

An investigation into the creation of entanglement mediated by interaction

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Abstract

This dissertation investigates the creation of entanglement through some form of interaction. We see that in our systems we may introduce an entanglement parameter, which is linked directly to the interaction term in our system. The entanglement parameter determines the correlation between our quantum particles. In order to quantify this we use two different measures; the Von-Neumann entanglement entropy and the linear entropy, which tell us about the correlations in our system. We find that the strength of correlation in the system, is dependent on the interaction term in the potential. The two potentials that we shall investigate in this dissertation are the Coulomb potential of the hydrogen atom and a toy model of two coupled quantum particles via a quadratic potential (two coupled harmonic oscillators). For the Coulomb potential our entanglement parameter is the Bohr radius a_0 and for our system with a quadratic potential we introduce the entanglement parameter κ , related to the coupling strength. We find that in the hydrogen atom the electron-proton system is strongly correlated for small values of a_0 and for larger values of a_0 the correlation between them becomes weaker. This is because in increasing a_0 we reduce the strength of interaction between the electron and proton. However, for the quadratic potential the results are very different. We find that not only does the system become highly correlated for low values of κ , but becomes maximally entangled for linear entropy as $\kappa \rightarrow \infty$.

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Contents

Introduction	6
1 Quantum formalism	9
1 Hilbert spaces and state vectors	10
2 Linear operators and tensor products	12
2.1 Linear operators	12
2.2 Projectors	13
2.3 Trace	13
2.4 Normal and Unitary Operators	14
2.5 The position and momentum operators	15
2.6 The Schödinger equation	17
2.7 Tensor products	18
3 Density matrix formalism	20
3.1 Density matrices	20
3.2 Partial trace and reduced states	22
2 Entanglement	24
4 The birth of entanglement	25
4.1 The mathematical definition of entanglement	26
4.2 Bell's inequalities in the CHSH form	27
4.3 Importance of entanglement	29
5 Measures of entanglement	31
5.1 Entanglement measures	31
5.2 Many body entanglement	35

3	Entanglement in physical systems	37
6	Electron-proton entanglement in the three dimensional hydrogen atom	38
6.1	The hydrogen atom in the position representation	38
6.2	The angular solution	41
6.3	The radial and complete solution	44
6.4	The hydrogen atom in the momentum representation	47
6.5	The starting point	48
6.6	The Coulomb potential	49
6.7	The radial equation in momentum space	49
7	Interaction has its part to play	50
7.1	The entanglement within the electron-proton system	51
7.2	The momentum wavefunction	51
7.3	Quantifying the entanglement in the hydrogen atom	54
8	A system of two coupled quantum particles	61
8.1	The coupled quantum particles	62
8.2	Quantifying the entanglement for the quadratic potential	66
	Conclusion	71
A	Appendix A	73
A.1	The humble commutator	73
B	Appendix B	74
B.1	Legendre polynomials	74
C	Appendix C	76
C.1	The Fourier transform of the momentum space wavefunction	76
	References	77

Introduction

The quantum property of entanglement was first discussed in 1935 by Einstein, Podolsky and Rosen (EPR) in their highly cited paper[EPR35] regarding the implications of what quantum mechanics means for the reality of the world. Entanglement is commonly referred to as ‘spooky action at a distance’ after the comments of Einstein, but is entanglement really so ‘spooky’ or is it something that we should be very grateful to have? Entanglement is a truly amazing feature of quantum mechanics, if we can harness entanglement as a resource then we have the opportunity to revolutionise the world around us, through the creation of a universal quantum computer and who knows what else. It is even believed that entanglement is actually a fundamental property of the geometry of space-time and that it is responsible for the creation of the universe that surrounds us[Oue15]. In this work specifically we shall be developing the ideas presented by Tommasini, Timmermans and de Toledo Piza in their paper regarding the entanglement between the electron and proton in the hydrogen atom [TTdTP98]. In the paper they take the well known wave-function for the hydrogen atom and show how it becomes entangled, which we shall discuss in more depth in chapter three; Entanglement in physical systems. They then state that in order to understand how entangled the system is, we must look at the reduced density matrix $\tilde{\rho}(\mathbf{k} = \frac{\mathbf{p}}{\hbar})$ in the momentum space, not the position space. The $\tilde{\rho}(\mathbf{k})$ turn out to be the eigenvalues of our system, with eigenstates given by normalised plane waves. Using the spectral data they then go on to calculate the standard deviation of the momentum distribution to find that the standard deviation Δp is proportional to $\frac{1}{a_0}$, where a_0 is the Bohr radius. They state that in this context the standard deviation is a measure of the strength of correlation, and that the stronger the correlation between the electron and proton the higher the value of a_0 . Now of course, I hear you cry “But isn’t the Bohr radius a fixed parameter dependent on the orbital quantum number n ?”

Well, in the usual sense yes it is, but in this context we can view it as some sort of entanglement parameter and this idea of an entanglement parameter will be at the centre of our investigations in chapter three.

Our investigations will focus on two systems, firstly we shall revisit the hydrogen atom, but this time to quantify the entanglement using two other measures, the Von-Neumann entanglement entropy and the linear entropy in terms of our entanglement parameter a_0 . The second system that we shall look at is a toy model describing two coupled quantum bosonic particles with a quadratic potential. We shall see in chapter three that this system also has an entangled wavefunction. The difference this time is that we have introduced a new entanglement parameter ‘ κ ’, related to the coupling strength. We then proceed again to quantify the amount of entanglement in the system, with the same measures we used for the hydrogen atom. We aim to see how the potentials in both of these systems effect the strength of the correlations between our quantum objects. This is because it is the potentials that induce the interaction between them. Of course this is important as it is the interaction that is responsible for the creation of entanglement in these two systems. We also see in chapter three that for a potential of the form $V \propto \frac{1}{r}$ (the Coulomb potential) that the entanglement is strongest near the origin and decreases rather rapidly as a_0 is increased, contrary to the statements made in [TTdTP98]. However, in observing the behaviour of our entanglement measures as a function of a_0 , the way in which they tend to zero is very different and presents many questions. Conversely, for a potential of the form $V \propto r^2$ (quadratic potential) we find that the system becomes increasingly correlated as our entanglement parameter κ is increased and for linear entropy as κ tends to infinity, the state becomes maximally entangled. Both entanglement measures have the same curve and agree strongly, unlike the case for $\frac{1}{r}$.

Of course, in order to understand these models we first need to understand the rules of the game, that being quantum mechanics. The first chapter of this dissertation is dedicated solely towards providing the tools for understanding the introductory ideas in quantum information science and providing the reader with the right knowledge of quantum mechanics to progress on to further chapters. This then enables us in chapter two to discuss the ideas of entanglement, what it means to be entangled, why something

is entangled and how we quantify entanglement as an amount. From which we can move on to chapter three to discuss our two physical examples; one with the Coulomb potential and the other with a quadratic potential, we derive the wavefunctions for both systems analytically. We then collect our thoughts and finish with a conclusion expressing further areas of interest and a discussion about the effects of interaction on the creation of entanglement.

Chapter 1

Quantum formalism

The aim of this chapter is to familiarise the reader with certain aspects of quantum mechanics, which will be important for understanding several areas of this dissertation. It is assumed that the reader will have some familiarity with the basic principles of quantum mechanics, such as the postulates. We shall also explore some of the introductory formalism of quantum information science, that will enable us to construct our entanglement measures.

1 Hilbert spaces and state vectors

Before we can admire the wonders of quantum mechanics, we need to define a framework within which we can develop a formalism that defines the actions of the quantum world. We do this by introducing the notion of a Hilbert space, where the Hilbert space encapsulates the idea of a linear space in which we have orthogonality.

Definition 1.1. : *Let \mathcal{H} be a finite dimensional complex linear space. An inner product on \mathcal{H} is a map $\langle \cdot | \cdot \rangle : \mathcal{H} \times \mathcal{H} \rightarrow \mathbb{C}$ satisfying the following conditions for all $|\psi\rangle, |\phi\rangle$ and $|\chi\rangle \in \mathcal{H}, \alpha \in \mathbb{C}$*

1. *Positivity* $\langle \psi | \psi \rangle \geq 0, \forall |\psi\rangle \in \mathcal{H}$
2. *Definiteness* $\langle \psi | \psi \rangle = 0$ if and only if $|\psi\rangle = 0$
3. *Additivity* $\langle \psi | \phi + \chi \rangle = \langle \psi | \phi \rangle + \langle \psi | \chi \rangle \forall |\psi\rangle, |\phi\rangle, |\chi\rangle \in \mathcal{H}$
4. *Homogeneity* $\langle \psi | \alpha \phi \rangle = \alpha \langle \psi | \phi \rangle$
5. *Conjugate symmetry* $\langle \psi | \phi \rangle = \langle \phi | \psi \rangle^*$

The norm of a vector $|\psi\rangle$ ¹ is defined as $\|\psi\| = \sqrt{\langle \psi | \psi \rangle}$. A space \mathcal{H} with an inner product $(|\cdot\rangle, |\cdot\rangle) = \langle \cdot | \cdot \rangle$ is called a Hilbert space.

By using the inner product of two ket vectors, it becomes possible to construct an orthonormal basis $\{|\chi_k\rangle\}$ such that:

$$(|\chi_i\rangle, |\chi_j\rangle) = \langle \chi_i | \chi_j \rangle = \delta_{ij} \quad (1.1)$$

Therefore suppose $|\psi\rangle = \sum_k \psi_k |\chi_k\rangle$, by multiplying $|\chi_k\rangle$ from the left we obtain $\langle \chi_k | \psi \rangle = \psi_k$, which is just a scalar. This enables us to express a wavefunction in terms of an orthonormal basis as:

$$|\psi\rangle = \sum_k \langle \chi_k | \psi \rangle |\chi_k\rangle = \sum_k |\chi_k\rangle \langle \chi_k | \psi \rangle$$

¹It is assumed that the reader is comfortable with Dirac notation and the notions of a dual space.

Since this is true for any $|\psi\rangle$, we define the completeness relation to be:

$$\sum_k |\chi_k\rangle\langle\chi_k| = \mathbb{I} \quad (1.2)$$

where \mathbb{I} is the identity operator in \mathcal{H} . The completeness relation can be expanded for systems with a continuous spectra as follows:

$$\int d\chi |\chi\rangle\langle\chi| = 1 \quad (1.3)$$

To give an idea of what a Hilbert space looks like we have included below some basic, yet important examples:

1. *Finite dimensional \mathcal{H}* : Given \mathbb{C}^n as the space of column vectors $z := (z_1, z_2, \dots, z_n)$ with inner product:

$$(|z\rangle, |\mu\rangle) = \langle z|\mu\rangle = \sum_{j=1}^n z_j^\dagger \mu_j = z^* \mu$$

where † represents the adjoint.

2. *Infinite dimensional \mathcal{H}* : L^2 the space of square integrable complex valued functions on some set A :

$$\langle\psi|\phi\rangle = \int_A \psi^*(x)\phi(x)dx < \infty$$

The second example will be of particular importance for the latter part of this dissertation. In creating a framework for our quantum world we can now introduce the state vector $|\psi\rangle \in \mathcal{H}_f$, where \mathcal{H}_f is the state space and is a complex Hilbert space associated to a closed quantum system. The state vector is usually a time-dependent unit vector and represents the quantum state of the system, however in this dissertation we shall be only dealing with time-independent state vectors, also called stationary states. The quantum state contains all the information we need to know about our particular system and in order to extract that information we must apply different linear operations to our state. This allows us to extract the spectral data, by which I mean the eigenvalues and the corresponding eigenvectors (eigenkets) which provide us with the information about

the associated outcomes of a linear operator representing a measurable quantity “An observable”. The general eigenvalue equation is as follows:

$$A |\psi_i\rangle = \lambda_i |\psi_i\rangle, \lambda_i \in \mathbb{R} \quad (1.4)$$

2 Linear operators and tensor products

2.1 Linear operators

Linear operators are used in many different areas of mathematics, from pure mathematics all the way through to computer science. One of their most important roles is to describe the operations of our quantum world, within the framework of a Hilbert space \mathcal{H} . They enable us to extract information about the spectrum of a state and help us to construct a picture of the evolution of that particular quantum state or states. We can represent any linear operator on a d -dimensional Hilbert space \mathcal{H} by some operator \hat{A} . Formally we say:

Definition 2.1. : Let $(\mathcal{H}, \langle \cdot | \cdot \rangle)$ be a Hilbert space. A linear operator on \mathcal{H} is a map $\hat{A} : \mathcal{H} \rightarrow \mathcal{H}$ satisfying the linearity condition $\hat{A}(\alpha |\phi\rangle + \beta |\psi\rangle) = \alpha \hat{A} |\psi\rangle + \beta \hat{A} |\phi\rangle$. $\forall |\psi\rangle, |\phi\rangle \in \mathcal{H}$ and $\alpha, \beta \in \mathbb{C}$

An important class of linear operators are the self-adjoint operators that represent observable quantities, where a self-adjoint operator is one such that $\hat{A} = \hat{A}^\dagger$. The operators must be self-adjoint because the eigenvalues of the operator represent the possible outcomes of a quantum state i.e. the measurement outcomes. These of course must be real and so the eigenvalues of the operator must also be real, which is true for all self-adjoint operators. Four important linear operators that are used throughout quantum mechanics and quantum information theory are the Pauli spin matrices:

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

2.2 Projectors

Projectors play a key role in quantum mechanics and have an especially important role in measurement. But what is a projector? Well, suppose U is a k -dimensional subspace of the Hilbert space \mathcal{H} , it can be shown that there exists a unique decomposition of a vector $|\psi\rangle$ in to its component in U and U^\perp , where U^\perp is the subspace orthogonal to U , so that we have:

$$|\psi\rangle = |\psi_U\rangle + |\psi_{U^\perp}\rangle$$

where $|\psi_U\rangle \in U$ and $|\psi_{U^\perp}\rangle \in U^\perp$. Thus the orthogonal projection onto U is defined as the map: $\mathbf{P}_U : |\psi\rangle \mapsto |\psi_U\rangle$, from which we define the projector operator:

Definition 2.2. *Let \mathcal{H} be a Hilbert space. A projection operator \hat{P} is a linear operator on \mathcal{H} satisfying:*

$$\text{Self-adjoint: } \hat{P} = \hat{P}^\dagger$$

$$\text{Idempotent: } \hat{P}^2 = \hat{P} \cdot \hat{P} = \hat{P}$$

In the general case where $U := \text{Range}(\hat{P})$ is multidimensional, we can choose an arbitrary orthonormal basis $\{|\chi_1\rangle, \dots, |\chi_d\rangle\} \in U$ and express \hat{P} as the sum of one-dimensional projectors onto these vectors:

$$\hat{P} = \sum_{k=1}^d |\chi_k\rangle\langle\chi_k| \tag{2.1}$$

(2.1) is one of the most useful tools in quantum information science for cutting through complexity and performing a range of different operations on our quantum system.

2.3 Trace

An important operation is the trace, which has a whole variety of uses throughout quantum mechanics and quantum information science. The trace will form an important part of our tool bag. In terms of state vectors we may define the trace as:

Definition 2.3. *Suppose $\{|\psi_i\rangle\}$ is a complete orthonormal basis set in \mathcal{H} . Since a linear operator on a d -dimensional Hilbert space can be represented as a matrix with elements*

$A_{ij} = \langle \psi_i | \hat{A} | \psi_j \rangle$, we can define the trace of an operator as follows:

$$\text{Tr}(\hat{A}) = \sum_{i=1}^d \langle \psi_i | \hat{A} | \psi_i \rangle \quad (2.2)$$

Below we have compiled a list of some of the basic properties of the trace:

1. *Linearity:* $\text{Tr}(\alpha\hat{A} + \beta\hat{B}) = \alpha\text{Tr}(\hat{A}) + \beta\text{Tr}(\hat{B})$
2. *Cyclicity:* $\text{Tr}(\hat{A}\hat{B}) = \text{Tr}(\hat{B}\hat{A})$
3. *Basis free representation:* If $\{|\mu_1\rangle, \dots, |\mu_d\rangle\}$ is another complete orthonormal basis in \mathcal{H} then:

$$\text{Tr}(\hat{A}) = \sum_{i=1}^d \langle \phi_i | \hat{A} | \phi_i \rangle = \sum_{i=1}^d \langle \mu_i | \hat{A} | \mu_i \rangle$$

4. $\text{Tr}(|\psi\rangle\langle\phi|) = \langle\phi|\psi\rangle$ for all $|\psi\rangle, |\phi\rangle \in \mathcal{H}$

2.4 Normal and Unitary Operators

In order to describe how a quantum state evolves in a isolated system we introduce a very important type of linear operator, the unitary operator \hat{U} . The unitary operator is a special type of normal operator, where an operator \hat{N} on \mathcal{H} is called normal if and only if $\hat{N}\hat{N}^\dagger = \hat{N}^\dagger\hat{N}$. The unitary operator is special, as $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \mathbb{I}$ and has the following formal definition:

Definition 2.4. : A operator \hat{U} is unitary if and only if the following holds $\hat{U}\hat{U}^\dagger = \hat{U}^\dagger\hat{U} = \hat{I}$ where \hat{U}^\dagger is the adjoint of \hat{U} . Unitary operators have the following interesting properties:

1. The rows and columns of \hat{U} form an orthonormal basis.
2. \hat{U} preserves inner products $\langle \psi | \hat{U}^\dagger \hat{U} | \phi \rangle = \langle \psi | \hat{U}^\dagger \hat{U} | \phi \rangle = \langle \psi | \phi \rangle$ which implies \hat{U} preserves norms and angles up to some phase.
3. The eigenvalues of \hat{U} are all of the form $\exp(i\theta)$.

4. Which means \hat{U} can be diagonalized in the following way:

$$\hat{U} = \begin{pmatrix} e^{i\theta_1} & 0 & \dots & 0 \\ 0 & \ddots & \ddots & 0 \\ \vdots & \ddots & \ddots & \vdots \\ 0 & \dots & 0 & e^{i\theta_a} \end{pmatrix}$$

Essentially the unitary operators ‘represent’ the observable time in quantum mechanics.

