KMS States in Quantum Statistical Mechanics

By

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Abstract

The algebraic description of quantum mechanics provides an abstract and generalised method for studying quantum systems. Within this framework, KMS states provide a natural candidate for equilibrium states in quantum statistical mechanics. The primary aim of this project was to investigate the properties of KMS states and the characterisation of KMS states as equilibrium states, and to study examples of simple quantum systems through an algebraic framework.

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Conventions

Inner products will be linear in the second variable, and will initially be denoted by $\langle \cdot, \cdot \rangle$. In section 3.2.1 we will slightly change notation to align with the bra-ket notation introduced there. All inner products used after section 3.2.1 will therefore be denoted by $\langle \cdot | \cdot \rangle$.

Hilbert spaces are assumed separable unless otherwise noted.

The natural numbers, denoted $\mathbb{N}$, are the positive integers $\{1, 2, 3, 4, \dots\}$. The non-negative integers, $\mathbb{N} \cup \{0\}$, will be denoted $\mathbb{N}_0$.

0.1 A note on units

When we describe the measurement of a physical quantity, we express that quantity as a ratio of the physically measured value and a specified, standard value. For example, when we measure the length of a football field to be 91 metres, we are really saying that the length of the field divided by the length of one metre is 91. Equivalently, we could express the length of the same field as 100 yards. In physics, it is important to express all numerical quantities with their associated units - a distance of 1 is meaningless if we don't know whether the units are centimetres or kilometres. A system of units is a specification of standard values for length, mass, time and other fundamental quantities. The most commonly used system of units is the S.I. (Systéme International) or metric system. In physics, certain physical quantities, such as the speed of light c or the universal gravitational constant G occur so frequently in equations and formulae that it is convenient to choose units such that these quantities are equal to 1. In this thesis, we will use whatever units are most convenient at the time, frequently choosing units such that $\hbar = 1$.

Chapter 1

Introduction

1.1 Historical background

1.1.1 Classical mechanics

Classical physics is the study of the physical laws of the universe describing the motion of macroscopic bodies under various forces. As a quantitative science, classical physics began around the 17th century with the work of Johannes Kepler, Galileo Galilei and most notably, Isaac Newton. Newton's laws of motions and his law of universal gravitation in his famous 'Principia Mathematica' [42] provided the first mathematical description of physical phenomena, and began the study of classical mechanics.

In the 18th and 19th centuries, Joseph-Louis Lagrange and William Rowan Hamilton, among others, reformulated classsical (Newtonian) mechanics using different mathematical formalisms. Lagrange developed a theory of mechanics based upon the principle of least action [30, 31] which is more flexible in the choice of coordinates used to describe a given system. Hamiltonian mechanics is an equivalent formulation [22, 23], which is a better description of systems when we are interested in conserved physical quantities (such as energy or momentum). These two generalisations of Newtonian mechanics abstract the mathematical formalism of classical mechanics, and in doing so provide a deeper conceptual understanding of the theory.

Towards the end of the 19th century, classical mechanics was thought to be a full description of the physical laws of nature, at least in principle. A famous quote, often attributed to William Thomson (Lord Kelvin) says

> *"There is nothing new to be discovered in physics now. All that remains is more and more precise measurement."*

There were, however, several experimental results which either conflicted with the results of classical physics or were unable to be explained by them. These included blackbody radiation, the photoelectric effect, spectral lines and the stability of the hydrogen atom. A select example is the hydrogen atom, which at the time was thought to consist of a dense, positively charged nucleus orbited by a light, negatively charged particle called an electron. According to the classical theory, any accelerating electric charge (such as an electron orbiting a nucleus) should lose energy by emitting radiation. This would cause the electron to lose kinetic energy and eventually fall into the nucleus. A short calculation shows that the predicted lifetime of the hydrogen atom is of the order of 10^{-11} seconds, which is significantly shorter than the observed lifetime. This result, as well as the others mentioned, indicated the need for a new theory to describe physics at the atomic scale.

1.1.2 Quantum mechanics

Quantum mechanics was developed independently in two different forms by Werner Heisenberg and Erwin Schrödinger. Heisenberg's quantum mechanics [24] was developed to predict the intensities of atomic spectral lines. Heisenberg, together with Max Born and Pascual Jordan, realised that observables (such as position q and momentum p) were more correctly described by non-commuting quantities which could be represented with infinite dimensional matrices, resulting in a theory known as 'matrix mechanics' [6]. Schrödinger's wave mechanics approach [51, 52, 53, 54] is considered an extension of de Broglie's wave-particle hypothesis, in which he posited that an electron orbiting a nucleus is described by a wave, and the allowed orbitals are those for which the circumference corresponds to an integer number of wavelengths. Schrödinger sought to find the wave equation describing the wave nature of electrons, and developed his famous equation

$$H\psi = i\hbar\frac{\partial}{\partial t}\psi,$$

where H is the Hamiltonian[1], ψ is the wavefunction and $\hbar$ is a positive constant. The equivalence of the approaches of Heisenberg and Schrödinger was shown by Schrödinger in [55], and both theories were embedded in a more general formalism by Paul Dirac [14],

[1] Here the Hamiltonian is a differential operator

although this formalism was not mathematically rigorous, relying on ill-defined delta functions. John von Neumann soon realised that a much more natural framework of quantum mechanics was provided by the abstract theory of Hilbert spaces and linear operators, and established a rigorous axiomatic framework in [66]. One considers a complex Hilbert space $\mathcal{H}$ and linear operators acting on it. To each measurable quantity one assigns a self-adjoint operator acting on $\mathcal{H}$, called an observable, and the spectrum of the operator corresponds to the possible measurements of that observable. These operators form an algebra called the algebra of observables. States are represented by normalised vectors in the Hilbert space. The time evolution of an observable A is then given by the quantum mechanical analogue of Hamilton's equation:

$$\frac{\partial A_t}{\partial t} = \frac{i(HA_t - A_t H)}{\hbar},$$

where H is the Hamiltonian, an observable which usually corresponds to the total energy of the system. The solution to this equation of motion is given by $A_t = e^{itH} A e^{-itH}$, where we have chosen units such that $\hbar = 1$. Stone's theorem [58, 59] asserts that this time evolution is a strongly continuous group of automorphisms of the algebra of observables. The Schrödinger picture is easily obtained from this structure with the identification $\mathcal{H} = L^2(\mathbb{R}^n)$.

