hubbard model commutes with $\widehat{N}_e$ and $\widehat{S}_z$ the spectrum can be calculated in each of the subspaces separately. In addition to these constants of motion we also find the higher order conserved quantity (Steeb [130])

$$\begin{aligned}\widehat{C} :=& \sum_{j=1}^{4}((c_{j\uparrow}^{\dagger}c_{j-1\uparrow}-c_{j-1\uparrow}^{\dagger}c_{j\uparrow})(n_{j\downarrow}+n_{j-1\downarrow})+(c_{j\downarrow}^{\dagger}c_{j-1\downarrow}-c_{j-1\downarrow}^{\dagger}c_{j\downarrow})(n_{j\uparrow}+n_{j-1\uparrow}))\\ &-\sum_{j=1}^{4}\sum_{s\in\{\uparrow,\downarrow\}}(c_{js}^{\dagger}c_{j-1s}-c_{j-1s}^{\dagger}c_{js}).\end{aligned}$$

The existence of this higher-order constant of motion (since $[\widehat{C},\widehat{H}]=0$) is related to the fact that the one-dimensional Hubbard model admits a Lax representation. The Hamilton operator admits the C_{4v} point-group symmetry and the C_2 symmetry of spin-reversal.

In Bloch representation the four point Hubbard model is given by

$$\widehat{H} := \sum_{k} \sum_{s\in\{\uparrow,\downarrow\}} \epsilon(k) c^{\dagger}_{ks} c_{ks} + \frac{U}{4} \sum_{k_{1,2,3,4}} \delta(k_1 - k_2 + k_3 - k_4) c^{\dagger}_{k_1\uparrow} c_{k_2\uparrow} c^{\dagger}_{k_3\downarrow} c_{k_4\downarrow}$$

where $\epsilon(k) = 2t\cos(k)$ and

$$k, k_1, k_2, k_3 \in \left\{ -\frac{\pi}{2}, 0, \frac{\pi}{2}, \pi \text{ modulo } 2\pi \right\}.$$

In this form the Hamilton operator commutes with the total momentum operator given by

$$\widehat{P} := \sum_{k} \sum_{s\in\{\uparrow,\downarrow\}} k n_{ks}.$$

Heilmann and Lieb [49] studied the six-point Hubbard Hamilton operator as a model for φ electrons in benzene. They computed all the energy levels for all values of the repulsion parameter. After extracting all the symmetry of the model they found many instances of permanent degeneracy of levels with different symmetry and also crossing of levels of the same symmetry. They demonstrated that there is no hidden symmetry to account for these effects.

Thus one can conclude that the Hamilton operator H has non-Abelian symmetry groups and these are dependent on U. Shastry [113] found many invariants .

Yuzbashyan et al [160] expanded upon the research of Heilmann and Lieb and looked at the relationship between the symmetry of a system and its degeneracies for the six point Hubbard model. We may define the Hamilton operator for the Hubbard model

$$\widehat{H} = t \sum_{j=1}^{N} \sum_{s\in\{\uparrow\downarrow\}} \left(c^{\dagger}_{js} c_{j+1s} + c^{\dagger}_{j+1s} c_{js} \right) + U \sum_{j=1}^{N} \left(\widehat{n}_{j\uparrow} - \frac{1}{2} I \right) \left(\widehat{n}_{j\downarrow} - \frac{1}{2} I \right)$$

where t represents the kinetic term and U the Coulomb interaction between electrons of opposite spin on the same site. $\widehat{n}_{js} := c^{\dagger}_{js} c_{js}$ is the number operator. We introduce the notation N representing the number of sites and M representing the number of electrons. Yuzbashyan et al [160] considered the case where there are equal spin up and spin down electrons so that $N = 2n$ and $M = 2m$. We may consider parameter independent and parameter dependent symmetries. For the purposes of studying the effect of parameter dependent symmetries on the system one needs to factor out the parameter independent symmetries.