2.5 The position and momentum operators

Two important operators that we will see throughout this dissertation are the position and momentum operators \hat{x} and \hat{p} . We say loosely, that these operators are the quantum analogues of their classical counterparts. This is because any set of operators defined in such a way that the following commutation relation² is satisfied:

$$[\hat{x}, \hat{p}] = \hat{x}\hat{p} - \hat{p}\hat{x} = -i\hbar \quad (2.3)$$

where typically \hbar is defined to be one, are suitable quantum operators for representing our position and momentum variables. The reason for this is quite technical and full of subtle points, but the crux of the argument is to do with the concept of canonical quantisation³, which is essentially a set of axioms to transform our classical ideas to the quantum world. As mentioned previously the given outcomes for a particular observable are determined by the spectrum of the linear operator representing that observable, this is of course true for the position and momentum. In the position representation using the basis $|x\rangle$ and the eigenvalue equation (1.4) we have:

$$\hat{x}|x\rangle = x|x\rangle \quad (2.4)$$

and by complex conjugation we have:

$$\langle x|\hat{x} = \langle x|x \quad (2.5)$$

²See appendix A for information regarding commutation relations

³See [Nak03] for a detailed discussion.

the eigenvalues must be real for observables. Thus multiplying (2.5) by $|\psi\rangle$ from the right we get:

$$\langle x|\hat{x}|\psi\rangle = x \langle x|\psi\rangle = x\psi(x) = x\psi_x \quad (2.6)$$

But how exactly do we represent the momentum operator \hat{p} , which has basis states $|p\rangle$, in terms of the position basis states $|x\rangle$? We begin by considering the following unitary operator:

$$\hat{U}(a) = e^{(-ia\hat{p})} \quad (2.7)$$

which satisfies the following relation:

$$\hat{U}(a) |x\rangle = |x + a\rangle \quad (2.8)$$

This can be seen by looking at the commutation relation between \hat{x} and $\hat{U}(a)$ and writing the exponential operation in terms of its Taylor series. If we then take $a = \varepsilon$, where ε is a infinitesimal number[Nak03], so that we can write (2.8) as:

$$\hat{U}(\varepsilon) |x\rangle = |x + \varepsilon\rangle \simeq (1 - i\varepsilon\hat{p}) |x\rangle$$

it follows that:

$$\hat{p}|x\rangle = \frac{|x + \varepsilon\rangle - |x\rangle}{-i\varepsilon} \text{ as } \varepsilon \rightarrow 0 = i \frac{d}{dx} |x\rangle \quad (2.9)$$

and so its dual is:

$$\langle x|\hat{p} = \frac{\langle x + \varepsilon| - \langle x|}{-i\varepsilon} \text{ as } \varepsilon \rightarrow 0 = -i \frac{d}{dx} \langle x| \quad (2.10)$$

therefore for any state $|\psi\rangle$ we obtain:

$$\langle x|\hat{p}|\psi\rangle = -i \frac{d}{dx} \langle x|\psi\rangle = -i \frac{d}{dx} \psi(x) \quad (2.11)$$

and so in the position representation $\hat{p} = -i \frac{d}{dx}$ or for multiple dimensions the derivative is replaced by the Laplacian. If instead we'd chosen to work in the momentum representation, which has eigenstates $|p\rangle$, then for every definition in the previous discussion we would just interchange \hat{x} with \hat{p} . Combining these definitions we arrive at the following:

$$\langle x|p\rangle = \frac{1}{(2\pi)^{\frac{1}{2}}} e^{(ipx)} \quad (2.12)$$

$$\langle p|x\rangle = \frac{1}{(2\pi)^{\frac{1}{2}}} e^{(-ipx)} \quad (2.13)$$

where $C = \frac{1}{(2\pi)^{\frac{1}{2}}}$ is the normalisation constant for the normalisation condition $\langle x|x'\rangle = \delta(x - x')$. From these relation we see how we can change from one representation to another i.e. $\psi(x) \rightarrow \psi(p)$:

$$\psi(p) = \langle p|\psi\rangle = \int dx \langle p|x\rangle \langle x|\psi\rangle = \int \frac{dx}{(2\pi)^{\frac{1}{2}}} e^{(-ipx)} \psi(x) \quad (2.14)$$

which is merely the Fourier transform of $\psi(x)$. Likewise to transform in the opposite direction we take the inverse Fourier transform. It is worth noting that all the definitions above can be easily extended to cope with multiple dimensions.

2.6 The Schrödinger equation

The Schrödinger equation has the equivalent quantum role as that of Newton's laws in classical mechanics; it enables us to predict the future behaviour of our quantum state. It does this via the wavefunction, which we find when we solve Schrödinger's equation. The wavefunction provides us with the probability distributions for a given event to occur. It should be noted however, that the wavefunction can only be found analytically in a few special cases, although there are several numerical and approximation methods that exist which provide us with some structural information about more complex wavefunctions. Thus without further delay, the time-independent Schrödinger equation is defined as:

$$\hat{H} |\psi\rangle = E |\psi\rangle \quad (2.15)$$

where \hat{H} represents our Hamiltonian operator, E we define to be the eigenvalues of the Hamiltonian operator which represent the Energy spectrum and $|\psi\rangle$ is our state vector. The wavefunction itself is defined according to the representation we are using, whether that be position, momentum etc. For example in position representation we say that $\psi_x = \langle x|\psi\rangle \in \mathbb{C}$ and since other representations have different basis vectors, the wavefunctions in those representations will be defined accordingly. Thus we can represent the state vector, in the position basis, as follows:

$$|\psi\rangle = \int dx |x\rangle \langle x|\psi\rangle = \int \psi(x) |x\rangle \quad (2.16)$$

where the probability of finding the particle in the interval $[x, x + dx]$ in the state $|\psi\rangle$ is determined by $|\psi(x)|^2 dx$. Thus it is natural to impose the following normalisation condition:

$$\int dx |\psi(x)|^2 = \langle \psi | \psi \rangle = 1 \quad (2.17)$$

2.7 Tensor products

In quantum mechanics, when we deal with multiple systems we require several different Hilbert spaces. In order to connect these spaces together, to form composite systems, we introduce the notion of a tensor product. To understand the tensor product, it is best to first look at its definition for matrices:

Definition 2.5. *Let $A \in M_{n,m}$ and $B \in M_{k,p}$ be two complex matrices. The tensor product $A \otimes B$ is the $nk \otimes np$ matrix with the following block structure*

$$A \otimes B = \begin{pmatrix} A_{11}B & A_{12}B & \dots & A_{1n}B \\ A_{21}B & A_{22}B & \dots & A_{2n}B \\ \vdots & \vdots & \ddots & \vdots \\ A_{m1}B & A_{m2}B & \dots & A_{mn}B \end{pmatrix} \quad (2.18)$$

as a simple example let us take the tensor product of two, two by one vectors:

$$\begin{pmatrix} 2 \\ 8 \end{pmatrix} \otimes \begin{pmatrix} 3 \\ 5 \end{pmatrix} = \begin{pmatrix} 6 \\ 10 \\ 24 \\ 40 \end{pmatrix} \quad (2.19)$$

We list below a few properties of the tensor product for matrices A, B, C and D and the scalars α, β and γ :

1. $A \otimes B \neq B \otimes A$
2. $A \otimes (\beta B + \gamma C) = \beta A \otimes B + \gamma A \otimes C$

3. $(\alpha A + \beta B) \otimes C = \alpha A \otimes C + \beta B \otimes C$
4. $(A \otimes B) \otimes C = A \otimes (B \otimes C)$
5. $(A \otimes B) \cdot (C \otimes D) = AC \otimes BD$ whenever the products exist.
6. $A^T \otimes B^T = (A \otimes B)^T$
7. $A^\dagger \otimes B^\dagger = (A \otimes B)^\dagger$

Now that we have introduced the tensor product for matrices, we are ready to move to a ‘basis free’ [Gut15] perspective by defining the tensor products of Hilbert spaces and operators.

Definition 2.6. *Let U and V be two linear vector spaces. The tensor product $U \otimes V$ is the linear space spanned by elements of the form $|\psi\rangle \otimes |\phi\rangle$, where $|\psi\rangle \in U$ and $|\phi\rangle \in V$ such that the following relations hold:*

1. $(|\psi\rangle + |\psi'\rangle) \otimes |\phi\rangle = |\psi\rangle \otimes |\phi\rangle + |\psi'\rangle \otimes |\phi\rangle$
2. $|\psi\rangle \otimes (|\phi\rangle + |\phi'\rangle) = |\psi\rangle \otimes |\phi\rangle + |\psi\rangle \otimes |\phi'\rangle$
3. $(\alpha |\psi\rangle) \otimes |\phi\rangle = |\psi\rangle \otimes (\alpha |\phi\rangle) = \alpha(|\psi\rangle \otimes |\phi\rangle)$

where $\alpha \in \mathbb{C}$ and $\phi' \in U$ and $\psi' \in V$ are arbitrary vectors.

Let \mathcal{H}_A and \mathcal{H}_B be two Hilbert spaces. The tensor product $\mathcal{H}_A \otimes \mathcal{H}_B$ becomes a Hilbert space when endowed with the inner product:

$$\langle \psi \otimes \phi | \psi' \otimes \phi' \rangle = \langle \psi | \psi' \rangle \langle \phi | \phi' \rangle$$

to a sesquilinear form $\langle \cdot | \cdot \rangle : \mathcal{H}_A \otimes \mathcal{H}_B \otimes \mathcal{H}_A \otimes \mathcal{H}_B \rightarrow \mathbb{C}$

To see how the tensor product acts on operators let $\hat{A} : \mathcal{H}_A \rightarrow \mathcal{H}_A$ and $\hat{B} : \mathcal{H}_B \rightarrow \mathcal{H}_B$ be linear operators on the spaces \mathcal{H}_A and \mathcal{H}_B respectively. The tensor product $\hat{A} \otimes \hat{B}$ is the linear operator on $\mathcal{H}_A \otimes \mathcal{H}_B$ whose action on a product vector is:

$$(\hat{A} \otimes \hat{B})(|\psi\rangle \otimes |\phi\rangle) = \hat{A}|\psi\rangle \otimes \hat{B}|\phi\rangle \tag{2.20}$$

We finish with a few additional properties regarding the tensor product and linear operators:

1. If both \hat{A} and \hat{B} are normal or self adjoint or unitary or positive then so is $\hat{A} \otimes \hat{B}$.
2. If \hat{A} and \hat{B} both have spectral decompositions $\hat{A} = \sum_i \lambda_i |\chi_i\rangle\langle\chi_i|$ and $\hat{B} = \sum_j \nu_j |\mu_j\rangle\langle\mu_j|$ for the orthonormal bases $\{|\chi_1\rangle, \dots, |\chi_{d_A}\rangle\} \in \mathcal{H}_A$ and $\{|\mu_1\rangle, \dots, |\mu_{d_B}\rangle\} \in \mathcal{H}_B$, then:

$$\hat{A} \otimes \hat{B} = \sum_{ij} \lambda_i \nu_j |\chi_i\rangle\langle\chi_i| \otimes |\mu_j\rangle\langle\mu_j| = \sum_{ij} \lambda_i \nu_j |\chi_i \otimes \mu_j\rangle\langle\chi_i \otimes \mu_j|$$

and its spectrum is : $\sigma(\hat{A} \otimes \hat{B}) = \{\lambda\nu : \lambda \in \sigma(\hat{A}), \nu \in \sigma(\hat{B})\}$.

3. The trace: $Tr(\hat{A} \otimes \hat{B}) = Tr(\hat{A})Tr(\hat{B})$

3 Density matrix formalism

3.1 Density matrices

We shall now move on to discuss the density matrix (operator) formalism, as a density matrix contains the equivalent information to our quantum state $|\psi\rangle$. We use the density operator language as it is notationally much more convenient to use. Another nice property of the density matrix is that its structure provides us with the probability distribution of all the possible measurements of the given system.

Definition 3.1. *Let $\{|\psi_1\rangle, \dots, |\psi_d\rangle\}$ be an orthonormal basis on \mathcal{H} , then the operator $\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i|$ on \mathcal{H} , such that $\sum_i p_i = 1$ is called a density matrix if it has the following properties:*

$$\text{Positivity: } \rho \geq 0$$

$$\text{Unit trace(normalisation): } Tr(\rho) = 1$$

⁴ d_A and d_B represent the respective dimensions of the spaces.

These conditions also hold true for what are called reduced (partial) states, which are states that contain information about one system of our composite space, we shall discuss reduced states in more detail later on.

In order to relate the density matrix to our linear operator \hat{A} , we recall the eigenvalue equation (1.4) and state that our operator \hat{A} has eigenvalues λ_i such that $\hat{A}|\chi_i\rangle = \lambda_i|\chi_i\rangle$, where $|\chi_i\rangle$ are the normalised eigenkets that form a complete set $\{|\chi_i\rangle\}$. Thus if we have a normalised state such that $|\psi\rangle = \sum_i a_i |\chi_i\rangle$, then we can define the expectation value of \hat{A} with respect to the state $|\psi\rangle$ as:

$$\langle \hat{A} \rangle_\psi = \langle \hat{A} \rangle = \langle \psi | \hat{A} | \psi \rangle = \sum_i \lambda_i |a_i|^2 \quad (3.1)$$

where $|a_i|^2$ is the probability of getting the outcome λ_i , such that $\sum_i |a_i|^2 = 1$ and the expectation value $\langle \hat{A} \rangle_\psi$ is the mean value found from multiple measurements on an ensemble of identically prepared systems. To relate this back to our density operator we say that if the state vector is known then a density operator of the form:

$$\rho = |\psi\rangle\langle\psi| \quad (3.2)$$

is called a pure state, this allows us to define the expectation value of \hat{A} as:

$$\langle \hat{A} \rangle = Tr \left(|\psi\rangle\langle\psi| \hat{A} \right) = Tr(\rho \hat{A}) \quad (3.3)$$

However, if the state is mixed then we have a density matrix of the form:

$$\rho = \sum_i p_i |\psi_i\rangle\langle\psi_i| \quad (3.4)$$

and so our expectation value is defined as:

$$\langle \hat{A} \rangle = Tr \left(\sum_i p_i |\psi_i\rangle\langle\psi_i| \hat{A} \right) = Tr(\rho \hat{A}) \quad (3.5)$$

We can also define the matrix elements ρ_{ji} of the density operator in any basis $\{|\chi_j\rangle\}$ as:

$$\rho_{ji} = \langle \chi_j | \rho | \chi_i \rangle = \rho_{ij}^* \quad (3.6)$$

3.2 Partial trace and reduced states

We are almost ready to talk about partial states, but before we can we must discuss the concept of the partial trace. The partial trace enables us to construct reduced states, as it only acts on one of the terms in the tensor product, leaving the other unchanged.

Definition 3.2. Let $\hat{A} \otimes \hat{B}$ be a tensor product operator on the space $\mathcal{H}_A \otimes \mathcal{H}_B$. Its partial traces over \mathcal{H}_A and \mathcal{H}_B are the operators on \mathcal{H}_A and respectively \mathcal{H}_B , defined as:

$$Tr_B(\hat{A} \otimes \hat{B}) = \hat{A} \cdot Tr(\hat{B})$$

$$Tr_A(\hat{B} \otimes \hat{A}) = \hat{B} \cdot Tr(\hat{A})$$

Any linear operator \hat{X} on $\mathcal{H}_A \otimes \mathcal{H}_B$ can be written as a linear combination of rank one tensor products, since the partial trace can be extended by linearity to all operators[Gut15]:

$$\hat{X} = \sum_{i_A, j_A, i_B, j_B} X_{i_A j_A, i_B j_B} |\chi_{i_A}\rangle\langle\chi_{i_B}| \otimes |\mu_{j_A}\rangle\langle\mu_{j_B}| = \sum_{i_A, j_A, i_B, j_B} X_{i_A j_A, i_B j_B} |\chi_{i_A} \otimes \mu_{j_A}\rangle\langle\chi_{i_B} \otimes \mu_{j_B}|$$

for orthonormal bases $\{|\chi_1\rangle, \dots, |\chi_{d_A}\rangle\}$ and $\{|\mu_1\rangle, \dots, |\mu_{d_B}\rangle\}$ then:

$$Tr_B(\hat{X}) = \sum_{i_A, i_B=1}^{d_A} \left(\sum_{j=1}^{d_B} X_{i_A j, i_B j} \right) |\chi_{i_A}\rangle\langle\chi_{i_B}| \quad (3.7)$$

$$Tr_A(\hat{X}) = \sum_{j_A, j_B=1}^{d_B} \left(\sum_{i=1}^{d_A} X_{i j_A, i j_B} \right) |\mu_{j_A}\rangle\langle\mu_{j_B}| \quad (3.8)$$

The partial trace has the following important properties:

1. Taking both partial traces give the trace:

$$Tr_A(Tr_B(\hat{X})) = Tr_B(Tr_A(\hat{X})) = Tr_{AB}(\hat{X}) = Tr(\hat{X}) = \sum_{i,j} X_{ij,ik}$$

2. Partial trace of rank one operators:

$$Tr_B(|\chi\rangle\langle\chi'| \otimes |\mu\rangle\langle\mu'|) = |\chi\rangle\langle\chi'| \cdot Tr(|\mu\rangle\langle\mu'|) = \langle\mu'|\mu\rangle |\chi\rangle\langle\chi'|$$

3. The partial trace is not cyclic:

$$Tr_A(\hat{X}\hat{Y}) \neq Tr_A(\hat{Y}\hat{X})$$

4. The partial trace of a positive operator is a positive operator:

$$\hat{X} \geq 0 \Rightarrow Tr_A(\hat{X}) \geq 0 \text{ and } Tr_B(\hat{X}) \geq 0$$

Now that we have the required formalism in place, we are in a position to discuss the idea of a reduced state. A reduced state on a bipartite system has exactly the same properties as a density matrix, except it only contains information about one of the systems. Formally we say that for some Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_B$, if $|\psi\rangle \in \mathcal{H}_A \otimes \mathcal{H}_B$ is a pure bipartite state, then the partial states of the two subsystems are given by the density matrices:

$$\rho_A = Tr_B(|\psi\rangle\langle\psi|) \tag{3.9}$$

$$\rho_B = Tr_A(|\psi\rangle\langle\psi|) \tag{3.10}$$

With the tools now in place, we are in a position to discuss the ideas and concepts regarding entanglement.

Chapter 2

Entanglement

In this chapter the reader shall be introduced to the foundations of entanglement, its importance and uses throughout quantum information science. The reader shall also be introduced to the difficulties the quantum community faces in trying to understand multipartite entanglement. We introduce also the notions for what it means for a state, specifically a bipartite state, to be entangled and ways in which we can quantify this entanglement.

4 The birth of entanglement

Entanglement was first described by Einstein, Podolski and Rosen (EPR) [EPR35] to demonstrate the conceptual differences between the quantum world and the classical world. Published in 1935, their paper argued that quantum mechanics was not a complete theory of Nature; that being there are hidden variables which are yet to be discovered. They showed this by presenting an example of an entangled quantum state, to which it is not possible to attribute some precise classical meaning that allows us to understand its behaviour with certainty. This stems from the fact that although the predictive powers of quantum mechanics are much greater than those of classical mechanics, classical systems deal with objects that are completely deterministic, which is the complete opposite to the quantum world, where we must consider all possible paths that our object can take. We can not attribute a definitive value, but we can say probabilistically what its outcome will be, as we know all possible outcomes of our quantum object (observable) are determined by the spectrum of the linear operator that represents it.

This strange nature of reality led EPR to assume that quantum mechanics was incomplete. The ideas presented by EPR were kept at the back of the minds of many a physicist, for many a decade and to some extent still play on the minds of those who have yearning for casuality.