Once the mathematical framework of quantum mechanics had been established, it was subject to mathematical analysis. Marshall Stone announced, in 1930, a uniqueness theorem for operators satisfying the canonical commutation relations[2] [58]. Von Neumann published a proof of this result in 1931 [65]. The resulting theorem is known as the Stone-von Neumann theorem, and asserts that any two pairs of operators satisfying the canonical commutation relations are unitarily equivalent.

1.1.3 Statistical mechanics

Statistical mechanics is the study of the bulk propeties of a system, such as temperature and pressure, using probability theory. The systems studied in statistical mechanics often deal with very large numbers of particles[3]. This makes a traditional treatment of

[2]The position and momentum operators q and p mentioned previously were known to satisfy the commutation relation $qp - pq = i\hbar$.

[3]Typical thermodynamics systems comprise of 10^{24} particles

the system, which relies on solving the equations of motions of the individual particles, untenable.

In 1738, Daniel Bernoulli published what is considered the first work on statistical mechanics, *Hydronimca* [3]. In this work, Bernoulli laid the basis for the kinetic theory of gases - the description of a gas as a large number of small particles which are in constant motion. The kinetic theory of gases is able to explain the macroscopic behaviour of large systems through the specification of the microscopic system. As an example of the power of this theory, consider a container of gas. The pressure of such a gas is explained through the kinetic theory of gases as the force exerted on the container walls by the impacts of the individual gas particles. One is able to derive, under this assumption, the connection between the pressure of the gas (P), the volume of the container (V), and the average kinetic energy of the particles (i.e. the temperature, T). This connection is known as the ideal gas law, and is succinctly stated as

$$PV = nRT,$$

where n is the amount of substance of gas, and R is the universal gas constant[4]. This result was first derived from the kinetic theory of gases independently by August Krönig in 1856 [28], and Rudolf Clausius in 1857 [9]. Between 1859 and 1866, James Clerk Maxwell, known primarily for his work on electromagnetic field theory, formulated the Maxwell distribution of molecular velocities for a system in equilibrium [33, 34, 35, 36, 37]. Maxwell's distribution gives the fraction of molecules in a gas moving with a specific velocity at a given temperature, and has greatly extended the range of Bernoulli's kinetic theory of gases. In 1868, Ludwig Boltzmann extended Maxwell's distribution to include external forces and systems not in equilibrium [5]. In 1876 and 1878, Josiah Willard Gibbs published a two-part, 300 page treatise on statistical mechanics, discussing phase equilibria, statistical ensembles, free energy as the driving force of chemical reactions and chemical thermodynamics [16, 17]. The work of Gibbs occurred before the advent of quantum mechanics, however much of his analysis survived the transition to quantum mechanics.

(Classical) statistical mechanics studies statistical ensembles of (classical) systems of particles, while quantum statistical mechanics is the study of statistical ensembles of

[4]The gas constant has an approximate value of 8.314 J K^{-1} mol^{-1}

quantum mechanical systems - i.e. physical systems which are described using quantum mechanics. The standard quantum mechanical formalism can incorporate statistical mechanics quite easily. In the standard description, states (also called pure states) are represented by vectors in a Hilbert space $\mathcal{H}$. The expectation value of an observable A in the state ψ is given by the inner product, $\langle \psi, A\psi \rangle$. A mixed state is a statistical ensemble of several pure states[5]. The expectation value of a mixed state ϕ is then defined to be a functional over the observables of the form

$$\phi(A) = \sum_i \lambda_i \langle \psi_i, A\psi_i \rangle ,$$

where $\lambda_i \geq 0$, $\sum_i \lambda_i = 1$ and $\|\psi_i\| = 1$. The quantities λ_i are the probabilities that the quantum system may be found in the state ψ_i. The expectation value of a mixed state ϕ, although not given by an inner product with a vector, can be written

$$\phi(A) = \mathrm{Tr}(\rho A),$$

where ρ is a positive trace class operator with trace equal to one, called a density matrix. The term state (within the context of operator algebras) has now come to mean a positive linear functional of norm one.

1.1.4 Operator algebras

Operator algebras is a branch of mathematics which studies collections of continuous linear operators on topological vector spaces. These operators form algebras with multiplication given by composition of mappings. The linear operators on a Hilbert space form a special and often studied operator algebra. In addition to their applications in the theory of quantum mechanics and quantum statistical mechanics, operator algebras have found applications in diverse fields of mathematics such as knot theory, non-commutative geometry, representation theory and probability.

In 1929, motivated in part by his work in quantum mechanics, von Neumann introduced a special type of operator algebra which is today referred to as a von Neumann algebra [67]. Originally referred to as rings of operators, von Neumann algebras are algebras of bounded operators on a Hilbert space containing the identity operator and closed

[5]Note that a mixed state is different to a quantum superposition of states. A quantum superposition ψ of two pure states ψ_1 and ψ_2 is itself a pure state, $\psi = \frac{1}{\sqrt{2}}(\psi_1 + \psi_2)$

in the weak operator topology. Francis Joseph Murray and John von Neumann developed the theory for these von Neumann algebras in a series of papers written in the 1930s and 1940s [38, 39, 40, 68, 69, 70].

A natural example of a von Neumann algebra is the algebra of bounded operators on a Hilbert space $\mathcal{H}$, denoted $\mathcal{B}(\mathcal{H})$. Subalgebras of $\mathcal{B}(\mathcal{H})$ are known as C^*-algebras, and were given an abstract characterisation by Israel Gelfand and Mark Naimark in 1943 [15] without any reference to a Hilbert space. In 1947, Irving Segal developed the mutual correspondence between states and representations[6] of a C^*-algebra [56]. In [57], Segal presents a series of postulates which, he argues, describe physical systems. His theory suggests that an algebraic rephrasing of quantum mechanics is more general, while still describing the physical system. An algebraic rephrasing of quantum mechanics is then given by defining an algebra of observables $\mathcal{A}$, which may be a von Neumann algebra or a C^*-algebra. States[7] are positive linear functionals of norm one on the algebra of observables, and the dynamics of the system is given by a strongly continuous one-parameter group of automorphisms of the algebra of observables.