Parameter independent symmetries (U -independent) fall into three categories namely *spatial symmetry* (or symmetry of the polygon), *spin symmetry* and *particle-hole symmetry* (Yuzbashyan et al [160]). Spatial symmetries are generated by rotations and reflections where

$$\widehat{\sigma} := \prod_{s=\uparrow\downarrow} \prod_{k=1}^{n-1} \widehat{J}_{ks;-ks}, \quad \widehat{\sigma}' := \prod_{s=\uparrow\downarrow} \prod_{k=1}^{n} \widehat{J}_{k-1,s;2n-k,s}$$

reflects a polygon in the line passing through the vertices n and $2n$ where

$$\widehat{J}_{js;j's'} := 1 - \widehat{n}_{js} - \widehat{n}_{j's'} + c^\dagger_{js}c_{j's'} + c^\dagger_{j's'}c_{js}$$

interchanges orbitals (js) and $(j's')$. Now the operator

$$\widehat{C}_{2n} := \widehat{\sigma}\widehat{\sigma}'$$

rotates the polygon by π/n. Spin symmetry is generated by $\widehat{S}^2$ and $\widehat{S}_z$ where we define

$$\widehat{S}_+ := (\widehat{S}_-)^\dagger = \sum_{j=1}^{2n} c^\dagger_{j\uparrow}c_{j\downarrow}, \quad \widehat{\mathbf{n}}_s := \sum_{j=1}^{2n} \widehat{n}_{js}$$

so that

$$\widehat{S}_z := \frac{\widehat{\mathbf{n}}_\uparrow - \widehat{\mathbf{n}}_\downarrow}{2}, \qquad \widehat{S}^2 := \frac{1}{2}\left(\widehat{S}_-\widehat{S}_+ + \widehat{S}_+\widehat{S}_-\right) + \widehat{S}_z^2.$$

To describe particle hole symmetry we define the operators

$$\widehat{J}^{(o)}_s := \prod_{j=0}^{n-1}(1 - 2\widehat{n}_{2j+1,s}), \quad \widehat{J}^{(h)}_s := \prod_{j=1}^{2n}\left(c^\dagger_{js} + c_{js}\right)$$

where $\widehat{J}^{(o)}_s$ changes the sign of the wavefunction each time there is a spin-s electron on an odd site and $\widehat{J}^{(h)}_s$ interchanges holes and particles for a spin direction s. We introduce the following operators

$$\widehat{J}^{(o)} = \widehat{J}^{(o)}_\uparrow \widehat{J}^{(o)}_\downarrow, \quad \widehat{J}^{(h)} = \widehat{J}^{(h)}_\uparrow \widehat{J}^{(h)}_\downarrow, \quad \widehat{I}^{(o)} = \widehat{J}^{(o)}\widehat{J}^{(h)}, \quad \widehat{Z}_\uparrow = \widehat{J}^{(o)}_\uparrow \widehat{J}^{(h)}_\downarrow.$$

The following commutation and anti-commutation relations hold

$$[\widehat{Z}_\uparrow, \widehat{H}]_+ = 0, \quad [\widehat{\sigma}, \widehat{H}]_+ = 0$$

$$[\widehat{I}^{(o)}, \widehat{H}] = [\widehat{J}^{(0)}, \widehat{t}]_+ = [\widehat{I}^{(o)}, \widehat{S}_z]_+ = [\widehat{I}^{(o)}, \widehat{S}^2] = 0$$

$$\widehat{I}^{(o)}\widehat{C}_{2n} - \widehat{C}_{2n}\widehat{I}^{(o)}(-1)^{\widehat{\mathbf{n}}} = \widehat{Z}_\uparrow\widehat{C}_{2n} + \widehat{C}_{2n}\widehat{Z}_\uparrow(-1)^{\widehat{\mathbf{n}_\downarrow}} = \widehat{Z}_\uparrow\widehat{\sigma} - (-1)^{n-1}\widehat{\sigma}\widehat{Z}_\uparrow = 0$$

where $\widehat{t}$ is the kinetic energy operator

$$\widehat{t} := t\sum_{j=1}^{N}\sum_{s=\uparrow\downarrow}\left(c^\dagger_{js}c_{j+1s} + c^\dagger_{j+1s}c_{js}\right).$$