But why? Well, quantum mechanics explained the behaviour of the nano-world and paved the way for semi-conductors, lasers and many other revolutionary areas of physics and technological advances. The problem was, quantum mechanics conceptually was unsatisfactory as a fundamental theory of Nature and the EPR argument enhanced that skepticism. It was not until 1964 when John Bell published his paper [B⁺64], regarding the validity of the EPR assumptions, that quantifying what it means for an object to be classical became a possibility. In the paper, Bell does not make any assumption about quantum mechanics. But instead assumes that our notion of a classical view of the world is true. In order to show this he considered a thought experiment where two causally disconnected observers share many identical pairs of physical systems (represented by the

random variables X_i and Y_j) and are allowed to perform two different types of measurements on their respective systems (represented by the Pauli matrices). The measurements performed in each pair are chosen at random and correspond to elements of ‘reality’. The expectation values of these observables depend on the probability associated with a given outcome and the actual value of the outcome. Bell then derived a set of inequalities, which are more succinctly written in the CHSH form, that bound the expectation value of a linear combination of the observables. However, certain entangled states will violate these inequalities. In order to understand whether or not the inequality is violated we must perform an experimental test of Bell’s inequalities, from which we can deduce whether or not the EPR assumptions are correct or quantum mechanics is indeed a true description of the world. This test was first experimentally realised with entangled pairs of photons in 1982 [AGR82] and it demonstrated the violation of Bell’s inequalities, which therefore implies that quantum mechanics is a true description of the world. This type of experimental test has subsequently been used to detect entanglement experimentally in other physical systems [VWZ02].

4.1 The mathematical definition of entanglement

The intricacies of defining what it means for something to be experimental entangled and mathematical entangled, almost look as if they are completely different descriptions of the same thing. Quite simply, mathematically one would say that a bipartite state is entangled if it cannot be written in the following way:

$$|\Psi_{AB}\rangle = |\Psi_A\rangle \otimes |\Psi_B\rangle \tag{4.1}$$

That is, we cannot write the state $|\Psi_{AB}\rangle \in \mathcal{H}_{AB}$ as the tensor product of two separate states $|\Psi_A\rangle \in \mathcal{H}_A$ and $|\Psi_B\rangle \in \mathcal{H}_B$. If a bipartite state can be written in this form then it is called separable. The Schmidt decomposition is a more generalised form of this result and is encapsulated in the following definition:

Definition 4.1. *Let $|\psi\rangle$ be a pure state of a composite system $\mathcal{H}_A \otimes \mathcal{H}_B$. Then there exists an integer $r \leq \min(d_A, d_B)$, and two sets of orthonormal vectors $\{|\chi_1\rangle, \dots, |\chi_r\rangle\}$*

in \mathcal{H}_A and $\{|\mu_1\rangle, \dots, |\mu_r\rangle\}$ in \mathcal{H}_B such that:

$$|\psi\rangle = \sum_{i=1}^r \sqrt{\lambda_i} |\chi_i\rangle \otimes |\mu_i\rangle \quad (4.2)$$

where λ_i are strictly positive and satisfy $\sum_{i=1}^r \lambda_i = 1$. The coefficients $\sqrt{\lambda_i}$ are called the Schmidt coefficients of $|\psi\rangle$.

From this expression we may extract the reduced states, for system A:

$$\begin{aligned} \rho_A &= \sum_{ij=1}^r \sqrt{\lambda_i \lambda_j} \text{Tr}_B(|\chi_i \otimes \mu_i\rangle \langle \chi_j \otimes \mu_j|) \\ &= \sum_{ij=1}^r \sqrt{\lambda_i \lambda_j} \text{Tr}_B(|\chi_i\rangle \langle \chi_j| \otimes |\mu_i\rangle \langle \mu_j|) \\ &= \sum_i^r \lambda_i |\chi_i\rangle \langle \chi_i| \end{aligned} \quad (4.3)$$

likewise for system B we obtain:

$$\rho_B = \sum_{j=1}^r |\mu_j\rangle \langle \mu_j| \quad (4.4)$$

Thus the two partial states have the same non-zero eigenvalues and eigenstates $|\chi_i\rangle$ and $|\mu_j\rangle$ respectively. The number r is called the Schmidt rank and together with the eigenvalues μ it quantifies the amount of entanglement between the systems A and B . A Schmidt rank greater $r > 1$ means that we have an entangled state.

4.2 Bell's inequalities in the CHSH form

In order to experimentally determine whether or not a state is entangled, it is a question of measurement and we must look at the statistical distributions of the observables and see whether or not we violate Bell's inequalities.

But what exactly are Bell's inequalities? Well, referring back to our original discussion we have two distant observers Alice and Bob who share many identical pairs of particles. Alice and Bob can perform two different measurements on their respective particles, represented by the random variables X_{A_1}, X_{A_2} for Alice and Y_{B_1}, Y_{B_2} for Bob. The

individual measurements are chosen randomly and have two possible outcomes $\{-1, 1\}$.

In the Clauser, Horne, Shimony and Holt (CHSH) form Bell's inequalities read:

$$\mathbb{E}(X_{A_1}Y_{B_1}) + \mathbb{E}(X_{A_2}Y_{B_1}) + \mathbb{E}(X_{A_2}Y_{B_2}) - \mathbb{E}(X_{A_1}Y_{B_2}) \leq 2 \quad (4.5)$$

We can prove (4.5) as follows [Gut15]:

$$X_{A_1}Y_{B_1} + X_{A_2}Y_{B_1} + X_{A_2}Y_{B_2} - X_{A_1}Y_{B_2} = (X_{A_1} + X_{A_2})Y_{B_1} + (X_{A_2} - X_{A_1})Y_{B_2} \quad (4.6)$$

Since $X_{A_1}, X_{A_2} \in \{-1, 1\}$ it follows that either $X_{A_1} + X_{A_2} = 0$ or $X_{A_1} - X_{A_2} = 0$, therefore (4.6) is equal to ± 2 . If the joint distribution of $(X_{A_1}, X_{A_2}, Y_{B_1}, Y_{B_2})$ is:

$$p(i, j, k, l) = \mathbb{P}(X_{A_1} = i, X_{A_2} = j, Y_{B_1} = k, Y_{B_2} = l)$$

then by taking the expectation of (4.6) we find:

$$\begin{aligned} \mathbb{E}(X_{A_1}Y_{B_1}) + \mathbb{E}(X_{A_2}Y_{B_1}) + \mathbb{E}(X_{A_2}Y_{B_2}) - \mathbb{E}(X_{A_1}Y_{B_2}) &= \sum_{ijkl \in \{+1, -1\}} p(i, j, k, l)(ik + jk + jl - il) \\ &= \sum_{ijkl \in \{+1, -1\}} p(i, j, k, l)2 = 2 \quad \square \end{aligned}$$

where the expectation value over the composite system with respect to some Bell basis state $|\psi\rangle$ is defined as:

$$\mathbb{E}(\hat{X}_{A_i}\hat{Y}_{B_j}) = \langle \psi | \hat{X}_{A_i} \otimes \hat{Y}_{B_j} | \psi \rangle = \text{Tr}[(\hat{P}_{A_i} \otimes \hat{P}_{B_j}) | \psi \rangle \langle \psi |] \quad (4.7)$$

where \hat{P}_{A_i} and \hat{P}_{B_j} are the eigenprojectors of Alice and Bob's observables respectively, corresponding to a particular outcome. In the quantum experiment Alice has operators, $\hat{X}_{A_1} = \sigma_3$ and $\hat{X}_{A_2} = \sigma_1$ and Bob has operators $\hat{Y}_{B_2} = \frac{-(\sigma_3 + \sigma_1)}{\sqrt{2}}$ and $\hat{Y}_{B_1} = \frac{(\sigma_3 - \sigma_1)}{\sqrt{2}}$. The Bell basis states are a set of entangled bipartite states that form an orthonormal basis and are defined as:

$$|\phi_+\rangle = \frac{(|0\rangle \otimes |0\rangle + |1\rangle \otimes |1\rangle)}{\sqrt{2}} \quad (4.8)$$

$$|\phi_-\rangle = \frac{(|0\rangle \otimes |0\rangle - |1\rangle \otimes |1\rangle)}{\sqrt{2}} \quad (4.9)$$

$$|\psi_+\rangle = \frac{(|0\rangle \otimes |1\rangle + |1\rangle \otimes |0\rangle)}{\sqrt{2}} \quad (4.10)$$

$$|\psi_-\rangle = \frac{(|0\rangle \otimes |1\rangle - |1\rangle \otimes |0\rangle)}{\sqrt{2}} \quad (4.11)$$

These definitions of entanglement make entanglement look like a rather simple and well understood concept, but in reality the truth is quite different. These ideas only hold for bipartite systems, not multipartite systems⁵ which are incredibly difficult to understand theoretically and generate experimentally. However, research in to entanglement has never been greater, it is an exciting area of quantum information science; both experimentally and theoretically. The idea of what it means for something to be entangled has been stripped to its core [AFOV08] [VPRK97a] [GF07] and a great body of work is currently being produced about it. However, can anyone say that we understand the fundamentals of entanglement, probably not. What we can say however is that we are finding a way to decrypt it. In fact, it is even believed now that entangled systems are just a subset of a more fundamental quantum property, quantum discord [OZ01][DLM⁺12].

4.3 Importance of entanglement

Although we do not truly know all of the potential uses of entanglement at this moment in time, for systems where entanglement can be used as some kind of information resource we see something remarkable. On the basic level what makes quantum mechanics so fascinating is the concept of linear superposition, where we have so called “Schrödinger cat” states that are in some superposition state:

$$|\psi\rangle = \alpha|0\rangle + \beta|1\rangle \tag{4.12}$$

where $\alpha, \beta \in \mathbb{C}$ and $|0\rangle$ and $|1\rangle$ are qubit basis states, typically represented by the vectors:

$$|0\rangle = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, |1\rangle = \begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

Combining the property of linear superposition and entanglement, we can entangle several copies of these states and so in theory we could construct a quantum computer that would have an exponential speed as compared to its classical counter part. This is because each

⁵There are methods to extend Bell’s inequalities to multipartite states [idZB02], however there are additional complexities with this.

qubit is $N = 2^n$ bits, where N is the number of classical bits required, and n the number of qubits, i.e. a 6-qubit quantum computer contains the same information as $N = 64$ -bit classical computer. Even a small n -qubit quantum computer could solve problems multiple times faster than our classical N -bit super computers. This of course has created an immense amount of buzz in the field of quantum information science. However, theoretically these “Schrödinger cat” states are easy to construct, but experimentally it is incredibly challenging as the system has to be completely isolated from outside noise. This is because the noise either causes the state to decohere back in to a classical bit or errors are induced, which we have to somehow account for. Classically, correcting errors is incredibly simple as we can make observations without destroying our deterministic state. This is not true quantum mechanically, as we can not perform multiple measurements on our system, if we would like it to remain in a state of linear superposition. This therefore means that we potentially have to be able to correct for an exponential amount of errors, of course destroying any potential speed up. However, we should not be so disheartened, research on an industrial scale is being carried out by the likes of Google, IBM, Toshiba and many other technological giants. It is believed that it will be and can be done, but when, well that is to be determined.

Other information resource uses of entanglement are primarily security based, such as quantum key distribution [Eke91] and quantum teleportation [BBC⁺93]. The name quantum teleportation is slightly misleading as we are not teleporting anything as such. When we talk about quantum teleportation, we refer to transferring the properties of a state that is coupled to Alice’s system, to Bob’s system via measurement and classical communications. In performing this process we destroy the original state, but via the information that Bob has received from the classical communications he is able to construct an exact replica of the state that Alice wanted to send. In this sense the state is ‘teleported’ from Alice to Bob.

What we have given here is purely a very brief overview of some of the more prominent

uses of entanglement, there are also several algorithms that we could have discussed, in particular Shor's algorithm [Sho96], which using the properties of quantum mechanics can factor prime numbers in a polynomial time. The uses of entanglement are only just being explored and the area as a whole is going through a wonderful age of discovery.

5 Measures of entanglement

After all that has been discussed regarding entanglement, you are probably beginning to wonder how do we actually quantify the amount of entanglement for a given system. For the systems that we are dealing with, it is relatively easy since they are pure bipartite systems and so there is a strong base of theory to describe the entanglement within these systems. However, the same is not true for mixed states and is especially not true for multipartite states.

5.1 Entanglement measures

A lot of work has been done by the quantum information community in order to formalise the idea of an entanglement measure. From this body of work came a list of axioms that are generally believed to be the minimum requirement that any Entanglement measure $E(\rho)$ should satisfy [PV07][VPRK97b]:

1. $E(\rho) = 0$ iff ρ is separable.
2. Local unitary operations leave $E(\rho)$ invariant, i.e. $E(\rho_{AB}) = E(\hat{U}_A \otimes \hat{U}_B \rho_{AB} \hat{U}_A^\dagger \otimes \hat{U}_B^\dagger)$
3. $E(\rho)$ is additive. The entanglement of several copies of a state adds up to n times the entanglement of a single copy i.e. $E(\rho^{\otimes n}) = nE(\rho)$.
4. $E(\rho)$ is subadditive. The entanglement of two states is not larger than the sum of the entanglement of both individual states i.e. $E(\rho_a \otimes \rho_b) \leq E(\rho_a) + E(\rho_b)$
5. $E(\rho)$ is convex. $E(\lambda\rho_a + (1 - \lambda)\rho_b) \leq \lambda E(\rho_a) + (1 - \lambda)E(\rho_b)$, for $0 \leq \lambda \leq 1$.

6. For a pure bipartite state ρ_{AB} , $E(\rho_{AB})$ reduces to the entropy of entanglement (5.1),

$$E(\rho_{AB}) = S(\text{Tr}_A(\rho_{AB})) = S(\text{Tr}_B(\rho_{AB}))$$

I should however state that there is no completely agreed upon list of axioms, although most authors will either use the axioms listed above, or a subset of them. The next remark will seem rather contradictory, but it is important to emphasise that the field is still in a rapid phase of development. Some of the most important entanglement measures do not actually satisfy some of the above axioms [PV07] and so we should always approach the situation we are dealing with, with some degree of caution.

We shall now introduce just a few entanglement measures for bipartite systems. One entanglement measure in particular is more dominant than the others, whose origins lie in thermodynamics and was later popularised and modified by Von-Neumann. It is of course the Von-Neumann entanglement entropy, which was included in our entanglement measure axioms. It is a quantity that enables us to understand the amount of information in a given quantum state and is defined as:

$$S(\rho) = -\rho \ln \rho = \sum_i \lambda_i \ln(\lambda_i) \quad (5.1)$$

where the Borel theorem has been used in order to write the Von-Neumann entanglement entropy in terms of the states spectrum. The Von-Neumann entanglement entropy is one of the few entanglement measures that actually satisfies all necessary criteria for an entanglement measure, it is also the reason why it is one of the most widely used methods for quantifying the entanglement within quantum systems. It shall also be one of our key entanglement measures for quantifying the entanglement in both the hydrogen atom and our toy model.

The Von-Neumann entanglement entropy can also be seen as a degree for understanding how mixed a state is. In light of this interpretation we introduce another quantity, the linear entropy, which is defined as[ZHP93]:

$$S^L = \frac{1}{q-1} \text{Tr}(\rho - \rho^q) \quad (5.2)$$

where q is a real, not necessarily positive number. As q approaches 1, we recover the Von-Neumann entanglement entropy. When $q = 2$, which is the case for us, the linear entropy reduces to:

$$S^L = 1 - \text{Tr}(\rho^2) = 1 - \sum_i \lambda_i^2 \quad (5.3)$$

which can be seen as follows:

$$\frac{1}{1}[\text{Tr}(\rho) - \text{Tr}(\rho^2)]$$

since the trace of any density matrix must be 1, we have (5.3). The linear entropy, like the Von-Neumann entanglement entropy also determines the degree of mixing in a state and will also play an important role in quantifying the entanglement in the systems that we shall investigate later. The following two entanglement measures shall not be used in this dissertation, but are merely given to give the reader an idea of just some of the tools that are currently available.

Our next measure of entanglement enables us to compare our state of interest ρ with some unentangled state $\rho_{ue} = \sum_i p_i \rho_A^i \otimes \rho_B^i$, where the p_i are positive and satisfy $\sum_i p_i = 1$. In comparing the given state and the unentangled state we gain a quantitative measure of entanglement. From which we construct the trace distance, which is the distance between our state and the nearest unentangled state[AFOV08][PWK04]:

$$D_{ent}(\rho) = \text{Inf}_{\rho_{ue}} \frac{1}{2} |\rho - \rho_{ue}| \quad (5.4)$$

where the state ρ_{ue} is chosen to give the minimum distance. This measure enables us to identify the unentangled state most similar to our entangled state and quantify the entanglement by our ability to discriminate between the two. As example let us consider the two-qubit entangled state:

$$\rho = \cos^2(\theta) |0\rangle |0\rangle + \sin^2(\theta) |1\rangle |1\rangle$$

where the nearest unentangled state is:

$$\rho_{ue} = \cos^2(\theta) |0\rangle\langle 0| \otimes |0\rangle\langle 0| + \sin^2(\theta) |1\rangle\langle 1| \otimes |1\rangle\langle 1|$$

and so the associated distance is:

$$D_{ent} = |\cos(\theta) \sin(\theta)| \quad (5.5)$$

This is of course zero for $\cos(\theta) = 0$ or $\sin(\theta) = 0$, but is maximal when $\theta = \frac{\pi}{4}$ and so our entangled state corresponds directly to a Bell basis state.

The next and final measure of entanglement that we shall discuss is concurrence, which along with the Von-Neumann entanglement entropy is one of the few measures that can be applied to multipartite states. We start by introducing the spin flip transformation, for a single qubit, which takes the form⁶:

$$\rho \rightarrow \bar{\rho}_1 = \sigma_2 \rho^* \sigma_2 \quad (5.6)$$

From [Gut15] we know that we can represent a qubit in terms of the pauli ‘spin’ operators and the position vector \mathbf{r} as follows⁷:

$$\rho = \frac{1}{2}(\hat{I} + \mathbf{r} \cdot \boldsymbol{\sigma}) \quad (5.7)$$

The effect of this transformation changes the sign to a minus sign and so:

$$\bar{\rho}_1 = \frac{1}{2}(\hat{I} - \mathbf{r} \cdot \boldsymbol{\sigma}) \quad (5.8)$$

We can extend this transformation naturally to two-qubits by:

$$\bar{\rho}_2 = \sigma_2 \otimes \sigma_2 \rho^* \sigma_2 \otimes \sigma_2 \quad (5.9)$$

from which we construct a positive operator \hat{R} in terms of ρ and $\bar{\rho}_2$ as:

$$\hat{R} = \sqrt{\rho} \bar{\rho}_2 \sqrt{\rho} \quad (5.10)$$

Let the four positive eigenvalues of \hat{R} be, in terms of decreasing size, $\lambda_1, \dots, \lambda_4$. The concurrence $\mathcal{C}(\rho)$ for an entangled state ρ is defined to be [Woo98]:

$$\mathcal{C}(\rho) = \max\{0, \lambda_1 - \lambda_2 - \lambda_3 - \lambda_4\} \quad (5.11)$$

The concurrence takes a zero value for an unentangled state and a positive value for an entangled state. For several examples and more insight see [Woo98].

⁶This is related to the notation of a quantum channel, see [Gut15]

⁷Here $\mathbf{r} \cdot \boldsymbol{\sigma} = r_i \sigma_i$, where $i = 1, \dots, 3$.

5.2 Many body entanglement

Many body entanglement is in its own right an incredibly vast, yet rich area of study, that is full of questions and answers regarding the complexity of entanglement. It is no exaggeration to say that trying to understand what multipartite entanglement is, is a bit like putting together a jigsaw puzzle with thousands of pieces, which has no picture, yet has the ability to change depending on what pieces are connected. If that analogy sounds complicated, it is because multipartite entanglement is complicated. We shall however try and give a very brief overview of the ideas developed to understand entanglement in multipartite systems.