In 1964, Rudolf Haag and Daniel Kastler developed an axiomatic framework for quantum field theory, in an attempt to unify quantum mechanics with special relativity in an algebraic way [20]. Their mathematical framework is stated in terms of nets of C^*-algebras of local observables, and is therefore called Algebraic Quantum Field Theory (AQFT), or local quantum field theory. Haag's 1992 book provides a gentle and thorough introduction to local quantum field theory [19].

1.1.5 Equilibrium states and the KMS condition

A thermodynamical system typically contains a large number of particles. The simplest states of a thermodynamical system to describe are equilibrium states. These are states in which all external influences are balanced and whose bulk properties, such as pressure and temperature, are not changing with respect to time. A convenient mathematical way of obtaining bulk properties of an equilibrium state for a given thermodynamical system is to start with a system of N particles enclosed in a box of volume $\mathcal{V}$ and energy E, and then calculate the quantity of interest (say, temperature) inside the box. Taking the limit

[6] A representation of a C^*-algebra $\mathcal{A}$ is a homomorphism from $\mathcal{A}$ to $\mathcal{B}(\mathcal{H})$.

[7] i.e. the expectation values of physical states

as $N \to \infty$, $\mathcal{V} \to \infty$, $E \to \infty$ we obtain what is known as the thermodynamic limit. Not all quantities have continuous transitions to the thermodynamic limit - after the infinite volume limit sharp discontinuities in the thermodynamic properties can appear. Physically, these discontinuities apply to phase transitions of the material, and are sometimes cited as justification of the limit process.

Starting with a finite system, one first considers a finite subset of space Λ, together with a collection of observables which form the self-adjoint elements of a C^*-algebra $\mathcal{A}_\Lambda$. Given two subsets $\Lambda_1 \subset \Lambda_2$ of space, the algebras should satisfy $\mathcal{A}_{\Lambda_1} \subset \mathcal{A}_{\Lambda_2}$. The union of these algebras then gives us the thermodynamical limit. It can be shown that this union is a C^*-algebra, which we interpret as the algebra of observables of the infinite system. Algebras obtained this way are known as qausi-local algebras.

For the finite system, there is a standard prescription for obtaining an equilibrium state, called a Gibbs state. For a system at inverse temperature[8] β with Hamiltonian H, the partition function Z is defined by $Z = \mathrm{Tr}(e^{-\beta H})$. The Gibbs state ϕ_β is then given by the density matrix

$$\rho = Z^{-1} e^{-\beta H}.$$

In 1957, Ryogo Kubo pointed out a special property satisfied by the Gibbs states [29], and in 1959 Paul C. Martin and Julian Schwinger used this property to construct thermodynamic Greens functions [32]. If the time evolution of the finite system above is given by $\tau_t(A) = e^{itH} A e^{-itH}$, then the Gibbs state at finite volume satisfies the following condition

$$\phi_\beta(A\tau_{i\beta}(B)) = \phi_\beta(BA).$$

In 1967, Rudolf Haag, N.M. Hugenholtz and Marinus Winnink proposed this condition as a criterion for equilibrium states, and called it the KMS (for Kubo, Martin, Schwinger) condition [21]. While Haag, Hugenholtz and Winnink were working on the algebraic formulation of the KMS condition, Minoru Tomita developed his theory of modular automorphism groups. Tomita's work, and the relation to the KMS condition, went largely unnoticed until 1970 when Masamichi Takesaki published an investigation and elaboration of Tomita's theory [61], including a proof that a state satisfies the KMS

[8] We define the inverse temperature $\beta = \frac{1}{k_B T}$, where T is the absolute temperature and k_B is Boltzmann's constant, which has the approximate value $k_B = 1.38 \times 10^{-23}$ J K^{-1}

condition with $\beta = -1$ with respect to the modular automorphism group associated to that state.

In 1979, the work of many authors who worked on KMS states and their applications to quantum statistical mechanics was collected and summarised by Ola Bratelli and Derek Robinson in the first volume of their two part *Operator Algebras and Quantum Statistical Mechanics* [7]. Volume one, subtitled "C^* and W^*-Algebras Symmetry Groups Decomposition of States", developed and presented theory for the analysis of equilibrium states in the algebraic formulation of quantum statistical mechanics. Volume two, subtitled "Equilibrium States. Models in Quantum Statistical Mechanics", applied the theory of the first volume to study systems in quantum statistical mechanics including continuous quantum systems and quantum spin systems [8]. This thesis is based largely on the theory and examples contained within these two volumes.

1.2 Outline of thesis

Chapter 2 gives primary definitions and main results in the theory of C^*-algebras. The structure theorems for commutative and non-commutative C^*-algebras are stated, as well as the double commutant theorem for von Neumann algebras. Unbounded operators are discussed, and the Tomita-Takesaki theory of modular automorphisms is introduced.

Chapter 3 introduces the notion of algebraic quantum mechanics. The algebraic formulation of quantum mechanics is motivated through physical principles and by analogy with the mathematical structure of classical mechanics. Included in this chapter are miscellaneous results from the mathematical theory of quantum mechanics - namely the theory of the bounded operators on a Hilbert space. Quantum statistical mechanics is introduced with a discussion of equilibrium states, and the KMS condition is defined and discussed.

Chapter 4 gives some examples of quantum systems which we describe using the KMS condition and the algebraic formulation of quantum mechanics. Results for the quantum harmonic oscillator are derived in both the one-dimensional and N-dimensional case. The mathematical description of an ideal Fermi gas is given.

Chapter 5 discusses interacting quantum systems through the language of perturbation theory. We discuss alternate notions of equilibrium, the Fermi-oscillator system, and

conclude with some final remarks.