When we consider parameter-dependent integrals of motion there are in principle an infinite number of these that can be obtained by methods outlined by Shastry [113], [114], [115]. On a finite lattice only a finite number of these integrals are independent. The general form for the rth conserved current is

$$\widehat{I}_r(U,t) := \sum_{k=0}^{\ell} U^k t^{\ell-k}\widehat{I}^k_r$$

where $\widehat{I}_r^k$ are parameter-independent operators. When we consider permanent degeneracies it is important to note that odd ($r = 2k + 1$) and even ($r = 2k$) transform differently under spatial reflections and partial particle-hole transformation

$$[\widehat{\sigma}, \widehat{I}_{2k+1}] = 0, \quad [\widehat{Z}_\uparrow, \widehat{I}_{2k+1}]_+ = 0, \quad [\widehat{\sigma}, \widehat{I}_{2k}]_+ = 0, \quad [\widehat{Z}_\uparrow, \widehat{I}_{2k}] = 0.$$

Odd currents have the same U-independent symmetry as the Hubbard Hamilton operator.

Chapter 8

Computer Algebra Implementation

In this chapter we provide Maxima programs ([161], Barnes and Chu [5], Steeb and Hardy [124]) for some of the problems discussed in the dissertation as well as some other interesting problems. Further examples of computer implementation for quantum computing and Fermi systems may be seen in works by Steeb and Hardy [131], [132] amongst others where Symbolic C++ is used instead of Maxima.

Some frequently used Maxima commands include

(a) Kronecker product between matrices A and B

```
kronecker_product(A,B)
```

(b) The complex conjugate transpose of a matrix A

```
ctranspose(A)
```

(c) The trace of an $n \times n$ matrix A

```
mat_trace(A)
```

(d) The determinant of an $n \times n$ matrix A

```
determinant(A)
```

(e) The Frobenius norm of a matrix A

```
mat_norm(A,frobenius)
```

Program 1. The following Maxima code is an implementation of the formula given in section 2.1.1 to determine *mutually unbiased bases* in a d-dimensional Hilbert space. The dimension d and the required base b is given as input.

```
genbase(b,d) := block(
  for count : 0 thru d-1 do (
    genm(count,b,d)
  )
)$
genm(m,b,d) := block(
  sum : 0,
  I : genmatrix(lambda([r,c],0),d,d),
  for i : 1 thru d do I[i,i] : 1,
  om : cos((2*%pi)/d)+%i*sin((2*%pi)/d),
  for j : 0 thru d-1 do (
    sum : sum+om^((b/2)*j*(j-1)-j*m)*transpose(I[j+1])
  ),
  S : ratsimp((1/(sqrt(d)))*sum),
  print(S)
)$
```

Where the dimension d and the required base b is specified. For the input

```
genbase(0,3);
```

we obtain the output

$$\begin{bmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{bmatrix}, \quad \begin{bmatrix} \frac{1}{\sqrt{3}} \\ \frac{2}{3i-\sqrt{3}} \\ -\frac{2}{3i+\sqrt{3}} \end{bmatrix}, \quad \begin{bmatrix} \frac{1}{\sqrt{3}} \\ -\frac{2}{3i+\sqrt{3}} \\ \frac{2}{3i-\sqrt{3}} \end{bmatrix}.$$

For the input

```
genbase(1,3);
```

we obtain the output

$$\begin{bmatrix} \frac{1}{\sqrt{3}} \\ \frac{1}{\sqrt{3}} \\ \frac{\sqrt{3}i-1}{2\sqrt{3}} \end{bmatrix}, \quad \begin{bmatrix} \frac{1}{\sqrt{3}} \\ \frac{2}{3i-\sqrt{3}} \\ \frac{2}{3i-\sqrt{3}} \end{bmatrix}, \quad \begin{bmatrix} \frac{1}{\sqrt{3}} \\ -\frac{2}{3i+\sqrt{3}} \\ \frac{1}{\sqrt{3}} \end{bmatrix}.$$

This may also be done for the input

```
genbase(2,3);
```

Larger dimensions may also be considered.