Our previous definitions for a bipartite system which defined whether or not a state is entangled are no longer useful, as if we have a multipartite state i.e. $|\phi\rangle = |\psi_1\rangle \otimes \dots \otimes |\psi_d\rangle$, where $d > 2$, then the state may have several decompositions, some of which are entangled and some of which are not. In addition to this, different parts of the system may also be entangled and actually determining whether a multipartite state is entangled is an NP-hard problem.

Thankfully, not all is hopeless, there are ways in which we can tackle parts of this problem. One such solution is the introduction of an Entanglement witness, W , a special type of positive map. It is a self-adjoint operator which is able to detect entanglement in a state. The basic idea is [VPRK97a] that the expectation value of the witness W for the state ρ under consideration exceeds certain bounds only when ρ is entangled. An expectation value of W within this bound, however, does not guarantee that the state is separable. Simple geometric ideas help to explain the witness operator W at work [VPRK97a]. Let \mathcal{T} be the set of all density matrices and let \mathcal{E} and \mathcal{S} be the subsets of entangled and separable states, respectively. The convexity of \mathcal{S} is a key property for witnessing entanglement. The entanglement witness is then an operator defining a hyperplane which separates a given entangled state from the set of separable states. We have the freedom to choose W such that $Tr(\rho_S W) \leq 0$ for all disentangled states $\rho_S \in \mathcal{S}$ and so for $Tr(\rho_E W) > 0$ implies that $\rho_E \in \mathcal{E}$ is entangled. A problem with the method is that it is not invariant

under local unitary operations [VPRK97a].

Another concept that we may look at is the negativity, which is a way to detect the presence of entanglement in multipartite systems. Consider, for example, a bipartite state ρ_{AB} which lives on the space $\mathcal{H}_A \otimes \mathcal{H}_B$. If we calculate a state $\rho_{AB}^{T_i}$, where T_i is the partial transpose of state $i = A$ or B , then finding the sum of the absolute negative eigenvalues of this state, gives the negativity N_{AB} , from which we define the logarithmic negativity for a bipartite system as:

$$E_N = \log_2 2(2N_{AB} + 1) \tag{5.12}$$

As a final point let us mention very briefly, in a non-mathematical context, the ideas regarding pairwise qubit entanglement in mixed states. The reason we must turn to mixed states is because in general the subsystems of a many-body pure state will generally be in a mixed state. To deal with this three important representatives were introduced in order to quantify the entanglement in the system, they are; the entanglement cost E_C , the distillable entanglement E_D and the entanglement of formation E_F . We shall not go in to more detail than this, purely due to complexity. For the interested reader see[VPRK97a] for a much deeper and more in depth explanation of E_C , E_D and E_F and multipartite entanglement.

Chapter 3

Entanglement in physical systems

In this chapter we aim to show the reader a derivation of the hydrogen atom in both the position and momentum space representations. We then aim to show how entanglement arises in the hydrogen atom due to the electrostatic interaction between the electron and proton, and how the amount of entanglement within the system can be quantified in terms of an ‘entanglement parameter’. This is not a parameter in the usual sense, but is dictated by the interaction between the quantum particles. We then go on to use the ideas presented in the case of the entangled hydrogen atom, to discuss and analyse a system of two interacting coupled bosonic quantum particles, the system is almost identical to the two coupled oscillator model. This system has a different entanglement parameter and a different type of interaction through which it becomes entangled.

6 Electron-proton entanglement in the three dimensional hydrogen atom

The electron-proton system is studied at least once in all undergraduate quantum mechanics modules, due to the fact that it is one of the few systems in quantum mechanics where Schrödinger's equation can be solved completely analytically. The fact that we can do this, means not only do we have something robust that we can test physically, but we can also probe the system a little more and see if we can extract anymore information.

6.1 The hydrogen atom in the position representation

The starting point for understanding any system in quantum mechanics begins with the Schrödinger equation, see chapter one. Given in the form of state vectors it is not so easy to see that Schrödinger's equation is actually some n^{th} -order partial differential equation (PDE), which in the case of the hydrogen atom is a 2^{nd} -order PDE. To analyse the hydrogen atom (see fig. 1) we require the form of the Hamiltonian operator, as with the Hamiltonian in the classical sense, the Hamiltonian operator describes the dynamics of the system. However, instead of in a deterministic sense, it is in terms of the spectral data of the state. Where the spectral data allows us to calculate a set of probabilities for our given system. For the hydrogen atom, the general Hamiltonian operator is written in the form:

$$\hat{H} = \frac{\hat{\mathbf{p}}_e^2}{2m_e} + \frac{\hat{\mathbf{p}}_p^2}{2m_p} - \frac{e^2}{4\pi\epsilon_0|\mathbf{r}_e - \mathbf{r}_p|} \quad (6.1)$$

where the kinetic term is represented by $\frac{\hat{\mathbf{p}}_e^2}{2m_e} + \frac{\hat{\mathbf{p}}_p^2}{2m_p}$ and the electro-static repulsion between the electron and proton is described by the central potential $V(\mathbf{r}) = -\frac{e^2}{4\pi\epsilon_0|\mathbf{r}_e - \mathbf{r}_p|}$. Unfortunately, the Hamiltonian expressed in this form can not be written as the product of separable solutions i.e. it can not be written as the tensor product of two states and so is incredibly difficult to solve. But, with a little mathematical trickery and making the

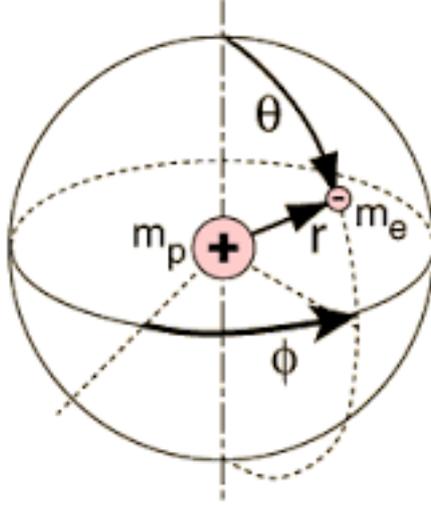


Figure 1: A classical picture of the hydrogen atom, which consists of one proton and one ‘orbiting’ electron [Hyp14].

following co-ordinate transforms:

$$\mathbf{r} = \mathbf{r}_e - \mathbf{r}_p \quad (6.2)$$

$$\mathbf{R} = \frac{m_e \mathbf{r}_e + m_p \mathbf{r}_p}{m_e + m_p} \quad (6.3)$$

where \mathbf{r} is the relative co-ordinate, \mathbf{R} is the co-ordinate at the centre of mass, we shall find that our Hamiltonian splits into two uncorrelated systems. Written in terms of our co-ordinate transform, the electron and proton positions are defined as:

$$\begin{aligned} \mathbf{r}_p &= \mathbf{R} + \frac{m_e}{M} \mathbf{r} \\ \mathbf{r}_e &= \mathbf{R} - \frac{m_p}{M} \mathbf{r} \end{aligned}$$

using these definitions we must also redefine the differential operators $\nabla^2 \mathbf{r}_p$ and $\nabla^2 \mathbf{r}_e$ of the respective momentum operators. Focusing on just one co-ordinate and using the chain rule, i.e. the x -co-ordinate of the proton, we write:

$$\begin{aligned} \frac{\partial \psi}{\partial x_p} &= \frac{\partial \psi}{\partial R_x} \frac{\partial R_x}{\partial x_p} + \frac{\partial \psi}{\partial r_x} \frac{\partial r_x}{\partial x_p} \\ \frac{\partial^2 \psi}{\partial x_p^2} &= \frac{\partial}{\partial R_x} \left(\frac{\partial \psi}{\partial x_p} \right) \frac{\partial R_x}{\partial x_p} + \frac{\partial}{\partial r_x} \left(\frac{\partial \psi}{\partial x_p} \right) \frac{\partial r_x}{\partial x_p} \\ &= \left(\frac{m_p}{M} \right)^2 \frac{\partial^2 \psi}{\partial R_x^2} + \left(\frac{2m_p}{M} \right) \frac{\partial^2 \psi}{\partial R_x \partial r_x} + \frac{\partial^2 \psi}{\partial r_x^2} \end{aligned}$$

likewise for $\frac{\partial^2 \psi}{\partial x_e^2}$ we get the following:

$$\frac{\partial^2 \psi}{\partial x_e^2} = \left(\frac{m_e}{M}\right)^2 \frac{\partial^2 \psi}{\partial R_x^2} - \left(\frac{2m_e}{M}\right) \frac{\partial^2 \psi}{\partial R_x \partial r_x} + \frac{\partial^2 \psi}{\partial r_x^2}$$

from which we can see that if we did this for the respective y and z co-ordinates that we would get the following expressions:

$$\nabla^2 \mathbf{r}_p = \left(\frac{m_p}{M}\right)^2 \nabla_{\mathbf{R}}^2 + \left(\frac{2m_p}{M}\right) \nabla_{\mathbf{R}} \nabla_{\mathbf{r}} + \nabla^2 \mathbf{r} \quad (6.4)$$

$$\nabla^2 \mathbf{r}_e = \left(\frac{m_e}{M}\right)^2 \nabla_{\mathbf{R}}^2 - \left(\frac{2m_e}{M}\right) \nabla_{\mathbf{R}} \nabla_{\mathbf{r}} + \nabla^2 \mathbf{r} \quad (6.5)$$

Therefore inserting these expressions back into (6.1) we get the following uncorrelated Hamiltonian:

$$\hat{H} = \hat{H}_{cm} + \hat{H}_{int} = \frac{\hat{\mathbf{p}}_R^2}{2M} + \frac{\hat{\mathbf{p}}_r^2}{2m_r} - \frac{e^2}{4\pi\epsilon_0|r|} \quad (6.6)$$

where \hat{H}_{cm} is the Hamiltonian at the centre of mass and \hat{H}_{int} is the internal Hamiltonian dependent on the relative co-ordinate \mathbf{r} , m_r is the reduced mass defined as:

$$m_r = \frac{m_e m_p}{m_e + m_p}$$

and M is the total mass defined as:

$$M = m_p + m_e$$

The following uncorrelated Hamiltonian now allows for separable solutions of the form:

$$\Psi(\mathbf{R}, \mathbf{r}) = \chi(\mathbf{R})\phi(\mathbf{r}) \quad (6.7)$$

We can now insert (6.7) and our uncorrelated Hamiltonian in to Schrödinger's equation to get the following:

$$\begin{aligned} \left(\frac{\hat{\mathbf{p}}_R^2}{2M} + \frac{\hat{\mathbf{p}}_r^2}{2m_r}\right) \chi(\mathbf{R})\phi(\mathbf{r}) - \left(\frac{e^2}{4\pi\epsilon_0|r|} - E\right) \chi(\mathbf{R})\phi(\mathbf{r}) &= 0 \\ \phi(\mathbf{r})\hat{H}_{cm}\chi(\mathbf{R}) + \chi(\mathbf{R})\hat{H}_{int}\phi(\mathbf{r}) &= E\chi(\mathbf{R})\phi(\mathbf{r}) \end{aligned}$$

where the total energy E is defined as [Oss13] $E = E'_{cm} + E'_{int}$ which gives us:

$$\phi(\mathbf{r})[\hat{H}_{cm}\chi(\mathbf{R}) - E'_{cm}\chi(\mathbf{R})] = -\chi(\mathbf{R})[\hat{H}_{int}\phi(\mathbf{r}) - E'_{int}\phi(\mathbf{r})]$$

We then divide through by the separable solution $\chi(\mathbf{R})\phi(\mathbf{r})$ to get two equations that are dependent on different variables, but are equal to one another. Therefore, since these equations are independent, both equations must be equal to some constant, i.e. E_0 . So we re-label the energies as $E_{cm} = E'_{cm} + E_0$ and $E_{int} = E'_{int} - E_0$ to get:

$$\hat{H}_{cm}\chi(\mathbf{R}) = E_{cm}\chi(\mathbf{R}) \quad (6.8)$$

$$\hat{H}_{int}\phi(\mathbf{r}) = E_{int}\phi(\mathbf{r}) \quad (6.9)$$

(6.8) can be shown quite simply to have plane wave solutions:

$$\chi(\mathbf{R}) = \frac{1}{\sqrt{V}}e^{i\mathbf{K}\cdot\mathbf{R}} \quad (6.10)$$

where the solutions have been normalised by the box normalisation scheme [TTdTP98], $\mathbf{K} = \frac{\mathbf{P}}{\hbar}$ is the wave-vector and \mathbf{P} is the momentum at the centre of mass. The factor $\frac{1}{\sqrt{V}}$ comes from the box normalisation scheme, which assumes that the ‘particle’ is confined to a large volume V . This regularisation is subtle, but is actually incredibly important as it ensures that the thermodynamic limit is satisfied. This in turn allows us to use our entanglement measures, well specifically the Von-Neumann entanglement entropy.

6.2 The angular solution

The difficult part is finding the solution to the relative part, due to the internal motion solution being dependent on the radial and angular variables. This is due to the fact that the potential, which is only dependent on the radial distance from the origin, is spherically symmetric. Thus the internal Hamiltonian has a solution which is separable in to spherical co-ordinates (r, θ, ϕ) :

$$\phi(\mathbf{r}) = R(r)Y(\theta, \phi) \quad (6.11)$$

But since our Laplacian for the internal Hamiltonian is written in terms of the relative distance, we must re-write it in terms of spherical co-ordinates:

$$\nabla_{\mathbf{r}}^2 = \frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial}{\partial r} \right) + \frac{1}{r^2 \sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial}{\partial \theta} \right) + \frac{1}{r^2 \sin^2(\theta)} \left(\frac{\partial^2}{\partial \phi^2} \right) \quad (6.12)$$

Inserting (6.12) into (6.9) we get:

$$-\frac{\hbar^2}{2m_r} \left[\frac{Y(\theta, \phi)}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) + \frac{R(r)}{r^2 \sin(\theta)} \left(\sin(\theta) \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{R(r)}{r^2 \sin^2(\theta)} \left(\frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} \right) \right] + (V(r) - E_{int})R(r)Y(\theta, \phi) = 0 \quad (6.13)$$

we then multiply through by $\frac{-2m_r r^2}{\hbar^2 R(r) Y(\theta, \phi)}$:

$$\left[\frac{1}{R(r)} \frac{\partial}{\partial r} \left(r^2 \frac{\partial R(r)}{\partial r} \right) - \frac{2m_r r^2}{\hbar^2} (V(r) - E_{int})R(r) \right] = -\frac{1}{Y(\theta, \phi)} \left[\frac{1}{\sin(\theta)} \frac{\partial}{\partial \theta} \left(\sin(\theta) \frac{\partial Y(\theta, \phi)}{\partial \theta} \right) + \frac{1}{\sin^2(\theta)} \left(\frac{\partial^2 Y(\theta, \phi)}{\partial \phi^2} \right) \right] = l(l+1) \quad (6.14)$$

which produces two independent equations. Therefore the only way for this statement to be true, is if the equations are both equal to the same constant. With hindsight available to us, we choose the constant to be $l(l+1)$, the eigenvalues to the angular momentum squared operator $\hat{\mathbf{L}}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$, where $l = 0, 1, 2, \dots$ will become our angular momentum quantum number. Focusing on the angular equation for $Y(\theta, \phi)$ first we notice that if we multiply by $Y(\theta, \phi) \sin^2(\theta)$ that we have a separable solution of the form:

$$Y(\theta, \phi) = \Theta(\theta)\Phi(\phi) \quad (6.15)$$

putting (6.15) back in to the angular equation and dividing through by $\Theta(\theta)\Phi(\phi)$ we get:

$$\frac{1}{\Theta(\theta)} \left[\sin(\theta) \frac{d}{d\theta} \left(\sin(\theta) \frac{d\Theta(\theta)}{d\theta} \right) \right] + l(l+1) \sin^2(\theta) = -\frac{1}{\Phi(\phi)} \frac{d^2\Phi(\phi)}{d\phi^2} = m^2 \quad (6.16)$$

where m^2 is our separation constant and leads to the magnetic quantum number m . Solving for the ϕ dependent equation is straight forward using standard ordinary differential techniques, from which we get:

$$\Phi(\phi) = A e^{(im\phi)} \quad (6.17)$$

where $m = \dots, -2, -1, 0, 1, 2, \dots$ and the constant factor can be absorbed into Φ . The reason why we have not written two linearly independent solutions is because $m \in \mathbb{Z}$. This is due to the fact that in the complex plane, if we rotate by 2π we get back to our

initial value i.e. $\Phi(\phi + 2\pi) = \Phi(\phi)$ is 2π -periodic. This implies $e^{(i2\pi m)} = 1$, which is true for all $m \in \mathbb{Z}$.