Chapter 2

The theory of C^*-algebras

This chapter recalls some of the mathematical theory of C^*-algebras. The definitions and results here are fairly standard and are covered quite thoroughly in various introductory textbooks such as [41, 13]. More advanced texts covering this material include [62, 63, 64, 25, 2].

2.1 Definitions

To define precisely what a C^*-algebra is, we first need some preliminary concepts. In the following, all vector spaces are considered to be complex vector spaces.

Definition 2.1.1. A **Banach space** is a normed vector space which is complete.

Norms will be denoted by $\|\cdot\|$.

Definition 2.1.2. An **algebra**, $\mathcal{A}$, is a vector space with an associative multiplication $(a, b) \in \mathcal{A} \times \mathcal{A} \mapsto ab \in \mathcal{A}$ which commutes with scalar multiplication and is distributive over addition.
A $*$**-algebra** is an algebra $\mathcal{A}$ equipped with an antilinear map $* : a \in \mathcal{A} \mapsto a^* \in \mathcal{A}$, which satisfies the following properties:

- $(a^*)^* = a \qquad \forall a \in \mathcal{A}$
- $(ab)^* = b^*a^* \qquad \forall a, b \in \mathcal{A}$

The map $*$ is called an **involution**.

Definition 2.1.3. A **Banach algebra** is a Banach space which is also an algebra, and for which the multiplication satisfies:

$$\|ab\| \leq \|a\|\|b\| \qquad \text{for all } a, b \in \mathcal{A}. \tag{2.1}$$

Definition 2.1.4. A C^***-algebra**, $\mathcal{A}$, is a Banach $*$-algebra which satisfies

$$\|a^*a\| = \|a\|^2 \tag{2.2}$$

for each $a \in \mathcal{A}$.

The property (2.1) is referred to as submultiplicativity of the norm, and property (2.2) is known as the C^*-identity. An immediate result that comes from these two properties is that involution on a C^*-algebra is isometric, i.e. norm-preserving. To see this, simply apply the submultiplicativity of the norm to $\|a\|^2 = \|a^*a\|$. This gives

$$\|a\|^2 = \|a^*a\| \leq \|a^*\|\|a\|,$$

which implies $\|a\| \leq \|a^*\|$ for any $a \in \mathcal{A}$. In particular, this property holds for the element a^*, and so $\|a^*\| \leq \|(a^*)^*\| = \|a\|$, establishing the equality $\|a\| = \|a^*\|$.

A C^*-algebra (or more generally any algebra) does not necessarily have a multiplicative identity. If it does have an identity, it is unique, and we say the algebra is **unital**. We denote the identity by $1_{\mathcal{A}}$, or simply 1 if it is clear which algebra we are talking about.

A C^*-algebra is **commutative** or **abelian** if the multiplication is commutative, i.e. if $ab = ba$ for every $a, b \in \mathcal{A}$.

Example 2.1.5. Let $\mathcal{H}$ be a Hilbert space. An operator $A : \mathcal{H} \to \mathcal{H}$ has a norm defined by

$$\|A\|_\infty = \sup\{\|Tx\| : x \in \mathcal{H} \text{ and } \|x\| \leq 1\}.$$

This norm is known as the operator norm, and we say that an operator is bounded if it has finite operator norm. The set of bounded linear operators on $\mathcal{H}$, denoted by $\mathcal{B}(\mathcal{H})$, forms a C^*-algebra with multiplication given by composition of operators and involution given by the operator adjoint.

Since operators don't generally commute, $\mathcal{B}(\mathcal{H})$ is a non-abelian algebra. It is unital because the linear operator $1 : x \mapsto x$ is bounded with norm 1.

Definition 2.1.6. Let $\mathcal{A}$ be a C^*-algebra, and suppose that $\mathcal{B}$ is a vector subspace of $\mathcal{A}$. We say $\mathcal{B}$ is a C^***-subalgebra** of $\mathcal{A}$ if it is closed under the product and involution (i.e. $a, b \in \mathcal{B}$ imply $ab \in \mathcal{B}$ and $a^* \in \mathcal{B}$), and if it is closed in the norm topology (i.e. if $\{a_n\}$ is a sequence in $\mathcal{B}$ and $a_n \to a$ in norm, then $a \in \mathcal{B}$).

Example 2.1.7. The compact operators $\mathcal{K}(\mathcal{H})$, on a Hilbert space $\mathcal{H}$, form a C^*-subalgebra of $\mathcal{B}(\mathcal{H})$. The compact operators are the natural extension of matrix operators to infinite dimensional vector spaces. To define the compacts, we first define an operator A to have **rank one** if it has the form $A = \theta_{x,y}$, where $\theta_{x,y} : z \mapsto \langle y, z \rangle\, x$. The name refers to the fact that this operator has a one-dimensional range. We now define the compacts to be the closed span of these rank one operators:

$$\mathcal{K}(\mathcal{H}) = \overline{\text{span}}\{\theta_{x,y} : x, y \in \mathcal{H}\}$$

If $\mathcal{H}$ is finite dimensional, then $\mathcal{K}(\mathcal{H}) = \mathcal{B}(\mathcal{H}) = M_n(\mathbb{C})$, the $n \times n$ matrices. If $\mathcal{H}$ is infinite dimensional, then $\mathcal{K}(\mathcal{H})$ is not unital.

Definition 2.1.8. A **homomorphism** between C^*-algebras $\mathcal{A}_1$, $\mathcal{A}_2$ is a linear map $\phi : \mathcal{A}_1 \to \mathcal{A}_2$ such that

$$\phi(ab) = \phi(a)\phi(b)$$
$$\phi(a^*) = \phi(a)^*.$$

An **isomorphism** is a bijective homomorphism. We say two C^*-algebras are isomorphic if there exists an isomorphism between them. An **automorphism** of a C^*-algebra $\mathcal{A}$ is an isomorphism $\phi : \mathcal{A} \to \mathcal{A}$. A homomorphism is **isometric** if it preserves the norm of every element, i.e. $\|a\| = \|\phi(a)\|$.

Note that here we are using the convention that a homomorphism is defined to be an involution preserving map. Some authors choose to omit this from the definition, and what we call a homomorphism they would call a $*$-homomorphism.