Program 2a. The following program provides a way of generating $n \times n$ *permutation matrices* for a given value of n as discussed in section 2.3.1.

```
permgen(n) := block([i,j,k,P,c],
 i : 1,
 cnt : 1,
 array(j,n),
 for k : 1 thru n do j[k] : 0,
 while i > 0 do (
  j[i] : j[i]+1,
  if equal(j[i],n+1) then (
    j[i] : 0, i : i-1
   ) else (
   if i > 0 then (
    c : 0,
    for k : 0 thru i-1 do if equal (j[k],j[i]) then c : c+1,
    if equal (c,0) then (
     i : i+1,
     if equal (i,n+1) then (
      P : genmatrix(lambda([r,c],0),n,n),
      for k : 1 thru n do P[k,j[k]] : 1,
      print(P),
      cnt : cnt+1,
      i : i-1
     )
    )
   )
  )
 )
)$
```

The input

```
permgen(3)
```

provides the output

$$\begin{bmatrix}1&0&0\\0&1&0\\0&0&1\end{bmatrix}, \quad \begin{bmatrix}1&0&0\\0&0&1\\0&1&0\end{bmatrix}, \quad \begin{bmatrix}0&1&0\\1&0&0\\0&0&1\end{bmatrix},$$

$$\begin{bmatrix}0&1&0\\0&0&1\\1&0&0\end{bmatrix}, \quad \begin{bmatrix}0&0&1\\1&0&0\\0&1&0\end{bmatrix}, \quad \begin{bmatrix}0&0&1\\0&1&0\\1&0&0\end{bmatrix}.$$

As expected there are $3! = 6$ matrices. There will be $n!$ output matrices for a given input n.

Program 2b. The above program may be adapted in various ways depending on what one needs the permutation matrices for. The following Maxima program is an adaptation of the above program to determine if there exists permutation matrices P_j such that $P_j^T H P_j = H$ for a given H.

```
permgen(H) := block([i,j,k,P,c],
 i : 1,
 n : length(H),
 count : 0,
 array(j,n),
 for k : 1 thru n do j[k] : 0,
 while i > 0 do (
  j[i] : j[i]+1,
  if equal(j[i],n+1) then (
    j[i] : 0, i : i-1
   ) else (
   if i > 0 then (
    c : 0,
    for k : 0 thru i-1 do if equal (j[k],j[i]) then c : c+1,
    if equal (c,0) then (
     i : i+1,
     if equal (i,n+1) then (
      P : genmatrix(lambda([r,c],0),n,n),
      for k : 1 thru n do P[k,j[k]] : 1,
      commutes(H,P),
      i : i-1
     )
    )
   )
  )
 )
)$
commutes(H,P) :=
 if equal(H.P,P.H) then (print('P[count]= P), count : count+1)$
permgen(matrix([U,t,t,0], [t,0,0,t], [t,0,0,t], [0,t,t,U]));
```

We obtain the output

$$\begin{bmatrix}1&0&0&0\\0&1&0&0\\0&0&1&0\\0&0&0&1\end{bmatrix}, \quad \begin{bmatrix}1&0&0&0\\0&0&1&0\\0&1&0&0\\0&0&0&1\end{bmatrix}, \quad \begin{bmatrix}0&0&0&1\\0&1&0&0\\0&0&1&0\\1&0&0&0\end{bmatrix}, \quad \begin{bmatrix}0&0&0&1\\0&0&1&0\\0&1&0&0\\1&0&0&0\end{bmatrix}.$$