Returning now to the equation for θ and trying to solve is a little more involved. Thankfully, as it is in the form of Legendre's equation(see appendix B) we can write the solution as:

$$\Theta(\theta) = AP_l^m(\cos(\theta)) \quad (6.18)$$

where P_l^m is called the associated Legendre function. The reason why there only exist one independent solution is because in order to avoid singularities, the constant of the non-polynomial solution is set to zero⁸. The associated Legendre function is generated in the following way:

$$P_l^{|m|}(w) = (1 - w^2)^{\frac{|m|}{2}} \left(\frac{d}{dw}\right)^{|m|} P_l(w) \quad (6.19)$$

and $P_l(w)$ is the l^{th} Legendre polynomial which can be generated via Rodrigues formula:

$$P_l(w) = \frac{1}{2^l l!} \left(\frac{d}{dw}\right)^l (w^2 - 1)^l \quad (6.20)$$

Now the associated Legendre functions satisfy the following orthogonality relation:

$$\int_{-1}^1 P_l^{|m|}(w) P_n^{|m|}(w) dw = \frac{2}{2l + 1} \frac{(l + |m|)!}{(l - |m|)!} \delta_{ln} \quad (6.21)$$

and so the associated Legendre functions satisfy the completeness relation for an infinite Hilbert space. We see also from equation (6.19) that $P_l^m = 0$ for any $m > l$, thus for any given l there are $2l + 1$ given values of m and so the possible values of m are:

$$m = -l, l + 1, \dots, -1, 0, 1, \dots, l - 1, l$$

We now have one final task to complete before we can write down our angular solution, that being we must now find the normalisation constant A . Using the orthogonal relation:

$$\int Y_{l',m'}^*(\theta, \phi) Y_{l,m}(\theta, \phi) d\Omega = \delta_{ll'} \delta_{mm'} \quad (6.22)$$

we find that A is equal to:

$$A = (-1)^m \sqrt{\frac{2l + 1}{4\pi} \frac{(l - m)!}{(l + m)!}}$$

⁸See appendix B for a discussion on Legendre polynomials

Thus our normalised angular wavefunctions, called spherical harmonics, are found to be:

$$Y_{lm}(\theta, \phi) = (-1)^m \sqrt{\frac{2l+1}{4\pi} \frac{(l-m)!}{(l+m)!}} P_l^m(\cos(\theta)) e^{im\phi} \quad (6.23)$$

6.3 The radial and complete solution

All that is left to solve is the radial component, equation (6.14). To do this we first make the substitution $R(r) = \frac{s(r)}{r}$, which makes our radial equation:

$$\frac{-\hbar^2}{2m_r} \frac{d^2 s}{dr^2} + \left[-\frac{e^2}{4\pi\epsilon_0} \frac{1}{r} + \frac{\hbar^2}{2m_r} \frac{l(l+1)}{r^2} \right] s(r) = E_{int} s(r) \quad (6.24)$$

We can tidy up this equation by introducing the following parameters:

$$\kappa = \frac{\sqrt{-2m_r E_{int}}}{\hbar} \quad (6.25)$$

$$\rho = \kappa r \quad (6.26)$$

$$\rho_0 = \frac{me^2}{2\pi\epsilon_0 \hbar^2 \kappa} \quad (6.27)$$

which results in the following:

$$\frac{d^2 s}{d\rho^2} = \left[1 - \frac{\rho_0}{\rho} + \frac{l(l+1)}{\rho^2} \right] s(\rho) \quad (6.28)$$

Rather than directly solving the problem, we first look at the asymptotic behaviour of (6.28) for large and small ρ , which allows us to guess a form for our general solution. For large ρ we find that:

$$s(\rho) \sim A e^{-\rho} \quad (6.29)$$

where the constant for e^ρ has been set to zero, to ensure that the radial function does not blow up for large ρ . Likewise as ρ tends to 0 we find:

$$s(\rho) \sim B \rho^{l+1} \quad (6.30)$$

which does not blow up for small ρ . Using the asymptotic behaviour we introduce a new function $t(\rho)$:

$$s(\rho) = \rho^{l+1} e^{-\rho} t(\rho) \quad (6.31)$$

which leads to the following:

$$\rho \frac{d^2 t}{d\rho^2} + 2(l+1-\rho) \frac{dt}{d\rho} + [\rho_0 - 2(l+1)] \rho = 0 \quad (6.32)$$

We now see that we can use Frobenius method to find a solution in the form of a power series in ρ :

$$t(\rho) = \sum_{j=0}^{\infty} a_j \rho^j \quad (6.33)$$

where our aim is to find the coefficients (a_0, a_1, \dots) . This series can now be put back in to (6.32) and using a dummy index $j \rightarrow j+1$ we can write all terms so that they are all multiplied by the same power of j . This of course does induce additional terms, but in this case the additional terms are removed due to zeros. So we are left with:

$$\begin{aligned} \sum_{j=0}^{\infty} j(j+1)a_{j+1}\rho^j + 2(l+1) \sum_{j=0}^{\infty} (j+1)a_{j+1}\rho^j - \\ 2 \sum_{j=0}^{\infty} j a_j \rho^j + [\rho_0 - 2(l+1)] \sum_{j=0}^{\infty} a_j \rho^j = 0 \end{aligned} \quad (6.34)$$

We can now equate the lowest powers of ρ^j which leaves us with the following recursion relation for a_j :

$$a_{j+1} = \left[\frac{2(j+l+1) - \rho_0}{(j+1)(j+2l+2)} \right] a_j \quad (6.35)$$

where we fix a_0 by normalisation, which then allows us to determine all other coefficients. Again we look at the asymptotic behaviour of the recursion relation and ensure that our solution doesn't blow up. For large j we see:

$$a_{j+1} \simeq \frac{2j}{j(j+1)} a_j = \frac{2}{j+1} a_j \quad (6.36)$$

The next trick is rather nice and allows us to find a function which fits our infinite series. We simply suppose that the asymptotic recursion relation is correct, which implies:

$$a_j = \frac{2^j}{j!} a_0 \quad (6.37)$$

thus:

$$t(\rho) = a_0 \sum_{j=0}^{\infty} \frac{2^j \rho^j}{j!} \quad (6.38)$$

$$= a_0 e^{2\rho} \quad (6.39)$$

which means

$$s(\rho) = a_0 \rho^{l+1} e^\rho \quad (6.40)$$

But there is a problem with this, $s(\rho)$ blows up for large ρ . In order to get rid of these non-normalisable solutions our series must terminate after a finite number of steps, i.e there is a j_{max} such that $a_{j_{max}} = 0$. From (6.35) this implies $2(j_{max} + l + 1) - \rho_0 = 0$, where we define our principle (orbital) quantum number to be:

$$n = j_{max} + l + 1 \quad (6.41)$$

which means $\rho_0 = 2n$. Since ρ_0 by definition determines E_{int} , we find that

$$E_{int} = -\frac{m_e e^2}{8\pi^2 \varepsilon_0^2 h^2 \rho_0^2} \quad (6.42)$$

and so the allowed energies are (dropping the subscript):

$$E_n = -\frac{E_1}{n^2} \quad (6.43)$$

which is Bohrs formula, where $n \in \mathbb{N}$. We can also define the Bohr radius⁹ as follows:

$$a_0 = \frac{1}{\kappa} = \frac{4\pi \varepsilon_0 h^2}{m_r e^2} \quad (6.44)$$

Putting everything together we can formulate the radial part to find:

$$R_{nl}(r) = \frac{1}{r} \rho^{l+1} e^{-\rho} t(\rho) \quad (6.45)$$

where $t(\rho)$ can be written as an associated Laguerre polynomial $t(\rho) = L_{n-l-1}^{2l+1}(2\rho)$, which has the following form:

$$L_{q-p}^p(x) = (-1)^p \left(\frac{d}{dx} \right)^p L_q(x) \quad (6.46)$$

where $L_q(x)$ is the q^{th} Laguerre polynomial, generated by:

$$L_q(x) = e^x \left(\frac{d}{dx} \right)^q (e^{-x} x^q) \quad (6.47)$$

⁹The Bohr radius a_0 is not to be confused with a_0 in our series solution.

Thus we can now construct our full wave equation. We combine (6.10), (6.45) and (6.23) and normalise (6.45) so that our full wavefunction in terms of all quantum numbers is defined as [Gri05]:

$$\Psi_{nlm}(\mathbf{R}, \mathbf{r}) = \frac{e^{(i\mathbf{K}\cdot\mathbf{R})}}{\sqrt{V}} \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-l-1)!}{2n[(n+1)!]^2}} e^{-\left(\frac{|r|}{na_0}\right)} \left(\frac{2|r|}{na_0}\right)^l \left[L_{n-l-1}^{2l+1}\left(\frac{2|r|}{na_0}\right) \right] Y_{lm}(\theta, \phi) \quad (6.48)$$

6.4 The hydrogen atom in the momentum representation

There are several reasons why the hydrogen atom is not discussed in the momentum space representation at undergraduate level; firstly complexity and secondly the mathematical tools required have usually not been developed. On the surface the problem seems quite innocent, as we know that to change between the different representations all we have to do is perform a Fourier transform. Unfortunately the three dimensional Fourier transform is very challenging. Several methods for finding the wavefunction in the momentum representation are described in detail by Fock [Foc35], Lévy [Lev50], Podolsky and Pauling [PP29], and others [Ave86] [Lom80]. As the methods would require the introduction of many new mathematical concepts, which for purely spacial reasons could not be contained within this work, I will summarise the main concepts, leaving out the more technical details and only quoting results. Since we only require the ground state radial equation for our investigation, we shall only derive an expression for the radial solution in terms of the orbital quantum number n , ignoring the angular part. Also, as the ground state Fourier transform from the position to the momentum space is moderately straight forward, we shall also include it, in section 7.

6.5 The starting point

We begin by defining the Fourier transform between each space, in atomic units,¹⁰ as:

$$\Psi(\mathbf{r}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int d^3\mathbf{p} e^{i\mathbf{r}\cdot\mathbf{p}} \phi(\mathbf{p}) \quad (6.49)$$

$$\phi(\mathbf{p}) = \int d^3\mathbf{r} e^{-i\mathbf{r}\cdot\mathbf{p}} \Psi(\mathbf{r}) \quad (6.50)$$

where the wavefunction $\phi(\mathbf{p})$ satisfies the normalisation condition:

$$\int d^3\mathbf{p} |\phi(\mathbf{p})|^2 = 1 \quad (6.51)$$

if $\Psi(\mathbf{r})$ is normalised to unity. We next proceed to write the Schrödinger equation in the form of an integral equation in momentum space:

$$(p^2 - 2E)\phi(\mathbf{p}) = -2 \int d^3\mathbf{p}' \phi(\mathbf{p}') V'(\mathbf{p} - \mathbf{p}') \quad (6.52)$$

where $V'(\mathbf{p})$ is the Fourier transform of $V(\mathbf{r})$ multiplied by $(2\pi)^{-\frac{3}{2}}$ and we restrict ourselves to potentials $V(\mathbf{r})$ which are only dependent on the distance \mathbf{r} , i.e. central potentials. This implies that $V'(\mathbf{p})$ is a function of the absolute value of \mathbf{p} only and is real. It also means that (6.52) is separable in spherical polar co-ordinates and has solutions of the form:

$$\phi(\mathbf{p}) = F_l(p) Y_{lm}(\theta, \phi) \quad (6.53)$$

where l and m retain the same definitions as previously discussed. This means that (6.52) can be reduced to a one-dimensional integral equation for $F_l(p)$ of form:

$$(p^2 - 2E)F_l(p) = -\lambda \int_0^\infty dp' p'^2 K_l(p, p') F_l(p') \quad (6.54)$$

where:

$$\lambda K_l(p, p') = 4\pi \int_{-1}^1 dx V' \left(\sqrt{p^2 + p'^2 - 2pp'x} \right) P_l(x) \quad (6.55)$$

The kernel K_l is symmetric in p and p' and depends on the value of l and the shape of the potential $V(r)$. The strength of the potential is contained in λ ‘the potential strength’ parameter. We assume that the energy E is given and λ is the eigenvalue to be determined and we define $P_l(x)$ as the un-normalised Legendre function of the first kind.

¹⁰Atomic units for the momentum are in terms of the Bohr momentum $p_0 = \frac{\hbar}{a_0}$

6.6 The Coulomb potential

For the Coulomb potential we may write, $V(r)$ in the momentum space as:

$$V'(p) = -\frac{1}{2\pi^2 p^2} \quad (6.56)$$

Substituting (6.56) in to (6.52) we find:

$$(p^2 - 2E)\phi(\mathbf{p}) = \frac{1}{\pi^2} \int d^3\mathbf{p}' \frac{\phi(\mathbf{p}')}{|\mathbf{p} - \mathbf{p}'|^2} \quad (6.57)$$

we note that (6.57) has partial wave solutions of the form (6.53) and $F_l(p)$ satisfies (6.54).

Using the addition theorem of the spherical harmonics and the orthogonality properties of the Legendre polynomials [WG89], we can evaluate the kernel K_l explicitly to give:

$$(p^2 - 2E)F_l(p) = \frac{2}{p\pi} \int_0^\infty dp' p' Q_l\left(\frac{p^2 + p'^2}{2pp'}\right) F_l(p') \quad (6.58)$$

where Q_l is a Legendre polynomial of the second kind and is related to the un-normalisable Legendre function of the first kind, P_l , by:

$$Q_l(z) = \frac{1}{2} \int_{-1}^1 dt \frac{P_l(t)}{z - t} \quad (6.59)$$

6.7 The radial equation in momentum space

Since $E < 0$, (6.58) has solutions F_{nl} , for a discrete spectrum of energy eigenvalues E_n , which is the same spectrum that we saw previously for $n \in \mathbb{N}$. Fock was the first to directly solve (6.58) [Foc35] for wavefunctions normalised such that:

$$\int_0^\infty dp p^2 |F_{nl}(p)|^2 = 1 \quad (6.60)$$

where p is expressed in atomic units. Since we will be treating the Bohr radius as a parameter, it would be more appealing to have a radial equation in terms of physical units. Thus, it is found that the solution is [PP29]:

$$F_{nl}(p) = \left(\frac{1}{2^{\frac{1}{2}}}\right) \frac{\pi(na_0)^{\frac{3}{2}} 2^{2l+4} l!}{(\hbar)^{\frac{3}{2}} (2\pi)^{\frac{1}{2}}} \left(\frac{n(n-l-1)!}{(n+l)!}\right)^{\frac{1}{2}} \left(\frac{\left(\frac{na_0 p}{\hbar}\right)^l}{\left(\left(\frac{na_0 p}{\hbar}\right)^2 + 1\right)^{l+2}}\right) C_{n-l-1}^{l+1} \left(\frac{\left(\frac{na_0 p}{\hbar}\right)^2 - 1}{\left(\frac{na_0 p}{\hbar}\right)^2 + 1}\right) \quad (6.61)$$

where $C_{p-q}^q(x)$ is the Gegenbauer function¹¹. We can write this in a better form in terms of the wavevector $k = p$, with $\hbar = 1$ as:

$$F_{nl}(k) = \left(\frac{1}{2^{\frac{1}{2}}}\right) \frac{\pi(na_0)^{\frac{3}{2}} 2^{2l+4} l!}{(2\pi)^{\frac{1}{2}}} \left(\frac{n(n-l-1)!}{(n+l)!}\right)^{\frac{1}{2}} \left(\frac{(na_0k)^l}{((na_0k)^2 + 1)^{l+2}}\right) C_{n-l-1}^{l+1} \left(\frac{(na_0k)^2 - 1}{(na_0k)^2 + 1}\right) \quad (6.62)$$

7 Interaction has its part to play

As we have now fully discussed the electron-proton system we are finally in a position to move towards the more interesting aspects of this dissertation. This being the electron-proton entanglement in the hydrogen atom, which is caused by the electrostatic interaction between the electron and proton. To my knowledge, the idea of electron-proton entanglement was first discussed by Tommasini, Timmermans and Toledo Piza. They came to the conclusion that by finding the reduced state of the electron system, which is found by integrating over the proton position basis eigenfunctions, and then transforming this state in to the momentum representation, that they were able to show how the standard deviation of the momentum distribution becomes a measure of correlation (entanglement) between the electron and proton. They found [TTdTP98] that the stronger the correlation between the electron and proton, the greater the value of the Bohr radius a_0 , where a_0 is directly linked to the interaction. In this section however, we shall see that by using established measures for quantifying entanglement, the opposite conclusion is reached, that being as a_0 increases the amount of correlation between the electron and proton decreases. To some degree, it seems very strange to vary a fixed parameter, but in viewing parameters that are related to the strength of interaction as having some effect on entanglement, leads to some interesting results and questions.

¹¹For a summary of Gegenbauer functions, visit Mathworld.

7.1 The entanglement within the electron-proton system

This is an important point, because in looking at equation (6.48) we know that it is separable and so can be decomposed in to the product of other states i.e. our separable solutions. But in order to do this we had to perform a mathematical trick, we changed our physical co-ordinates to some fictitious co-ordinates based on the centre of mass and the relative distance between the electron and proton, which did not actually describe the physical system. If we write (6.48) more succinctly in terms of the fictitious co-ordinates we have:

$$\Psi_{nlm}(\mathbf{R}, \mathbf{r}) = \phi(\mathbf{r}) \frac{e^{(i\frac{\mathbf{P}}{\hbar} \cdot \mathbf{R})}}{\sqrt{V}} \quad (7.1)$$

We next insert our original definitions for the relative (6.2) and centre of mass (6.3) co-ordinates in to (7.1), from which we see the following:

$$\Psi_{nlm}(\mathbf{r}_e, \mathbf{r}_p) = \phi(\mathbf{r}_e - \mathbf{r}_p) \frac{e^{(i\frac{\mathbf{P}}{\hbar} \cdot \frac{[m_e \mathbf{r}_e + m_p \mathbf{r}_p]}{M})}}{\sqrt{V}} \quad (7.2)$$

which means that our relative wavefunction is no longer separable due to its dependence on the electron and proton co-ordinates, as we have exponential terms and linear terms in the relative part which are dependent on $|r_e - r_p|$, which is of course not separable. This means that it no longer has a solution that can be written in terms of separable functions and so by the definitions discussed in chapter two, is entangled.

7.2 The momentum wavefunction

In quantum mechanics, when we deal with an observable we need to find its spectral data, i.e. the eigenvalues and eigenvectors of the linear operator that represents it. This is because it is the spectrum that gives us a wealth of information, regarding the possible outcomes of the system and the associated probabilities of those outcomes. For this system, things are no different and it is found that the eigenvalues are the partial states of the electron system in momentum space, with eigenvectors that are plane waves. But why is this so? Well, the state that we are dealing with is a pure state, which means its spectrum simply consists of the eigenvalues 0 and 1. But this is quite problematic,

especially if we would like to calculate the Von-Neumann entanglement entropy (5.1), as the eigenvalues of a pure state would imply a Von-Neumann entanglement entropy of zero. This means that we gather no understanding or information about how entangled our state is, despite the fact that (7.2) is mathematically entangled. It is for this reason that we look at the partial states of a pure system, as they are mixed states, and mixed states have a varying spectrum.

With this in mind let us now show why the eigenvalues are represented by partial states in the momentum representation. We begin by using a homogenous state $\rho(\mathbf{r}-\mathbf{r}') = \rho(\mathbf{r}, \mathbf{r}')$, which means that the state remains unchanged via translations. Next we define the following Fourier transform:

$$\rho(\mathbf{r}-\mathbf{r}') = \frac{1}{(2\pi)^3} \int d^3\mathbf{k} \tilde{\rho}(\mathbf{k}) e^{i\mathbf{k}\cdot[\mathbf{r}-\mathbf{r}']} \quad (7.3)$$

where \mathbf{k} is the wave vector. The Fourier transform plays a dual role, it is proportional to the momentum distribution of the system and provides us with the spectral data of the density matrix [TTdTP98]. For the first assertion we evaluate the momentum expectation value $\langle \hat{\mathbf{p}} \rangle$ for a pure system, with respect to the quantum state $|\psi\rangle$:

$$\langle \hat{\mathbf{p}} \rangle = \langle \psi | \hat{\mathbf{p}} | \psi \rangle$$

we first use the completeness relation over the position basis:

$$\begin{aligned} &= \int d^3\mathbf{r} \int d^3\mathbf{r}' \langle \psi | \mathbf{r} \rangle \langle \mathbf{r} | \hat{\mathbf{p}} | \mathbf{r}' \rangle \langle \mathbf{r}' | \psi \rangle \\ &= \int d^3\mathbf{r} \int d^3\mathbf{r}' \langle \mathbf{r} | \hat{\mathbf{p}} | \mathbf{r}' \rangle \rho(\mathbf{r}, \mathbf{r}') \end{aligned}$$

we then use the following relation $\langle \mathbf{r} | \hat{\mathbf{p}} | \mathbf{r}' \rangle = -\delta(\mathbf{r}-\mathbf{r}') i\hbar \nabla_{\mathbf{r}}$, which comes from using the completeness relation over the momentum basis states to write:

$$\langle \hat{\mathbf{p}} \rangle = -i\hbar \int d^3\mathbf{r} \int d^3\mathbf{r}' \delta(\mathbf{r}-\mathbf{r}') \nabla_{\mathbf{r}} \rho(\mathbf{r}, \mathbf{r}')$$

using (7.3) we find:

$$\begin{aligned} &= \frac{1}{(2\pi)^3} \int d^3\mathbf{r} \int d^3\mathbf{r}' \delta(\mathbf{r}-\mathbf{r}') \int d^3\mathbf{k} \hbar \mathbf{k} \tilde{\rho}(\mathbf{k}) e^{i\mathbf{k}\cdot[\mathbf{r}-\mathbf{r}']} \\ &= \frac{V}{(2\pi)^3} \int d^3\mathbf{k} \hbar \mathbf{k} \tilde{\rho}(\mathbf{k}) \end{aligned} \quad (7.4)$$

where the momentum is equal to $\mathbf{p} = \hbar\mathbf{k}$, which means $\tilde{\rho}(\mathbf{k})$ is a function of momentum $f(\mathbf{p})$, thus we acquire the first moment and a way to construct higher order moments. Thus the Fourier transform is proportional to the momentum distribution of the system. The volume V has been introduced as a large quantisation volume to avoid problems related to states of an infinite norm, also known as density of states or box normalisation. The fact that this acts as a distribution function means that we can define the standard deviation of the momentum distribution as follows:

$$\Delta\mathbf{p} = \sqrt{\langle\hat{\mathbf{p}}^2\rangle - \langle\hat{\mathbf{p}}\rangle^2} \quad (7.5)$$

In the paper [TTdTP98] they work in the centre of mass frame which means $\langle\hat{\mathbf{p}}\rangle^2 = 0$ and so we can use (7.4) and (7.5) to find that:

$$\Delta\mathbf{p} = \sqrt{\int d^3\mathbf{p} \mathbf{p}^2 f(\mathbf{p})} \quad (7.6)$$

In [TTdTP98] it is calculated that $\Delta\mathbf{p} = \frac{\hbar}{a_0}$.