Definition 2.1.9. Let $\mathcal{A}$ be a Banach algebra and $I \subset \mathcal{A}$. We say I is an **ideal** of $\mathcal{A}$ if it is a vector subspace, and $a \in I$, $b \in \mathcal{A}$ imply $ab \in I$ and $ba \in I$. If $\mathcal{A}$ is a $*$-algebra, then we also require that $a \in I$ implies $a^* \in I$.

Example 2.1.10. The compact operators, $\mathcal{K}(\mathcal{H})$, form an ideal of the C^*-algebra $\mathcal{B}(\mathcal{H})$.

Definition 2.1.11. Let $\mathcal{A}$ be a unital Banach $*$-algebra and $a \in \mathcal{A}$. Then the **spectrum** of a, denoted $\sigma(a)$, is the set of complex numbers λ for which $a - \lambda 1$ is not invertible.

The spectrum generalises the concept of eigenvalues to operators acting on infinite dimensional spaces. The spectrum of an operator contains all its eigenvalues, but could be strictly larger.

Example 2.1.12. Consider $M_n(\mathbb{C})$, the algebra of complex valued $n \times n$ matrices. The spectrum of a matrix $A \in M_n(\mathbb{C})$ is the set of complex numbers λ for which $A - \lambda I$ is not invertible. Since a matrix is not invertible if and only if it has determinant zero, the spectrum of A is

$$\sigma(A) = \{\lambda \in \mathbb{C} : \det(A - \lambda I) = 0\},$$

which is exactly the set of eigenvalues of the matrix A.

Example 2.1.13. Consider the Hilbert space $\mathcal{H} = \ell^2(\mathbb{N})$, and $T \in \mathcal{B}(\mathcal{H})$ defined by

$$T : (x_1, x_2, x_3, \dots) \mapsto (0, x_1, x_2, \dots).$$

This operator has no eigenvalues, but a non-empty spectrum. To see this, assume that $x = (x_1, x_2, x_3, \dots) \in \ell^2(\mathbb{N})$ is a non-zero eigenvector of T with eigenvalue λ. Then

$$Tx = \lambda x,$$

i.e.

$$(0, x_1, x_2, \dots) = (\lambda x_1, \lambda x_2, \lambda x_3, \dots). \tag{2.3}$$

If $\lambda = 0$, then $x = 0$, which would give a contradiction since x is non-zero. We therefore suppose that $\lambda \neq 0$. Since $\lambda \neq 0$, Equation (2.3) says that $x_1 = 0$, which then implies that $x_2 \neq 0$, and so on, giving $x = 0$, which is a contradiction. To show that the spectrum of T is non-empty, it is enough to show that $T + 1$ is not an invertible operator. We assume, for contradiction, that the vector $x = (1, 0, 0, \dots)$ is in the range of $T + 1$. This means that for some $y = (y_1, y_2, y_3, \dots) \in \ell^2(\mathbb{N})$,

$$\begin{aligned}(1, 0, 0, \dots) &= (T + 1)y \\ &= Ty + y \\ &= (y_1, y_1 + y_2, y_2 + y_3, \dots).\end{aligned}$$

This tells us that $y_1 = 1$, $y_2 = -1$, $y_3 = 1$ and in general that $y_n = (-1)^{n+1}$. This gives a contradiction since $y = (1, -1, 1, -1, \dots) \notin \ell^2(\mathbb{N})$. Thus $T + 1$ is not surjective, and therefore not invertible, so that -1 is in the spectrum of T.

2.2 Main results from the theory of C^*-algebras

The first result for this section relates to commutative C^*-algebras. It says that every commutative C^*-algebra is isomorphic to the continuous functions on some topological space. Moreover, given any (locally compact Hausdorff) topological space, we can associate a unique commutative C^*-algebra. The second result is a statement about any C^*-algebra. It says that every C^*-algebra is isomorphic to a subalgebra of the bounded linear operators acting on a Hilbert space. These are two powerful results and form the main motivation for the introduction and subsequent development of algebraic quantum mechanics. We conclude this section with a brief introduction to the continuous functional calculus for C^*-algebras, which allows us to define $f(a)$ when a is a normal element of our C^*-algebra and f is a continuous function.

2.2.1 Commutative C^*-algebras

Definition 2.2.1. Let X be a locally compact Hausdorff space. A function $f : X \to \mathbb{C}$ is said to **vanish at infinity** if, given any $\varepsilon > 0$, there exists a compact subset $K \subset X$ such that $|f(x)| < \varepsilon$ for all $x \notin K$.

Lemma 2.2.2. *Let X be a locally compact Hausdorff space. The set of continuous functions on X which vanish at infinity, denoted by $C_0(X)$, is a C^*-algebra under pointwise addition and multiplication with involution given by pointwise complex conjugation. Furthermore, $C_0(X)$ is unital if and only if X is compact and then we write $C(X)$ instead of $C_0(X)$.*

This is the standard example of a commutative C^*-algebra, and in fact, the following theorem asserts that every commutative C^*-algebra is isomorphic to $C_0(X)$, for some X. For a proof of the following theorem, see [62, Theorem I.3.11 and Theorem I.4.4].

Theorem 2.2.3 (Gelfand-Naimark Theorem for commutative C^*-algebras)**.** *Let $\mathcal{A}$ be a commutative C^*-algebra . Then $\mathcal{A}$ is isometrically isomorphic to $C_0(X)$, for some locally*

compact Hausdorff space X. Furthermore, X is determined uniquely up to homeomorphism.

If $\mathcal{A}$ is unital, then the Gelfand-Naimark theorem says that $\mathcal{A}$ is isometrically isomorphic to $C(X)$, the continuous functions on a compact space. The topological space X in the Gelfand-Naimark theorem can be realised as the set $\Delta(\mathcal{A})$ of all characters on $\mathcal{A}$, namely

$$\Delta(\mathcal{A}) = \{\phi : \mathcal{A} \to \mathbb{C} : \phi \text{ is a non-zero homomorphism}\}.$$

Before we discuss the non-commutative version of Theorem 2.2.3, we introduce a special class of objects called states. States are important both mathematically in the theory of C^*-algebras, and also in physical applications such as the description of physical states in algebraic quantum mechanics.