Program 3. The following Maxima program is an implementation of the *finite Heisenberg group* of order n as introduced in chapter 2.3.2

```
heisgroup(n) := block(
   om : cos(2*%pi/n)+%i*sin(2*%pi/n),
   Qn : genmatrix(lambda([r,c],0),n,n),
   for j : 1 thru n do Qn[j,j] : ratsimp(om^(j-1)),
   Pn : genmatrix(lambda([r,c],0),n,n),
   for r : 1 thru n do(
     for c : 1 thru n do (
       if equal(mod(c,n), mod(r-1,n)) then Pn[r,c] : 1
   )
   ),
   count : 0,
   for j : 0 thru n-1 do (
     for k : 0 thru n-1 do (
       for l : 0 thru n-1 do (
         Hn : (om^j)*(Qn^^k).(Pn^^l),
         print(H[count]),
         print(Hn),
         count : count+1
)
)
)
)$
```

For the input

```
heisgroup(2);
```

we obtain the output

$$\begin{bmatrix}1&0\\0&1\end{bmatrix},\quad \begin{bmatrix}0&1\\1&0\end{bmatrix},\quad \begin{bmatrix}1&0\\0&-1\end{bmatrix},\quad \begin{bmatrix}0&1\\-1&0\end{bmatrix},$$

$$\begin{bmatrix}-1&0\\0&-1\end{bmatrix},\quad \begin{bmatrix}0&-1\\-1&0\end{bmatrix},\quad \begin{bmatrix}-1&0\\0&1\end{bmatrix},\quad \begin{bmatrix}0&-1\\1&0\end{bmatrix}.$$

As expected for larger values of n the output will increase exponentially since the order of the finite Heisenberg group is n^3.

Program 4. The following Maxima program tests the *Yang-Baxter equation* introduced in the braid group section of chapter 2.3.2.

```
I2 : matrix([1,0],[0,1]);
R : matrix([0,0,0,a],[0,b,0,0],[0,0,c,0],[d,0,0,0]);
LHS : ratsimp(kronecker_product(R,I2).
      kronecker_product(I2,R).kronecker_product(R,I2));
RHS : ratsimp(kronecker_product(I2,R).
      kronecker_product(R,I2).kronecker_product(I2,R));
D : ratsimp(LHS-RHS);
```

If D is the zero matrix then we see that the equation is satisfied. In the case of unknown variables one may easily solve each element to equal zero. Any 4×4 matrix may be used as input for R.

Program 5. The following Maxima program is an implementation of the *Heisenberg uncertainty relation* introduced in chapter 3.2 and computes both the weaker and the stronger relation.

```
heis(A,B,psi) := block(
  I : genmatrix(lambda([r,c],0),length(A),length(A)),
  for j : 1 thru length(A) do I[j,j] : 1,
  eA : ctranspose(psi).A.psi,
  eA2 : ctranspose(psi).(A.A).psi,
  dA : sqrt(eA2-(eA)^2),
  eB : ctranspose(psi).B.psi,
  eB2 : ctranspose(psi).(B.B).psi,
  dB : sqrt(eB2-(eB)^2),
  LHSw : dA.dB,
  RHSw : (1/2)*abs(ctranspose(psi).(A.B-B.A).psi),
  LHSs : (dA^2).(dB^2),
  RHSs : (1/4)*abs(ctranspose(psi).(A.B-B.A).psi) +
         (1/4)*(abs(ctranspose(psi).((A-eA.I).(B-eB.I) +
         (B-eB.I).(A-eA.I)).psi))^2,
  print("LHS weak"),
  print(LHSw),
  print("RHS weak"),
  print(RHSw),
  print("LHS strong"),
  print(LHSs),
  print("RHS strong"),
  print(RHSs)
)$
```