We next see how the Fourier transform provides us with the spectral data. We begin with the following:

$$\int d^3\mathbf{r}' \rho(\mathbf{r} - \mathbf{r}') \frac{e^{i\mathbf{k}\cdot\mathbf{r}'}}{\sqrt{V}} =$$

then using (7.3) we write:

$$\begin{aligned} &= \frac{1}{(2\pi)^3} \int d^3\mathbf{k}' \tilde{\rho}(\mathbf{k}') \frac{e^{i\mathbf{k}'\cdot\mathbf{r}}}{\sqrt{V}} \int d^3\mathbf{r}' e^{i[\mathbf{k}-\mathbf{k}']\cdot\mathbf{r}'} \\ &= \tilde{\rho}(\mathbf{k}) \frac{e^{i\mathbf{k}\cdot\mathbf{r}}}{\sqrt{V}} \end{aligned} \quad (7.7)$$

which is precisely the eigenvalue equation seen in chapter one, although structurally it looks a little different. This is because for a given reduced density matrix we may write the eigenvalue equation as follows:

$$\sum_k \rho_{ik}^e U_{kl} = \lambda_l U_{il} \quad (7.8)$$

This is because for a bipartite state the reduced density matrices have the same eigenvalues, but different eigenkets (see Schmidt decomposition chapter two). The superscript e

represents which partial state we are dealing with and the unitary matrix U_{kl} enables us to diagonalise ρ^e , which is in the basis $|\mathbf{r}_{e_i}\rangle$.

There are two things to notice when comparing (7.7) and (7.8). First, one is continuous and the other is discrete, we will address this issue later. Second, a pure state has eigenvalues $\tilde{\rho}(\mathbf{k}_i) = 1$ for $j = i$ and $\tilde{\rho}(\mathbf{k}_j) = 0$ for all $j \neq i$, which implies the eigenstates are $\langle \mathbf{r} | \Psi \rangle = \frac{e^{i\mathbf{k}_i \cdot \mathbf{r}}}{\sqrt{V}}$. But, this represents a particle with definite momentum, i.e zero standard deviation. This adds to the reason for requiring a mixed state, as a mixed state has a varied spectrum $\tilde{\rho}(\mathbf{k}_j)$, thus a non-zero standard deviation. It is for this reason that Tommasini, Timmermans and Toledo Piza [TTdTP98] assume that the standard deviation may be interpreted as a measure of correlation. This of course ultimately leads to them, and now us, viewing the Bohr radius a_0 as a correlation parameter.

Returning back to the first point, in order convert between continuous and discrete spaces we will require the idea of density of states, to ensure the the trace of the density matrix remains set to unity. We can summarise this idea as follows:

$$1 = \int d^3\mathbf{r} \rho(0) = \rho(0)V = \frac{V}{(2\pi)^3} \int d^3\mathbf{k} \tilde{\rho}(\mathbf{k}) \rightarrow \sum_{\mathbf{k}} \tilde{\rho}(\mathbf{k}) \quad (7.9)$$

and so in using any trace formulas in the continuous spectrum we will have to integrate over the whole spectrum and we shall acquire a factor of $(\frac{L}{2\pi})^d$ which is dependent on the dimension, d , of the system.

7.3 Quantifying the entanglement in the hydrogen atom

Now that the background and understanding have been put in place, we may now proceed to use the ground state wavefunction in the momentum representation, to calculate first the density state of the whole system and second, the partial state for the electron subsystem. Once this is completed, we can then quantify the entanglement in the system as a function of the Bohr radius, using our chosen entanglement measures.

In the position representation the density state for the hydrogen atom is given as:

$$\rho(\mathbf{r}, \mathbf{r}') = |\Psi_{nlm}\rangle\langle\Psi_{nlm}| = \Psi_{nlm}(\mathbf{r}_e, \mathbf{r}_p)\Psi_{nlm}^*(\mathbf{r}'_e, \mathbf{r}_p) \quad (7.10)$$

and so we can extract our partial state, by integrating over the proton basis set of co-ordinate eigenfunctions:

$$\begin{aligned} \rho(\mathbf{r}_e, \mathbf{r}'_e) &= \int d^3\mathbf{r}_p \Psi_{nlm}(\mathbf{r}_e, \mathbf{r}_p)\Psi_{nlm}^*(\mathbf{r}'_e, \mathbf{r}_p) \\ &= \frac{e^{(-\frac{im_e\mathbf{P}}{\hbar M}\cdot[\mathbf{r}_e-\mathbf{r}'_e])}}{V} \int d^3\mathbf{r}_p \phi_e(\mathbf{r}_e - \mathbf{r}_p)\phi_e^*(\mathbf{r}'_e - \mathbf{r}_p) \\ &= \frac{e^{(-\frac{im_e\mathbf{P}}{\hbar M}\cdot[\mathbf{r}_e-\mathbf{r}'_e])}}{V} \rho_e(\mathbf{r}_e, \mathbf{r}'_e) \end{aligned} \quad (7.11)$$

where ρ_e simply represents the electron density matrix for electrons in atoms at rest, i.e. $\mathbf{P} = 0$ and so $\rho(\mathbf{r}_e, \mathbf{r}'_e) = \rho_e(\mathbf{r}_e, \mathbf{r}'_e)$. Thus we can now calculate the electron density state in the electron co-ordinate basis by setting $n = 1$ and $l = m = 0$ in (7.11) to get the ground state wavefunction. But, as we discussed earlier we require the density state in the momentum representation. In order to do this we must Fourier transform (7.10) in to the momentum space:

$$\begin{aligned} V\rho_e(\mathbf{r}_e, \mathbf{r}'_e) &= \int d^3\mathbf{r}_p \frac{1}{(2\pi)^6} \int d^3\mathbf{k} \phi_e(\mathbf{k}) e^{i\mathbf{k}\cdot[\mathbf{r}_e-\mathbf{r}_p]} \int d^3\mathbf{k}' \phi_e^*(\mathbf{k}') e^{-i\mathbf{k}'\cdot[\mathbf{r}'_e-\mathbf{r}_p]} \\ &= \frac{1}{(2\pi)^3} \int d^3\mathbf{k} \int d^3\mathbf{k}' \phi_e(\mathbf{k}) \phi_e^*(\mathbf{k}') e^{i\mathbf{k}\cdot\mathbf{r}_e - i\mathbf{k}'\cdot\mathbf{r}'_e} \frac{1}{(2\pi)^3} \int d^3\mathbf{r}_p e^{i\mathbf{r}_p\cdot(\mathbf{k}'-\mathbf{k})} \end{aligned}$$

since the last integral is simply the Fourier transform of the dirac delta function, we have:

$$\begin{aligned} &= \frac{1}{(2\pi)^3} \int d^3\mathbf{k} \int d^3\mathbf{k}' \phi_e(\mathbf{k}) \phi_e^*(\mathbf{k}') e^{i\mathbf{k}\cdot\mathbf{r}_e - i\mathbf{k}'\cdot\mathbf{r}'_e} \delta(\mathbf{k}' - \mathbf{k}) \\ &= \frac{1}{(2\pi)^3} \int d^3\mathbf{k} |\phi_e(\mathbf{k})|^2 e^{i\mathbf{k}\cdot[\mathbf{r}_e-\mathbf{r}'_e]} \end{aligned}$$

therefore:

$$\tilde{\rho}_e(\mathbf{k}) = \frac{|\phi_e(\mathbf{k})|^2}{V} \quad (7.12)$$

which means we require the wavefunction in the momentum representation. This we find by using (6.62):

$$\begin{aligned} F_{10}(\mathbf{k}) &= \frac{2^4}{2} \frac{\pi}{\sqrt{\pi}} (a_0)^{\frac{3}{2}} \frac{1}{((a_0k)^2 + 1)^2} 1 \\ &= \frac{(2^2 a_0 \pi^{\frac{1}{3}})^{\frac{3}{2}}}{((a_0\mathbf{k})^2 + 1)^2} \end{aligned} \quad (7.13)$$

As we said we would do, we shall also calculate this expression via a direct Fourier transform of the ground state. To do this we first choose to Fourier transform the following momentum space wavefunction $\phi(\mathbf{p}) = \frac{1}{\sqrt{\pi}}e^{-\mathbf{p}}$ which can be performed by using (6.49)¹². We can then relate this to a general position wavefunction as follows:

$$(2\pi)^{\frac{3}{2}}\Phi(\mathbf{r}) = \frac{8\pi}{(1+r^2)^2} \quad (7.14)$$

which we can then use to compare to the ground state position wavefunction:

$$\begin{aligned} \phi_e(\mathbf{k}) &= \int d^3\mathbf{r} \phi_{100e}(\mathbf{r}) e^{-i\mathbf{k}\cdot\mathbf{r}} \\ &= \int d^3\mathbf{r} \frac{1}{\sqrt{\pi}} \left(\frac{1}{(a_0)^{\frac{3}{2}}} \right) e^{\frac{|\mathbf{r}|}{a_0}} e^{-i\mathbf{k}\cdot\mathbf{r}} \end{aligned} \quad (7.15)$$

making the following substitution $\frac{\mathbf{r}}{a_0} = \mathbf{R}$ allows us to write:

$$\begin{aligned} &= \frac{(a_0)^{\frac{3}{2}}}{\sqrt{\pi}} \int d^3\mathbf{R} e^{-\mathbf{R}} e^{-ia_0\mathbf{k}\cdot\mathbf{R}} \\ &= \frac{(a_0)^{\frac{3}{2}}}{\sqrt{\pi}} \frac{8\pi}{((a_0\mathbf{k})^2 + 1)^2} \end{aligned} \quad (7.16)$$

which is precisely (7.13). Now that we have the ground state in the momentum space representation, we can calculate the electron density state by using (7.12):

$$\tilde{\rho}_e(\mathbf{k}) = \frac{(a_0)^3 64\pi}{((a_0\mathbf{k})^2 + 1)^4} \frac{1}{V} \quad (7.17)$$

Thus, we are finally in a position to calculate our first entanglement measure, the Von-Neumann entanglement entropy. However, before we calculate it we must tread carefully, as we refer back to the point that the spectrum in our case is continuous. So, when we calculate the Von-Neumann entanglement entropy, which will have to be transformed in to the continuous spectrum, we must ensure that we apply the density of states procedure by using (7.9). Recalling that the Von-Neumann entanglement entropy is given by:

$$S_e = \sum_{\mathbf{k}} \tilde{\rho}_e(\mathbf{k}) \ln(\tilde{\rho}_e(\mathbf{k}))$$

¹²See appendix C for more details

and so in applying the density of states procedure $\sum_{\mathbf{k}} \rightarrow \frac{V}{(2\pi)^3} \int d^3\mathbf{k}$ transforms the measure to:

$$= -\frac{V}{(2\pi)^3} \int d^3\mathbf{k} \tilde{\rho}_e(\mathbf{k}) \ln(\rho(\mathbf{k})) \quad (7.18)$$

Thus, we can now calculate the entanglement entropy:

$$= -\frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} d^3\mathbf{k} \frac{64\pi a_0^3}{(1+a_0^2 k^2)^4} \ln\left(\frac{64\pi a_0^3}{V(1+a_0^2 k^2)^4}\right)$$

we can convert this integral in to spherical co-ordinates to give:

$$= -\frac{1}{(2\pi)^3} \int_0^{\infty} dk \frac{k^2 256\pi^2 a_0^3}{(1+a_0^2 k^2)^4} \ln\left(\frac{64\pi a_0^3}{V(1+a_0^2 k^2)^4}\right) \quad (7.19)$$

To make our lives simpler we notice that if we group the following terms in the logarithm such that $\ln\left(\frac{64\pi a_0^3}{V} \frac{1}{1+(a_0^2 k^2)^4}\right)$ then we can actually apply the logarithm rule $\ln(AB) = \ln(A) + \ln(B)$, as the dimensions in each part are dimensionless, i.e for $A = \frac{64\pi a_0^3}{V} \rightarrow [A] = L^3 L^{-3} = []$, which is also true for B as $[k] = L^{-1}$. Thus we have the following integrals to solve:

$$I_1 = -\frac{1}{(2\pi)^3} \int_0^{\infty} dk \frac{k^2 256\pi^2 a_0^3}{(1+a_0^2 k^2)^4} \ln\left(\frac{64\pi a_0^3}{V}\right) \quad (7.20)$$

$$I_2 = \frac{1}{(2\pi)^3} \int_0^{\infty} dk \frac{k^2 256\pi^2 a_0^3}{(1+a_0^2 k^2)^4} 4 \ln(1+a_0^2 k^2) \quad (7.21)$$

We begin by first tackling I_1 , for which we see that we must solve an integral of the form:

$$I_Q = \left[\frac{k}{(1+a_0^2 k^2)^2} \right]^2 a_0^3$$

We can evaluate this integral through several different substitutions. Our first substitution is chosen to be $u = a_0 k$, which gets rid of a_0 in I_Q . Since we have a term $1+u^2$ we try a hyperbolic function and so let $\sinh(x) = u$. The limits remain the same and our integral reduces to the following:

$$I_Q = \int dx \tanh^2(x) \operatorname{sech}^5(x) \quad (7.22)$$

we next use the substitution $y = \tanh(x)$ together with the relation $\operatorname{sech}^2(x) = 1 - \tanh^2(x)$, this time the integration limits do change $\infty \rightarrow 1$ ¹³ and 0 remains 0, thus we

¹³Technically we mean $\lim_{x \rightarrow \infty} \tanh(x) = 1$.

can write:

$$I_Q = \int_0^1 dy y^2 (1 - y^2)^{\frac{3}{2}} \quad (7.23)$$

which has the solution:

$$= \left[\frac{1}{48} (y \sqrt{(1 - y^2)} (-3 + 14y^2 - 8y^4) + 3 \arcsin(y)) \right]_0^1 \quad (7.24)$$

$$I_Q = \frac{\pi}{32} \quad (7.25)$$

which means after cancellations that I_1 is equal to:

$$\begin{aligned} I_1 &= -\ln\left(\frac{64\pi a_0^3}{V}\right) \\ &= \ln\left(\frac{V}{64\pi a_0^3}\right) \end{aligned} \quad (7.26)$$

as all factors cancel. Moving now to I_2 we want to solve an integral of the form:

$$I_U = \left[\frac{k}{(1 + a_0^2 k^2)^2} \right]^2 a_0^3 \ln(1 + a_0^2 k^2) \quad (7.27)$$

using similar substitutions to our first integral we find:

$$I_U = \frac{1}{192} \pi (-5 + \ln(2^{12})) \quad (7.28)$$

therefore after cancellations:

$$I_2 = \ln(2^8) - \frac{10}{3} \quad (7.29)$$

and so the Von-Neumann entanglement entropy is found to be:

$$S_e = \ln\left(\frac{16V}{3V_0}\right) - \frac{10}{3} \quad (7.30)$$

where $V_0 = \frac{4\pi a_0^3}{3}$ is the volume dependent on the size of the Bohr radius.

Now that we have a complete expression for the Von-Neumann entanglement entropy, which is dependent on the Bohr radius a_0 and some finite volume V , we can plot it as a function of a_0 , see fig. 2. Although, it does seem rather strange to treat the Bohr radius

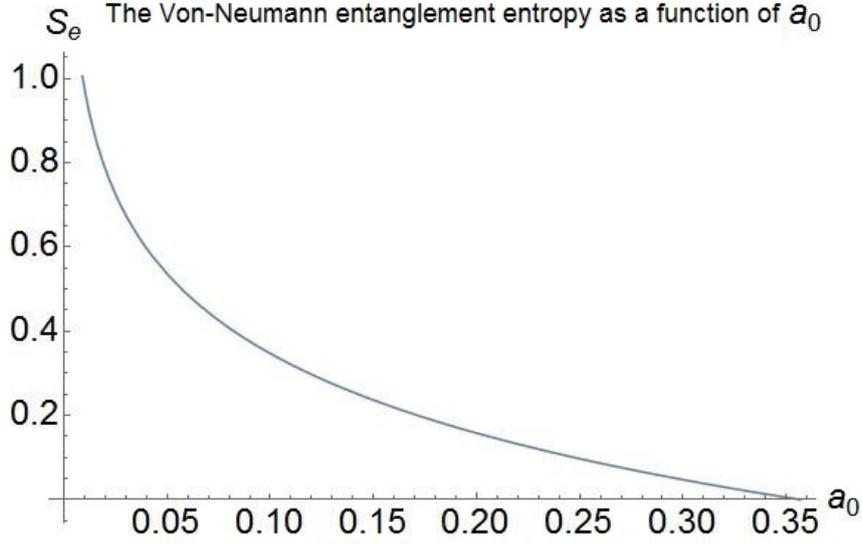


Figure 2: A plot of the entanglement entropy of the electron-proton system as a function of the Bohr radius a_0 . As the volume V is arbitrary, we have set it to unity.

as some kind of entanglement parameter, it does show something very interesting. First we see that the electron and proton are most entangled at the most probable distance between them in the ground state, i.e. $a_0 = 0.0529 * 10^{-9}$, which we should expect. But as the distance between the two increases, we see that the entanglement between them becomes weaker. This is because as the distance increases between the electron and proton, the electrostatic forces decrease in magnitude. This implies that in this particular case of entanglement, that the interaction between the electron and proton is the driving force for the creation of entanglement.