States

For the following, let $\mathcal{A}$ be a C^*-algebra.

Definition 2.2.4. A **linear functional** on $\mathcal{A}$ is a map $\phi : \mathcal{A} \to \mathbb{C}$ such that

$$\phi(\lambda a + \mu b) = \lambda\phi(a) + \mu\phi(b) \qquad \text{for all } \lambda, \mu \in \mathbb{C} \text{ and } a, b \in \mathcal{A}.$$

A linear functional, ϕ, is **positive** if $\phi(a^*a) \geq 0$ for all $a \in \mathcal{A}$.

The set of bounded linear functionals on a C^*-algebra forms a Banach space with norm

$$\|\phi\| = \sup\{\phi(a) : \|a\| = 1\}.$$

Definition 2.2.5. A **state** is a positive linear functional of norm 1.

The set of states, denoted $\mathcal{S}(\mathcal{A})$, is a convex set. A state ϕ is a **pure state** if, for $\lambda \in [0, 1]$ and $\psi_1, \psi_2 \in \mathcal{S}(\mathcal{A})$, we have

$$\phi = \lambda\psi_1 + (1 - \lambda)\psi_2, \quad \Longrightarrow \quad \phi = \psi_1 = \psi_2.$$

That is, ϕ is a pure state if it is an extremal point of the set of states. A positive state, or more generally a positive linear functional, defines a sesquilinear form on $\mathcal{A}$ by

$$(a, b) = \phi(a^*b).$$

We choose to use round brackets to denote this sesquilinear form because it is not definite[1], and therefore not an inner product. Although this sesquilinear form is not an inner product, the Cauchy-Schwarz inequality does still apply.

Theorem 2.2.6 (Cauchy-Schwarz inequality)**.** *Let ϕ be a positive linear functional on a C^*-algebra $\mathcal{A}$. The sequilinear form $(a,b) := \phi(a^*b)$ satisfies the following two conditions*

- $(a,b) = \overline{(b,a)}$ *for all* $a, b \in \mathcal{A}$
- $|(a,b)|^2 \leq (a,a)(b,b)$ *for all* $a, b \in \mathcal{A}$

Proof. For the first condition, we fix $a, b \in \mathcal{A}$. Then for any $\lambda \in \mathbb{C}$, we have

$$\begin{aligned} 0 &\leq (a+\lambda b, a+\lambda b) \\ &= \phi((a+\lambda b)^*(a+\lambda b)) \\ &= \phi(a^*a) + \overline{\lambda}\phi(b^*a) + \lambda\phi(a^*b) + |\lambda|^2\phi(b^*b). \end{aligned} \tag{2.4}$$

Since $\phi(a^*a) + |\lambda|^2\phi(b^*b)$ is always real, we must have

$$\Im(\overline{\lambda}\phi(b^*a) + \lambda\phi(a^*b)) = 0,$$

where $\Im(z)$ denotes the imaginary component of z. This is true for any $\lambda \in \mathbb{C}$, and so for $\lambda = 1$ we obtain

$$\Im(\phi(a^*b)) = -\Im(\phi(b^*a)),$$

while for $\lambda = i$ we obtain

$$\Re(\phi(a^*b)) = \Re(\phi(b^*a)),$$

where $\Re(z)$ denotes the real component of z. We therefore conclude that $\phi(a^*b) = \overline{\phi(b^*a)}$. For the second condition, we first note that $(a,a) \geq 0$ and $(b,b) \geq 0$. If $(a,a) = (b,b) = 0$, then (2.4) implies that for each $\lambda \in \mathbb{C}$,

$$\overline{\lambda}\phi(b^*a) + \lambda\phi(a^*b) \geq 0.$$

This is true for all λ, and in particular for $\lambda = -(b,a)$. We then have

$$-2(a,b)(b,a) \geq 0,$$

[1]There may be some non-zero $a \in \mathcal{A}$ with $(a,a) = 0$.

which implies

$$|(a,b)|^2 \leq 0$$

and so $(a,b) = 0$, giving the required inequality. We now suppose that at least one of (a,a) or (b,b) is non-zero. Since $|(a,b)|^2 = |(b,a)|^2$, we suppose without loss of generality that $(a,a) \neq 0$. For any $z \in \mathcal{A}$, the positivity of ϕ gives $(z,z) = \phi(z^*z) \geq 0$. In particular, this is true for $z = b - \frac{(a,b)}{(a,a)}a$, and therefore

$$\begin{aligned} 0 &\leq \left(b - \frac{(a,b)}{(a,a)}a, b - \frac{(a,b)}{(a,a)}a\right) \\ &= (b,b) - \frac{(a,b)(b,a)}{(a,a)} \\ &= (b,b) - \frac{|(a,b)|^2}{(a,a)}. \end{aligned}$$

Multiplying by (a,a) and rearranging gives the required inequality. □

Corollary 2.2.7. *Let ϕ be a positive linear functional on a unital C^*-algebra $\mathcal{A}$ with $\phi(1) = 1$. Then ϕ is a state.*

Proof. The element $\|a\|^2 1 - a^*a$ of a unital C^*-algebra $\mathcal{A}$ can be written in the form c^*c for some $c \in \mathcal{A}$. To see that this is true, apply the results of [25, Proposition 4.2.3 (ii) and Theorem 4.2.6], together with the C^*-identity to the element a^*a. If ϕ is a positive linear functional, then

$$\phi(\|a\|^2 1 - a^*a) = \phi(c^*c) \geq 0$$

and hence

$$\phi(a^*a) \leq \|a\|^2 \phi(1). \tag{2.5}$$

We now suppose $\phi(1) = 1$ as in the statement. Then $\|\phi\| \geq 1$ follows directly from the definition of $\|\phi\|$. To obtain $\|\phi\| \leq 1$ we calculate

$$\begin{aligned} |\phi(a)|^2 &= |\phi(1^*a)|^2 \\ &\leq \phi(1^*1)\phi(a^*a) \qquad \text{By the Cauchy-Schwarz inequality} \\ &\leq \|a\|^2, \end{aligned}$$

and thus $|\phi(a)| \leq \|a\|$. Putting this into the definition of $\|\phi\|$ gives us $\|\phi\| \leq 1$. Thus $\|\phi\| = 1$ and ϕ is a state. □

2.2.2 Non-commutative C^*-algebras

The non-commutative analogue of the Gelfand-Naimark theorem asserts that every C^*-algebra is isometrically isomorphic to a closed subalgebra of $\mathcal{B}(\mathcal{H})$. Homomorphisms from a C^*-algebra to $\mathcal{B}(\mathcal{H})$ are called representations, and the Gelfand-Naimark theorem for non-commutative C^*-algebras is framed in terms of representations.