Program 6. The following Maxima program is an implementation of the *Cayley transform* introduced in chapter 4.1.1.

```
caley(H) := block(
  In : genmatrix(lambda([r,c],0),length(H),length(H)),
  for j: 1 thru length(H) do In[j,j]:1,
  A : H-%i*In,
  B : H+%i*In,
  V : ratsimp(A.invert(B)),
  print(V)
)$
```

The input

```
caley(matrix([1/2,1/2],[1/2,1/2]));
```

provides the output

$$\begin{bmatrix} \frac{i(i-1)}{2} & -\frac{i(i+1)}{2} \\ -\frac{i(i+1)}{2} & \frac{i(i-1)}{2} \end{bmatrix}$$

and the input

```
caley((1/sqrt(2))*matrix([0,1,0],[1,0,1],[0,1,0]));
```

provides the output

$$\begin{bmatrix} -\frac{1}{2} & -\frac{i}{\sqrt{2}} & \frac{1}{2} \\ -\frac{i}{\sqrt{2}} & 0 & -\frac{i}{\sqrt{2}} \\ \frac{1}{2} & -\frac{i}{\sqrt{2}} & -\frac{1}{2} \end{bmatrix}$$

Any $n \times n$ hermitian matrix may be used as input.

Program 7. The following Maxima code provides the Pauli matrices together with their eigenvectors (and the conjugate transpose of their eigenvectors).

```
I2 : matrix([1,0],[0,1])$
sx : matrix([0,1],[1,0])$
sy : matrix([0,-%i],[%i,0])$
sz : matrix([1,0],[0,-1])$
u1 : (1/sqrt(2))*matrix([1],[1])$
u1t : ctranspose(u1)$
u2 : (1/sqrt(2))*matrix([1],[-1])$
u2t : ctranspose(u2)$
v1 : (1/sqrt(2))*matrix([1],[%i])$
v1t : ctranspose(v1)$
v2 : (1/sqrt(2))*matrix([1],[-%i])$
v2t : ctranspose(v2)$
w1 : matrix([1],[0])$
w1t : ctranspose(w1)$
w2 : matrix([0],[1])$
w2t : ctranspose(w2)$
r1 : kronecker_product(u1,kronecker_product(v1,w1))$
r1t : ctranspose(r1)$
r2 : kronecker_product(u1,kronecker_product(v1,w2))$
r2t : ctranspose(r2)$
r3 : kronecker_product(u1,kronecker_product(v2,w1))$
r3t : ctranspose(r3)$
r4 : kronecker_product(u1,kronecker_product(v2,w2))$
r4t : ctranspose(r4)$
r5 : kronecker_product(u2,kronecker_product(v1,w1))$
r5t : ctranspose(r5)$
r6 : kronecker_product(u2,kronecker_product(v1,w2))$
r6t : ctranspose(r6)$
r7 : kronecker_product(u2,kronecker_product(v2,w1))$
r7t : ctranspose(r7)$
r8 : kronecker_product(u2,kronecker_product(v2,w2))$
r8t : ctranspose(r8)$
A : r1.r1t+r2.r2t+r3.r3t+r4.r4t+r5.r5t+r6.r6t+r7.r7t+r8.r8t;
S :  exp(-%i*(3*om1+3*om2+om3)*t)*r1.r1t
   + exp(-%i*(om1-om2-om3)*t)*r2.r2t
   + exp(-%i*(om1-om2-om3)*t)*r3.r3t
   + exp(-%i*(-om1-om2-om3)*t)*r4.r4t
   + exp(-%i*(om1-om2-om3)*t)*r5.r5t
   + exp(-%i*(-om1-om2+om3)*t)*r6.r6t
   + exp(-%i*(-om1-om2+om3)*t)*r7.r7t
   + exp(-%i*(-3*om1+3*om2-om3)*t)*r8.r8t;
```

From this we see that the identity matrix may be partitioned.