We shall now calculate our second chosen measure of entanglement, the linear entropy (5.3). As discussed previously the linear entropy is closely related to the Von-Neumann entanglement entropy, in terms of our reduced state we write:

$$S_e^L = 1 - Tr(\rho_e^2)$$

As before we convert the system from a discrete spectrum to a continuous using the

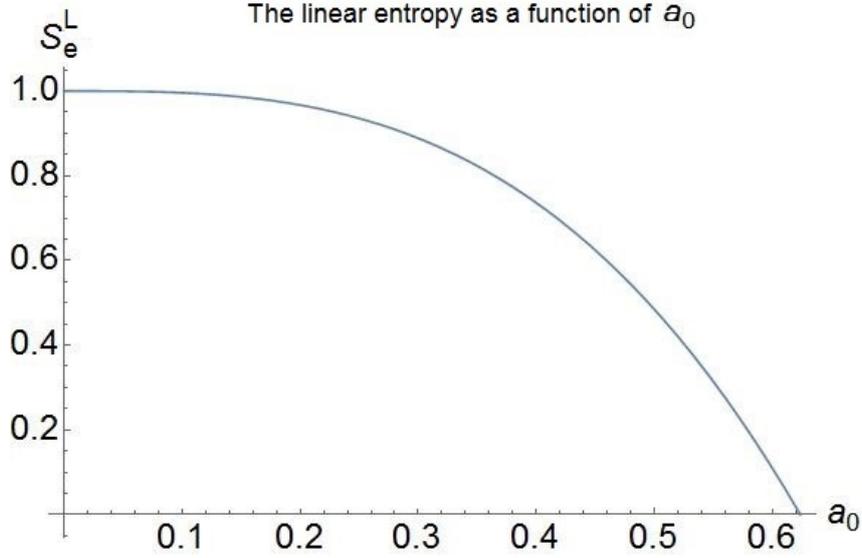


Figure 3: A plot of the linear entropy of the electron-proton system as a function of a_0 . Since the volume is arbitrary again, it is chosen to be unit.

density of states:

$$= 1 - \frac{V}{(2\pi)^3} \int_{-\infty}^{\infty} d^3\mathbf{k} \frac{(64\pi a_0^3)^2}{V^2(1 + a_0^2 k^2)^8}$$

Converting to spherical co-ordinates:

$$= 1 - \frac{1}{(2\pi)^3} \int_0^{\infty} dk \frac{k^2 4\pi (64\pi a_0^3)^2}{V(1 + a_0^2 k^2)^8}$$

using very similar substitutions to the integrals we evaluated for the Von-Neumann entanglement entropy we find:

$$S_e^L = 1 - \frac{33}{8} \frac{(a_0)^3}{V} \quad (7.31)$$

Having an expression for the linear entropy allows us to plot it as a function of a_0 fig. 3. Although the starting and end points of the linear entropy plot (fig. 3) are almost exact to the Von-Neumann entanglement entropy plot (fig. 2), the curvature of the graphs is very different and this means some caution is needed in its interpretation. If the linear entropy were to be taken as our only entanglement measure, it would tell us that the electron-proton system not only remains highly entangled for smaller distances of a_0 , but

it remains entangled for a larger range of a_0 . Where as we see for the Von-Neumann entanglement entropy fig. 2, that the strength of entanglement decays much quicker. It is interesting to see how two entanglement measures can give quite different answers about how correlated the electron and proton are. It would be nice if there were many other entanglement measures that we could compare it to, but for this type of pure bipartite system we are limited. So what can we definitely say about entanglement in this system? Well, both measures agree that the state is indeed entangled and both also agree that the electron and proton are most strongly correlated at the well known value of the Bohr radius in the ground state $a_0 = 0.0529 \times 10^{-9}$. Although the curves are different, both measures still decrease as the strength of the interaction also decreases and so we see a direct link between interaction and entanglement.

8 A system of two coupled quantum particles

We now progress onwards to a different physical system, a toy model of two coupled bosonic particles, whose interaction is determined by a quadratic potential, with coupling constant (our entanglement parameter) κ . This system is essentially that of two coupled harmonic oscillators in one-dimension. We shall see that this system again has a Hamiltonian, that although originally correlated, can be written in the form of two uncorrelated Hamiltonians after some fictitious co-ordinate transform. We see that our uncorrelated internal Hamiltonian is precisely the Hamiltonian governing the one dimensional quantum harmonic oscillator and so can be solved accordingly. The Hamiltonian at the centre of mass will have the same plane wave solution as before, with the box normalisation scheme and is one-dimensional. We then carry out the same analysis as that of the electron-proton system, except this time we have a different coupling in the wavefunction and a different entanglement parameter κ .

8.1 The coupled quantum particles

For this system we introduce an entanglement parameter κ , which is typically a measure of the coupling between two particles A and B . In using this parameter we shall proceed with a similar analysis to that of the electron-proton system, by calculating the reduced density matrix of one system in the momentum representation and investigate what happens to our entanglement measures as κ is varied .

To begin we require our equations of motion, which are contained within our Hamiltonian operator. Once we have written down our Hamiltonian operator we can then proceed to use Schrödinger's equation to calculate the wavefunction for this system. We begin by assuming we have two quantum particles A and B , which are connected by a quantum coupling (see fig.4), where the strength of the coupling is given by κ . The Hamiltonian will be very similar to the hydrogen atom, except this time we will have a different potential to describe a different interaction. Therefore we write:

$$\hat{H} = \frac{\hat{p}_a^2}{2m_a} + \frac{\hat{p}_b^2}{2m_b} + \frac{1}{2}m_x\kappa^2(x_a - x_b)^2 \quad (8.1)$$

we should also have the additional term $\frac{k}{2}(x_a^2 + x_b^2)$, but we have set $k = 0$. We can then use the methods presented in the electron-proton system to write the Hamiltonian in terms of the the internal Hamiltonian, which is dependent on the relative co-ordinate and governs the interaction and the Hamiltonian at the centre of mass:

$$\hat{H} = \frac{\hat{p}_R^2}{2M} + \frac{\hat{p}_r^2}{2m_x} + \frac{1}{2}m_x\kappa^2r^2 \quad (8.2)$$

where $r = x_a - x_b$ is the relative distance between our quantum particles, κ is our entanglement parameter, R represents the centre of mass co-ordinate, with respect to particle A of mass m_a and particle B of mass m_b . We also introduce the quantity m_x , which is analogues to the reduced mass m_r , except $e \rightarrow a$, $p \rightarrow b$ and we set $m_a = m_b$. Carrying out a similar analysis to before, we know that this Hamiltonian has separable solutions of the form:

$$\Phi(R, r) = \chi(R)\psi(r) \quad (8.3)$$

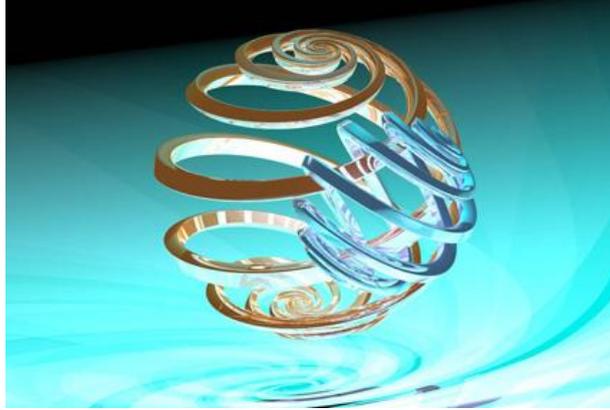


Figure 4: An artists impression of two coupled quantum particles[Sim11].

As we already know that the centre of mass Hamiltonian will just have plane wave solutions, we can go straight to finding the relative wavefunction $\psi(r)$, which is given by:

$$\frac{1}{2m_x} \left[\hat{p}_r^2 + \kappa^2 m_x^2 r^2 \right] \psi(r) = E \psi(r) \quad (8.4)$$

This of course is precisely the equation for a one dimensional quantum harmonic oscillator, which can be solved directly using ladder operators, a treatment first introduced by Dirac. We first introduce two operators, one to destroy and one to create, we define these operators as:

$$\hat{a} = \sqrt{\frac{1}{2\hbar m_x \kappa}} (m_x \kappa \hat{r} + i \hat{p}) \quad (8.5)$$

$$\hat{a}^\dagger = \sqrt{\frac{1}{2\hbar m_x \kappa}} (m_x \kappa \hat{r} - i \hat{p}) \quad (8.6)$$

where \dagger represents the self-adjoint (our creation operator). We then notice the following relations:

$$\hat{a}^\dagger \hat{a} = \frac{1}{2\hbar m_x \kappa} \left[(m_x \kappa \hat{r})^2 - i m_x \kappa [\hat{r}, \hat{p}] + \hat{p}^2 \right] = \frac{\hat{H}}{\hbar \kappa} - \frac{1}{2} \quad (8.7)$$

$$(8.8)$$

likewise the product $\hat{a} \hat{a}^\dagger$ is equal to:

$$\hat{a} \hat{a}^\dagger = \frac{\hat{H}}{\hbar \kappa} + \frac{1}{2} \quad (8.9)$$

combining both expressions together we see the following:

$$[\hat{a}, \hat{a}^\dagger] = 1 \quad (8.10)$$

We next introduce an hermitian operator, the number operator $\hat{N} = \hat{a}^\dagger \hat{a}$, which acts on a eigenket $|n\rangle$ to produce a real eigenvalue n , that represents an observable. The number operator allows us to write the Hamiltonian \hat{H} in the following way:

$$\hat{H} = \hbar\kappa(\hat{N} + \frac{1}{2}) \quad (8.11)$$

Therefore, upon applying the Hamiltonian operator to the number ket we find an expression for the discrete energy levels:

$$\hat{H} |n\rangle = E |n\rangle = \hbar\kappa(n + \frac{1}{2}) |n\rangle \quad (8.12)$$

which implies $E = \hbar\kappa(n + \frac{1}{2})$ and so the ground state $|0\rangle$ has energy $E_0 = \frac{\hbar\kappa}{2}$ i.e. everything is always moving. But what exactly is the ground state wavefunction for the quantum harmonic oscillator? It is identified as finding the state for which $\hat{a}|0\rangle = 0$. We can express this in the co-ordinate basis as follows:

$$\langle r' | \hat{a} | r \rangle = \delta(r - r') \frac{1}{\sqrt{2\hbar m_x \kappa}} \left(m_x \kappa r' + \hbar \frac{\partial}{\partial r'} \right)$$

where the ground state is defined as $\langle r | 0 \rangle = \psi_0(r)$, and we can use the completeness relation $\int dr |r\rangle \langle r| = \mathbb{I}$ to see the following:

$$\langle r | \hat{a} | 0 \rangle = 0 = \int dr \langle r | \hat{a} | r' \rangle \langle r' | 0 \rangle = \left(m_x \kappa r + \hbar \frac{\partial}{\partial r} \right) \psi_0(r)$$

which means we have to solve a simple separable first order differential equation:

$$\left(m_x \kappa r + \hbar \frac{\partial}{\partial r} \right) \psi_0(r) = 0 \quad (8.13)$$

solving this we find that our ground state is:

$$\psi_0(r) = \langle r | 0 \rangle = C e^{-r^2 \frac{m_x \kappa}{2\hbar}} \quad (8.14)$$

In order to ensure that our ground state is normalised we enforce the condition :

$$\int_{-\infty}^{\infty} dr \psi_0^*(r) \psi_0(r') = \delta(r - r') \quad (8.15)$$

which after a simple calculation of a Gaussian integral gives us the following normalisation constant:

$$C = \left(\frac{m_x \kappa}{\hbar \pi} \right)^{\frac{1}{4}}$$

thus the ground state wavefunction is:

$$\psi_0(r) = \langle r|0\rangle = \left(\frac{m_x \kappa}{\hbar \pi} \right)^{\frac{1}{4}} e^{(-r^2 \frac{m_x \kappa}{2\hbar})} \quad (8.16)$$

The nice property of Dirac's method, is that in order to generate higher states, we simply act on the ground state with the creation operator \hat{a}^\dagger . From this we find the normalised excited state wavefunctions are as follows :

$$\psi_n(r) = \langle r|n\rangle = \sqrt{\frac{1}{2^n n!}} \left(\frac{m_x \kappa}{\pi \hbar} \right)^{\frac{1}{4}} e^{(-\frac{m_x \kappa r^2}{2\hbar})} H_n \left(\frac{m_x \kappa}{\hbar} r \right) \quad (8.17)$$

where the functions $H_n(x)$ are the Hermite polynomials defined as:

$$H_n(x) = (-1)^n e^{x^2} \frac{d^n}{dx} (e^{-x^2}) \quad (8.18)$$

and any number ket $|n\rangle$, may be generated from the ground state as follows:

$$|n\rangle = \frac{(\hat{a}^\dagger)^n}{\sqrt{n!}} |0\rangle \quad (8.19)$$

Thus our complete wavefunction for the one dimensional harmonic oscillator is:

$$\Phi(R, r) = \frac{1}{\sqrt{L}} e^{(i\frac{p}{\hbar}R)} \sqrt{\frac{1}{2^n n!}} \left(\frac{m_x \kappa}{\pi \hbar} \right)^{\frac{1}{4}} e^{(-\frac{m_x \kappa r^2}{2\hbar})} H_n \left(\frac{m_x \kappa}{\hbar} r \right) \quad (8.20)$$

where $k = \frac{p}{\hbar}$. If we insert our original definitions for r and R back in to (8.20) then we find that we have a non-separable entangled state of the form:

$$\Phi(x_a, x_b) = \frac{1}{\sqrt{L}} e^{iK \left(\frac{m_a x_a + m_b x_b}{m_a + m_b} \right)} \psi(x_a - x_b) \quad (8.21)$$

This is due to the fact that in the exponential we have the term $(x_a - x_b)^2 = x_a^2 + x_b^2 - 2x_a x_b$, where the last term of the expansion is of course not separable in the exponential, thus creating our entangled state. In the case of the hydrogen atom we had the modulus $\mathbf{r} = |\mathbf{r}_e - \mathbf{r}_p|$, which of course is not separable either in the exponential. Of course this is very interesting from a mathematical perspective as there are quite a few systems with potentials of this form, when solved via the Schrödinger equation, give rise to this behaviour in the exponential term. Although whether or not this is truly entanglement or just clever mathematical manipulation, is of course debatable.

8.2 Quantifying the entanglement for the quadratic potential

Since most of the ideas have already been established in the previous example, we can easily move from step to step, quickly calculating the quantities that we require. In order to quantify entanglement in this system, we must first proceed with step one, finding the spectrum i.e. the partial state of system A in momentum space. We can do this by either finding the ground state wavefunction in the momentum space and continuing accordingly, or we can calculate the reduced density matrix for system A in the position space and then Fourier transform in to the momentum space using (6.50). Once we have the partial state for system A in the momentum representation we can then evaluate our entanglement measures.

Taking the latter approach we can write the partial state of system A in the position representation by integrating over system B 's basis set of coordinate eigenfunctions¹⁴:

$$\begin{aligned}\rho(x_a, x'_a) &= \frac{1}{L} \int dx_b \psi_0(x_a - x_b) \psi_0^*(x'_a - x_b) \\ &= \frac{1}{L} \int dx_b \left(\frac{2\tilde{\kappa}}{\hbar\pi} \right)^{\frac{1}{2}} e^{-[(x_a - x_b)^2 - (x'_a - x_b)^2] \frac{\tilde{\kappa}}{\hbar}}\end{aligned}$$

let $y = x'_a - x_b$, which means the limits would be from ∞ to $-\infty$ and so to flip this we induce another minus sign, which cancels the minus sign we get from the Jacobi factor:

$$\rho(x_a, x'_a) = \frac{1}{L} \left(\frac{2\tilde{\kappa}}{\hbar\pi} \right)^{\frac{1}{2}} e^{-((x_a - x'_a)^2 \frac{\tilde{\kappa}}{\hbar})} \int dy e^{-(2y^2 + 2y(x_a - x'_a)) \frac{\tilde{\kappa}}{\hbar}}$$

in completing the square and making the substitution $\tilde{y} = \sqrt{2\frac{\tilde{\kappa}}{\hbar}}(y + \frac{(x_a - x'_a)}{2})$ we can make the integral of Gaussian form to find that the reduced state is:

$$\rho_A(x_a, x'_a) = \frac{1}{L} e^{-((x_a - x'_a)^2 \frac{\tilde{\kappa}}{2\hbar})} \quad (8.22)$$

We next Fourier transform our reduced state for system A in to the momentum space, which we do by first defining the co-ordinate $r_a = x_a - x'_a$:

$$\tilde{\rho}_A(k) = \frac{1}{L} \int dr_a e^{-ikr_a} e^{-\left(\frac{r_a^2 \tilde{\kappa}}{2\hbar}\right)} \quad (8.23)$$

¹⁴We set $\tilde{\kappa} = \frac{1}{2}m_x\kappa$.

¹⁵The centre of mass momentum has been set to $P = \hbar K = 0$.

scaling r_a with $\tilde{r}_a = \sqrt{\frac{\tilde{\kappa}}{2\hbar}} r_a$ leaves us with:

$$= \frac{1}{L} \sqrt{\frac{2\hbar}{\tilde{\kappa}}} \int d\tilde{r}_a e^{-\left(\tilde{r}_a^2 + i\sqrt{\frac{2\hbar}{\tilde{\kappa}}} \tilde{r}_a^2 k\right)}$$

completing the square and making the substitution $y = \left(\tilde{r}_a + \frac{i}{2}\sqrt{\frac{2\hbar}{\tilde{\kappa}}} k\right)$ converts the integral in to Gaussian form:

$$\tilde{\rho}_A(k) = \frac{1}{L} \sqrt{\frac{2\hbar}{\tilde{\kappa}}} e^{-k^2 \left(\frac{2\hbar}{4\tilde{\kappa}}\right)} \int_{-\infty}^{\infty} dy e^{-y^2}$$

and so the partial state for system A in the momentum space is:

$$\tilde{\rho}_A(k) = \frac{1}{L} \sqrt{\frac{2\pi\hbar}{\tilde{\kappa}}} e^{-k^2 \left(\frac{\hbar}{2\tilde{\kappa}}\right)} \quad (8.24)$$

Now that we have the partial state of system A we can calculate the first of our entanglement measures, the Von-Neumann entanglement entropy. Setting $\hbar = 1$ and remembering to include a factor of $\left(\frac{L}{2\pi}\right)$ due to the density of states, we write:

$$S_A = - \left(\frac{L}{2\pi}\right) \int_{-\infty}^{\infty} dk \frac{1}{L} \left(\frac{2\pi}{\tilde{\kappa}}\right)^{\frac{1}{2}} e^{-k^2 \left(\frac{1}{2\tilde{\kappa}}\right)} \ln \left(\left(\frac{2\pi}{L^2 \tilde{\kappa}}\right)^{\frac{1}{2}} e^{-k^2 \left(\frac{1}{2\tilde{\kappa}}\right)} \right) \quad (8.25)$$

we next write the logarithm in the following way $\frac{1}{2} \ln \left(\frac{2\pi}{L^2 \tilde{\kappa}}\right) - k^2 \left(\frac{1}{2\tilde{\kappa}}\right)$. We can only do this as the dimensions in each part are dimensionless, for example the dimensions in the first part, remembering that $\hbar = 1$, are $[\] = \frac{[ML^2T^{-1}]}{[L^2MT^{-1}]}$ and likewise for the second part. Therefore we have two separate integrals:

$$I_1 = - \int_{-\infty}^{\infty} dk \frac{1}{4\pi} \left(\frac{2\pi}{\tilde{\kappa}}\right)^{\frac{1}{2}} e^{-k^2 \left(\frac{1}{2\tilde{\kappa}}\right)} \ln \left(\frac{2\pi}{L^2 \tilde{\kappa}}\right) \quad (8.26)$$

$$I_2 = \frac{1}{2\pi} \int_{-\infty}^{\infty} dk \left(\frac{2\pi}{\tilde{\kappa}}\right)^{\frac{1}{2}} \left(\frac{1}{2\tilde{\kappa}}\right) k^2 e^{k^2 \left(\frac{1}{2\tilde{\kappa}}\right)} \quad (8.27)$$