Definition 2.2.8. Let $\mathcal{A}$ be a C^*-algebra. A **representation** of $\mathcal{A}$ on a Hilbert space $\mathcal{H}$ is a homomorphism $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$. A representation π is

- **non-degenerate** if $\text{span}\{\pi(a)x : a \in \mathcal{A}, x \in \mathcal{H}\}$ is dense in $\mathcal{H}$.
- **faithful** if it is injective.
- **irreducible** if $\pi(\mathcal{A})$ has no non-trivial closed invariant subspaces, i.e. the only subspaces, $S \subset \mathcal{H}$, for which $\pi(a)S \subset S$ are $S = \{0\}$ or $S = \mathcal{H}$.

In $\mathcal{B}(\mathcal{H})$, every vector $\xi \in \mathcal{H}$ determines a linear functional on $\mathcal{B}(\mathcal{H})$ by

$$\phi_\xi : a \mapsto \langle \xi, a\xi \rangle .$$

These linear functionals are states when $\|\xi\| = 1$. States on $\mathcal{B}(\mathcal{H})$ which have this form are called **vector states**. The following theorem tells us that every state of a C^*-algebra is a vector state in some representation.

Theorem 2.2.9 (GNS representation)**.** *Let ϕ be a state on a unital C^*-algebra $\mathcal{A}$. Then there is a Hilbert space $\mathcal{H}_\phi$ and a representation $\pi_\phi : \mathcal{A} \to \mathcal{B}(\mathcal{H}_\phi)$. Furthermore, within $\mathcal{H}_\phi$ there is a unit vector Ω_ϕ such that*

$$\{\pi_\phi(a)\Omega_\phi : a \in \mathcal{A}\} \text{ is dense in } \mathcal{H}_\phi, \text{ and } \phi(a) = \langle \Omega_\phi, \pi_\phi(a)\Omega_\phi \rangle .$$

Given a representation $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$, we say that a vector $\Omega \in \mathcal{H}$ is **cyclic** if $\{\pi(a)\Omega : a \in \mathcal{A}\}$ is dense in $\mathcal{H}$. A representation $\pi : \mathcal{A} \to \mathcal{B}(\mathcal{H})$ is said to be a cyclic representation if there exists a cyclic vector in $\mathcal{H}$. The GNS (Gelfand-Naimark-Segal) representation says that for every state on a C^*-algebra, there is an associated non-degenerate cyclic representation. We will denote this representation, Hilbert space and cyclic vector by the triple $(\mathcal{H}_\phi, \pi_\phi, \Omega_\phi)$, and refer to the triple as the GNS representation of $\mathcal{A}$ associated to ϕ. It turns out that there are enough pure states so that we can

obtain a faithful representation by "stitching" together the GNS representations of all the pure states[2]. The following lemma tells us that "stitching" together representations does actually give us another representation.

Lemma 2.2.10. *Let S be a set, and suppose that for each $s \in S$ there is a representation π_s of $\mathcal{A}$ on a Hilbert space $\mathcal{H}_s$. Then the map*

$$\bigoplus_{s\in S} \pi_s : \mathcal{A} \to \mathcal{B}\left(\bigoplus_{s\in S} \mathcal{H}_s\right)$$

defined by

$$\left(\bigoplus_{s\in S} \pi_s\right)(a) = \bigoplus_{s\in S} \pi_s(a)$$

is a representation of $\mathcal{A}$ on the Hilbert space direct sum $\bigoplus_{s\in S} \mathcal{H}_s$, and this representation is non-degenerate if each of the π_s are.

Definition 2.2.11. Let $\mathcal{A}$ be a C^*-algebra and $\Phi \subset \mathcal{S}(\mathcal{A})$ be the set of pure states of $\mathcal{A}$. For each $\phi \in \Phi$, let π_ϕ denote the GNS representation of $\mathcal{A}$ on $\mathcal{H}_\phi$. The **Gelfand-Naimark representation** of $\mathcal{A}$ is defined to be the representation

$$\bigoplus_{\phi\in\Phi} \pi_\phi : \mathcal{A} \to \bigoplus_{\phi\in\Phi} \mathcal{H}_\phi$$

of $\mathcal{A}$ on the Hilbert space $\bigoplus_{\phi\in\Phi} \mathcal{H}_\phi$.

This representation is simply the direct sum of the GNS representations of pure states, which is well-defined by Lemma 2.2.10. We will use this representation to state the Gelfand-Naimark Theorem for non-commutative C^*-algebras.

Theorem 2.2.12 (Gelfand-Naimark theorem)**.** *Let $\mathcal{A}$ be a C^*-algebra. Then the Gelfand-Naimark representation of $\mathcal{A}$ is a faithful non-degenerate representation.*

Corollary 2.2.13. *Let $\mathcal{A}$ be a C^*-algebra. Then $\mathcal{A}$ is isometrically isomorphic to a closed subalgebra of $\mathcal{B}(\mathcal{H})$, for some Hilbert space $\mathcal{H}$.*

While it is true that every abstract C^*-algebra is isometrically isomorphic to a concrete subalgebra of $\mathcal{B}(\mathcal{H})$ for some $\mathcal{H}$, many C^*-algebras arise independently of a Hilbert space representation. An obvious example is $C_0(X)$.

[2]Here "stitching" corresponds to taking the direct sum.