Program 8. The following Maxima code determines the *discrete Fourier transform* of a given basis in $\mathbb{C}^4$ introduced in chapter 4.1.3

```
DFT(a0,a1,a2,a3) := block(
  A : matrix([a0,a1,a2,a3]),
  for count : 0 thru 3 do (
    genb(count,A)
  )
)$
genb (count,A) := block(
  sum : 0,
  om : %i,
  for k : 0 thru 3 do (
    sum : sum+om^(count*k)*A[1,k+1]
  ),
  b : (1/2)*sum,
  bnorm : ratsimp((1/mat_norm(b,frobenius))*b),
  print(B[count]),
  print(bnorm)
)$
```

Program 9. The following program determines if a given vector is *maximally entangled* as described in chapter 5.1

```
maxent(n,psi) := block(
  I : genmatrix(lambda([r,c],0),n,n),
  for j : 1 thru n do I[j,j] : 1,
  A : genmatrix(lambda([r,c],0),n,n),
  for r : 1 thru n do(
    for c : 1 thru n do (
      A[r,c] : a[r,c]
)
),
LHS : ratsimp(ctranspose(psi).(kronecker_product(A, I)).psi),
RHS : ratsimp((1/n)*mat_trace(A)),
print("If following not 0, not maximally entangled:"),
print(ratsimp(LHS-RHS))
)$
maxent(2,(1/sqrt(2))*matrix([1],[0],[0],[1]));
```

The inputs for the program are the vector $|\psi\rangle \in \mathcal{H} \otimes \mathcal{H}$ and the dimension n of the Hilbert space $\mathcal{H}$.

Program 10. The following Maxima code is an implementation of the *3-tangle* introduced in chapter 5.3.

```
epps(n1,n2) := block(
  if equal(n1,n2) then e : 0 else(
   if equal(n1,0) then e : 1 else e : -1
 )
)$
ntangle(c) := block(
itau : 0,
for a1 : 0 thru 1 do (
for a2 : 0 thru 1 do (
for a3 : 0 thru 1 do (
for b1 : 0 thru 1 do (
for b2 : 0 thru 1 do (
for b3 : 0 thru 1 do (
for g1 : 0 thru 1 do (
for g2 : 0 thru 1 do (
for g3 : 0 thru 1 do (
for d1 : 0 thru 1 do (
for d2 : 0 thru 1 do (
for d3 : 0 thru 1 do (
    itau : itau + ((c[1+a1*4+a2*2+a3,1])*(c[1+b1*4+b2*2+b3,1])*
                   (c[1+g1*4+g2*2+g3,1])*(c[1+d1*4+d2*2+d3,1])*
                   (epps(a1,b1))*(epps(a2,b2))*(epps(g1,d1))*
                   (epps(g2,d2))*(epps(a3,g3))*(epps(b3,d3)))
)
)
)
)
)
)
)
)
)
)
)
),
tau : 2*abs(itau),
print("The 3-tangle is"),
print(tau)
)$
c : matrix([1/sqrt(2)],[0],[0],[0],[0],[0],[0],[1/sqrt(2)]);
ntangle(c);
```

In this example we use the GHZ-state, any vector in $\mathbb{C}^8$ may be used.

Chapter 9

Conclusion

In this dissertation our focus was on entanglement and energy level crossing in spin and Fermi Hamilton operators. We introduced basic mathematical concepts as well as quantum theory. Important matrix properties and linear operators were discussed. We investigated exceptional points of Hermitian and non-Hermitian operators and diabolic points of spin systems. A chapter with sample Maxima programs was included.

There are open problems that one may investigate in future research. Many new entanglement measures are being discussed in the literature, especially for multipartite entanglement. It would be worthwhile to study these new measures of entanglement focusing on points where energy level crossing occurs.

Furthermore in this dissertation we found that the Fourier transform does not preserve entanglement. This can be investigated further considering other questions such as whether or not the ordering of the states affects the outcome of the Fourier transform.

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Index