Again both integrals can easily be solved by converting them to Gaussian form. Making the substitution $\tilde{k} = k \left(\frac{1}{2\tilde{\kappa}}\right)^{\frac{1}{2}}$ in I_1 gives us:

$$I_1 = \frac{1}{4\pi} (2\tilde{\kappa})^{\frac{1}{2}} \left(\frac{2\pi}{\tilde{\kappa}}\right)^{\frac{1}{2}} \ln \left(\frac{2\pi}{L^2 \tilde{\kappa}}\right) \int_{-\infty}^{\infty} d\tilde{k} e^{-\tilde{k}^2} = -\frac{1}{2} \ln \left(\frac{2\pi}{L^2 \tilde{\kappa}}\right) \quad (8.28)$$

and making the exact same substitution in I_2 gives us:

$$I_2 = (2\tilde{\kappa})^{\frac{1}{2}} \left(\frac{1}{2\pi}\right) \left(\frac{2\pi}{\tilde{\kappa}}\right)^{\frac{1}{2}} \int_{-\infty}^{\infty} d\tilde{k} \tilde{k}^2 e^{-\tilde{k}^2} = \frac{1}{2} \quad (8.29)$$

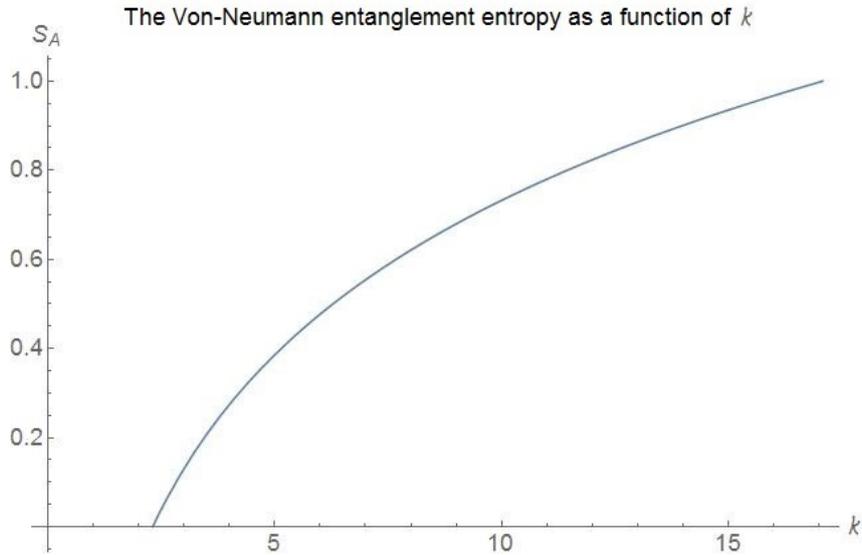


Figure 5: A plot of the Von-Neumann entanglement entropy as a function of κ for the quadratic potential, with $L = 1$ and $m_x = 2$.

Thus combining our answers for I_1 and I_2 we find the Von-Neumann entanglement entropy to be:¹⁶

$$S_A = \frac{1}{2} \left[1 - \ln \left(\frac{2\pi}{L^2 \bar{\kappa}} \right) \right] \quad (8.30)$$

We set L to unity and $m_x = 2$. This allows us to plot the Von-Neumann entanglement entropy as a function of κ fig.5. It is quite interesting to see in fig. 5 that due to a different interaction, the way in which our coupled quantum particles entangle is very different to the electron-proton system. We see that for small values of our entanglement parameter κ that our state is not very entangled, however, as κ is increased the degree of entanglement within the system also increases. The problem however is that this system is not bound, the Von-Neumann entanglement entropy will continue to increase and it doesn't really make sense to have a Von-Neumann entanglement entropy greater than one. As if it is greater than one, it would imply a state that is more maximally entangled than the maximally entangled state. So it may mean one of two things, either our model is incorrect or we have overlooked something. However, the Von-Neumann entanglement

¹⁶The logarithm is indeed dimensionless remember that $\hbar = 1$.

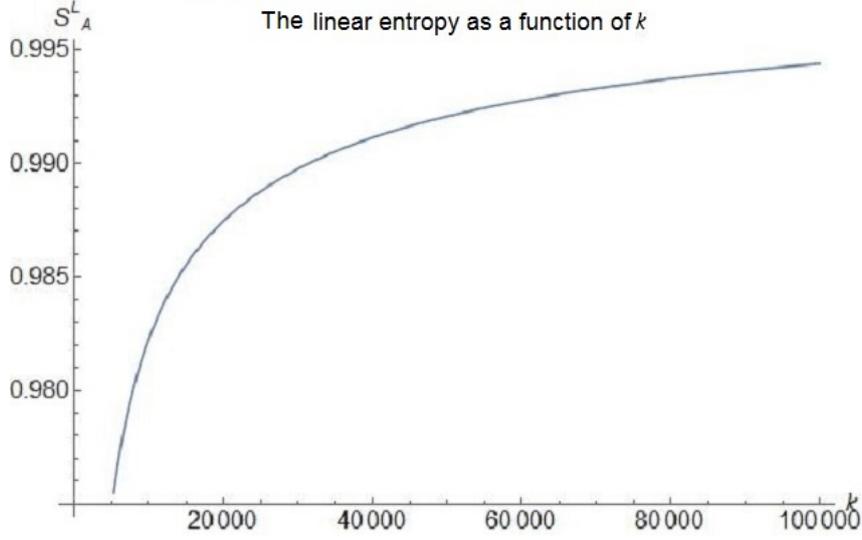


Figure 6: A plot of the linear entropy for large κ , with $L = 1$ and $m_x = 2$

entropy is directly related to the Shannon-Boltzmann equation through the thermodynamic limit and in breaking down the Von-Neumann entanglement entropy, we may see it as a measure of entropy of our system i.e it is telling us the uncertainty contained within our system and so from that perspective the Von-Neumann entropy can be much greater than one. Of course we can address this problem by fixing the values of κ , to ensure that we get entanglement entropies between zero and one, which relate to what we expect theoretically.

In light of our previous calculations, let us now calculate the linear entropy. Recalling that the linear entropy is defined as $S_A^L = 1 - Tr(\rho_A^2)$ and using (8.24) we can write:

$$S_A^L = 1 - \frac{L}{2\pi} \int_{-\infty}^{\infty} \frac{1}{L^2} \left(\frac{2\pi}{\tilde{\kappa}} \right) e^{(-k^2 \frac{1}{\tilde{\kappa}})} \quad (8.31)$$

using the scaling $\tilde{k} = \frac{k}{\tilde{\kappa}}$ we find:

$$\begin{aligned} &= 1 - \frac{1}{L} \left(\frac{1}{\tilde{\kappa}} \right)^{\frac{1}{2}} \int_{-\infty}^{\infty} e^{-\tilde{k}^2} d\tilde{k} \\ S_A^L &= 1 - \frac{1}{L} \left(\frac{\pi}{\tilde{\kappa}} \right)^{\frac{1}{2}} \quad (8.32) \end{aligned}$$

Now that we have an explicit formula for the linear entropy we may now plot it as a

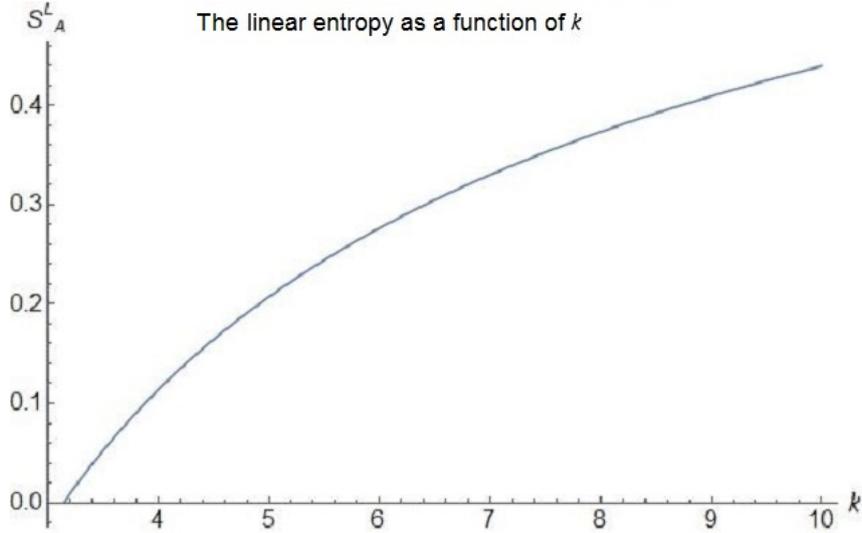


Figure 7: A plot of the linear entropy for small κ , with $L = 1$ and $m_x = 2$

function of our entanglement parameter κ , where $L = 1$ and $m_x = 2$. This time however, we shall do two plots, one for large κ (fig. 6) and one for small κ (fig. 7).

When κ is large we see how the linear entropy approaches a maximally entangled state (fig. 6), in fact it shall only have a linear entropy of one in the limit as κ tends to infinity. We equally see that even when κ is small fig. 7, the particles are strongly correlated, which is similar to the behaviour seen in fig. 5. Additionally, unlike the case of the electron-proton system, both the entanglement measures have very similar curves. We can of course set bounds on the value of κ , as we did for a_0 to plot our entanglement measures, so that the Von-Neumann entanglement entropy does not exceed one. So we could argue, in essence, the following, that if $\kappa > \kappa_{bound}$ then it is not a physical solution. But then this it self creates another question, why should we put a bound on κ when the linear entropy requires a very large κ to become maximally entangled? From a purely physical perspective it would not make sense to have an infinitely strong coupling constant, and so it is right that we should have some κ_{bound} , which we state is the value for which the Von-Neumann entanglement entropy is equal to one, i.e. $\kappa_{bound} = \frac{2\pi e^{\frac{1}{2}}}{L^2}$ where L can be chosen accordingly.

Conclusion

As we come to a close, let us collect our results and reflect on what we have found from our two models, regarding the creation of entanglement via interaction. In both the electron-proton system and our toy model of two interacting coupled particles, we see that the original Hamiltonian could not be solved via separation of variables, as it was correlated due to the interaction term. However, in switching to a set of fictitious co-ordinates, which are purely a mathematical transform and do not describe the actual physical system, we found that the Hamiltonian splits in to two uncorrelated parts; one describing the internal motion, the other the centre of mass. We find the wavefunction and it seems to be uncorrelated. This is of course true for any system of two interacting particles, for which we have a central potential, i.e. a potential which is solely dependent on radial positions and so is spherically symmetric. However, in actually changing back to the original co-ordinate system, which is dependent on the physical system, we find that we now have an entangled wavefunction. This means that for all systems where we have two quantum particles, whose interaction is mediated by a potential of this form, will have an ‘entangled’ wavefunction. The essential point here is that entanglement is not an absolute property of quantum states. Entanglement is a property of a quantum state relative to a given set of subsystems.

In comparison of the two systems and the entanglement measures we used on each system, we very clearly see that the plots of the measures are heavily dependent on the shape of the potential. For the hydrogen atom we see this decaying behaviour, especially so for the Von-Neumann entanglement entropy, although it is less so for the linear entropy. For our toy model of two coupled quantum particles, the effect of interaction on the correlations in this system is very different to that of the hydrogen atom. We see that the entanglement in the system increases as the coupling strength κ is increased, whereas we have an inversion of this for the hydrogen atom. Both the Von-Neumann entanglement entropy and the linear entropy for this system showed how interaction was the driving force behind the strength of the correlations between our quantum particles A and B . However,

one cravat we faced was the that the Von-Neumann entanglement entropy would become much greater than one, for larger values of κ , whereas the linear entropy would become maximally entangled and so we have two different polarisations, something that is within physical bounds and something that is not. In order to rectify this problem we introduced a κ_{bound} for which the Von-Neumann entanglement entropy is a less than or equal to one and we state that all $\kappa > \kappa_{bound}$ are nonphysical values for our parameter.

This dissertation has aimed to provide an insight in to the creation of entanglement by interaction and some of the fundamental concepts behind what it means for something to be entangled. It should also be noted that we do necessarily even need any form of interaction to entangle two systems [PBWZ98]. For future work and further directions looking in to thermal entanglement via a common heat bath would be a natural extension from the coupled quantum particles example as there are similarities in the formulation of the two. Another direction is to try and extend these ideas to many body systems, but we fear that this may be too challenging for merely a year long project, due to the shear complexity of decrypting multipartite entanglement. For our final words, we leave the reader with the following statement; if mathematically it depends on the frame in which we are placed whether or not a state is entangled, can we say the same for the experimentalist, does the entanglement that they observe, depend upon where the ‘eyes’(the measurement device) of our observer is looking?

A Appendix A

A.1 The humble commutator

The commutator plays an important role in quantum mechanics, as it is a way of determining whether or not two observables can be simultaneously measured, which of course is something that we do not have to worry about classically. We say that if two operators \hat{A} and \hat{B} commute, that is $[\hat{A}, \hat{B}] = 0$, then the observables corresponding to \hat{A} and \hat{B} are simultaneously measurable, which means the operators have a common basis of simultaneous eigenstates [Oss13].

The structure of the commutator that we would like in quantum mechanics is directly related to a Lie algebra, that is we would like our operators to obey the following properties given operators \hat{A}, \hat{B} and \hat{C} and $\alpha \in \mathbb{C}$:

$$\begin{aligned} \text{Bi-linear: } [\hat{A} + \alpha\hat{C}, \hat{B}] &= [\hat{A}, \hat{B}] + \alpha[\hat{C}, \hat{B}] \\ \text{Anti-symmetric: } [\hat{A}, \hat{B}] &= -[\hat{B}, \hat{A}] \\ \text{Jacobi-Identity: } [\hat{A}, [\hat{B}, \hat{C}]] + [\hat{B}, [\hat{C}, \hat{A}]] + [\hat{C}, [\hat{A}, \hat{B}]] &= 0 \end{aligned}$$

B Appendix B

B.1 Legendre polynomials

A Legendre function simply put, is a function which satisfy Legendre's equation of order n :

$$(1 - x^2)y'' = 2xy' + n(n + 1)y = 0 \quad (\text{B.1})$$

For applications n is usually an integer, however, if n is a non integer we must be a little careful. We first note that (B.1) is invariant under the transformation $x \rightarrow -x$. Thus if $P_n(x)$ is a solution to (B.1) so is $P_n(-x)$. However, for non-integer n , $P_n(-x)$ is not a multiple of $P_n(x)$ and so they are linearly independent. Thus the general solution to (B.1) is:

$$y(x) = AP_n(x) + BP_n(-x) \quad (\text{B.2})$$

where A and B are arbitrary constants. An important property of $P_n(x)$ is that it is singular at $x = -1$ for n non-integer. Therefore solutions of (B.1) have a singularity at, at least one of the points $x = 1$ and $x = -1$ for n non-integer.

Taking this into account we find two series solutions of the form:

$$\begin{aligned} y_0(x) &= 1 + \sum_{m=1}^{\infty} \left[(-1)^m x^{2m} \left(\frac{n(n-2) \cdots (n-2m-2)}{(2m)!} \right) \times ((n+1) \cdots (n+2m+1)) \right] \\ y_1(x) &= x + \sum_{m=1}^{\infty} \left[(-1)^m x^{2m+1} \left(\frac{(n-1) \cdots (n-2m+1)}{(2m+1)!} \right) \times ((n+2) \cdots (n+2m)) \right] \end{aligned}$$

It is interesting to note that for n an even integer, the series for $y_0(x)$ will terminate when $m = \frac{n}{2} - 1$ and if n is an odd integer the series $y_1(x)$ terminates when $m = \frac{n+1}{2}$. Such solutions are known as Legendre polynomials and the first few in normalised form are given as:

$$P_0(x) = 1$$

$$P_1(x) = x$$

$$P_2(x) = \frac{1}{2}(3x^2 - 1)$$

$$P_3(x) = \frac{1}{2}(5x^3 - 3x)$$

In order to generate the n^{th} Legendre polynomial we use Rodrigues formula:

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} [(x^2 - 1)^n] \quad (\text{B.3})$$

For n an integer we construct our general solution to (B.1) by first noting that the polynomials generated by (B.3) are non-singular and second, that $P_n(-x) = (-1)^n P_n(x)$. Where the latter point means $P_n(x)$ and $P_n(-x)$ are linearly dependent, but as (B.1) is a second order ordinary differential equation (ODE) we require two linearly independent solutions. Thus we denote the second solution, for n an integer as $Q_n(x)$, where $Q_n(x)$ is non-polynomial and singular at the points $x = \pm 1$. Thus for n an integer the general solution is of the form:

$$y(x) = AP_n(x) + BQ_n(x) \quad (\text{B.4})$$

where A and B are arbitrary constants.

C Appendix C

C.1 The Fourier transform of the momentum space wavefunction

We want to calculate explicitly the Fourier transform of the following momentum wavefunction $\psi(\mathbf{p}) = \frac{1}{\sqrt{\pi}}e^{-p}$ in the position representation $\psi(\mathbf{r})$. We do this by first using (6.49), which allows us to write:

$$\psi(\mathbf{r}) = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} e^{i\mathbf{r}\cdot\mathbf{p}} \psi(\mathbf{p}) dp_x dp_y dp_z \quad (\text{C.1})$$

we can convert this integral in to spherical co-ordinates with the z -axis chosen in the direction of \mathbf{r} [Oss13], so that $\mathbf{r} \cdot \mathbf{p} = |r||p| \cos(\theta)$, therefore:

$$\psi(\mathbf{r}) = \left(\frac{1}{2\pi}\right)^{\frac{3}{2}} \int_0^{2\pi} d\phi \int_0^{\pi} d\theta \sin(\theta) \int_0^{\infty} p^2 e^{irp \cos(\theta)} \frac{1}{\pi^{\frac{1}{2}}} e^{-p} \quad (\text{C.2})$$

The $d\phi$ integral gives us a factor of 2π and then for $d\theta$ integral we make the substitution $v = \cos(\theta)$, which makes the region of integration from 1 to -1 , to flip the limits we induce a minus sign and so integrating we find:

$$\psi(\mathbf{r}) = \left(\frac{1}{2}\right)^{\frac{1}{2}} \frac{1}{\pi} \int_0^{\infty} dp p^2 e^{-p} \left[\frac{e^{irpv}}{irp} \right]_{-1}^1$$

and so we are left with the following expression:

$$\frac{1}{2^{\frac{1}{2}} \pi ir} \int_0^{\infty} dp p (e^{-p(1-ir)} - e^{-p(1+ir)}) \quad (\text{C.3})$$

which can be integrated using the following relation:

$$\int_0^{\infty} dp p^n e^{-\beta p} = \frac{n!}{\beta^{n+1}}, \text{ where } n = 0, 1, 2, \dots \quad (\text{C.4})$$

as $n = 1$ and $\beta = (1 \pm ir)$ we have:

$$\psi(\mathbf{r}) = \frac{2^{\frac{3}{2}}}{\pi(1+r^2)^2} \quad (\text{C.5})$$

from which we recover (7.14).

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