2.2.3 Continuous functional calculus

Given an element a of a unital C^*-algebra $\mathcal{A}$, we are able to form a C^*-algebra $C^*(a)$. The algebra $C^*(a)$ is defined to be the closure of the subalgebra of $\mathcal{A}$ consisting of all linear combinations of elements of the form

$$a^{m_1}(a^*)^{n_1}a^{m_2}(a^*)^{n_2}\cdots a^{m_p}(a^*)^{n_p}$$

with $m_i, n_i \in \mathbb{N}_0$ and $a^0 := 1_{\mathcal{A}}$. This is referred to as the C^*-algebra generated by a and 1. If the element a commutes with its adjoint, then this C^*-algebra is simply expressed as the closed linear span of elements of the form $a^m(a^*)^n$, i.e.

$$C^*(a) = \overline{\text{span}}\left\{\sum \lambda_{m,n}a^m(a^*)^n\right\}.$$

Definition 2.2.14. An element a of a C^*-algebra $\mathcal{A}$ is **normal** if $aa^* = a^*a$.

For a normal element a, the C^*-algebra generated by a and 1 is a commutative, unital C^*-algebra, and we can therefore apply the Gelfand-Naimark theorem for commutative C^*-algebras. This tells us that for every continuous function[3] f, there exists a corresponding element, $f(a)$, in $\mathcal{A}$, and that these $f(a)$ behave algebraically the way we would expect them to. The continuous functional calculus allows us to take functions of operators in $\mathcal{B}(\mathcal{H})$, or more generally for arbitrary, unital C^*-algebras.

Theorem 2.2.15 (The continuous functional calculus)**.** *Let a be a normal element of a unital C^*-algebra $\mathcal{A}$. Then there is a unique homomorphism $\gamma_a : C(\sigma(a)) \to \mathcal{A}$ which takes the identity function[4] ι to a. Furthermore, γ_a is an isomorphism from $C(\sigma(a))$ to $C^*(a)$.*

Remark 2.2.16. If $a \in \mathcal{A}$ is normal, the image of a continuous function f under the continuous functional calculus homomorphism is often written as $f(a)$. That is,

$$f(a) := \gamma_a(f).$$

To show that this is what we expect for $f(a)$, we give a few examples. We already know that if f is the identity function, then

$$f(a) = \gamma_a(\iota) = a.$$

[3]The function f must be defined and continuous on the spectrum of a.

[4]The identity function is defined by $\iota : z \mapsto z$. Note that this is not the same as the identity element $1 \in C(\sigma(a))$, which is defined to be the constant function $1 : z \mapsto 1$.

For the following three examples let $\mathcal{A}$ be a unital C^*-algebra and suppose $a \in \mathcal{A}$ is normal.

Example 2.2.17. Let $f(z) = \sum c_n z^n$ be a polynomial. That is,

$$f = \sum c_n \iota^n. \tag{2.6}$$

Then, since γ_a is a homomorphism,

$$f(a) = \gamma_a(f) = \gamma_a\left(\sum c_n \iota^n\right) = \sum c_n(\gamma_a(\iota))^n = \sum c_n a^n.$$

Example 2.2.18. Let $f(z) = \bar{z}$. In $C(\sigma(a))$, f is the adjoint of the identity function, so

$$f(a) = \gamma_a(f) = \gamma_a(\iota^*) = a^*.$$

Example 2.2.19. Let $f(z) = \sqrt{z}$. When $\sigma(a) \subset \mathbb{R}^+$, f is defined and continuous on $\sigma(a)$, so the continuous functional calculus guarantees the existence of some element $b = f(a) \in \mathcal{A}$ such that $b^2 = a$.

Positive elements

Before we conclude the section on the continuous functional calculus, we recall that elements of a C^*-algebra which have a spectrum contained in $[0, \infty)$ all have the form b^*b, for a suitable b. We call such elements positive elements because this property allows us to define an ordering on the C^*-algebra.

Definition 2.2.20. Let $\mathcal{A}$ be a unital C^*-algebra. An element $a \in \mathcal{A}$ is **positive** if $\sigma(a) \subset [0, \infty)$. We denote the set of positive elements of $\mathcal{A}$ by $\mathcal{A}_+$.

Theorem 2.2.21. *Let $\mathcal{A}$ be a unital C^*-algebra. Then $a \in \mathcal{A}$ is positive if and only if $a = b^*b$ for some $b \in \mathcal{A}$.*

Proof. If a is positive, then the continuous functional calculus guarantees the existence of an element $b = \sqrt{a}$ for which $b = b^*$ and $a = b^2$. For a proof that $a = b^*b$ implies that a is positive, we refer the reader to [62, Theorem 6.1]. □

Remark 2.2.22. We are able to define an order relation on a C^*-algebra by specifying $a \geq b$ if $a - b \in \mathcal{A}_+$. In particular if $\mathcal{A}$ is unital, the result used in the beginning of the proof of Corollary 2.2.7 is equivalent to the statement $a^*a \leq \|a\|^2 1_{\mathcal{A}}$. Note also that as an immediate result of Theorem 2.2.21 and Definition 2.2.4, a linear functional ϕ is positive if and only if $\phi(a) \geq 0$ for all $a \in \mathcal{A}_+$.

2.3 Von Neumann algebras

The Gelfand-Naimark theorem asserts that commutative C^*-algebras are isomorphic to the algebra of continuous functions on a suitable topological space, and consequently, the theory of arbitrary (i.e. non-commutative) C^*-algebras is sometimes referred to as non-commutative topology. There are a special class of C^*-algebras known as von Neumann algebras which occur as concrete subalgebras of $\mathcal{B}(\mathcal{H})$ for a Hilbert space $\mathcal{H}$. All commutative von Neumann algebras are isomorphic to $L^\infty(X, \mu)$, for some measure space (X, μ), and so the theory of arbitrary (i.e. non-commutative) von Neumann algebras is sometimes referred to as non-commutative measure theory [11]. This section introduces von Neumann algebras.

2.3.1 Operator topologies

Given a Hilbert space $\mathcal{H}$, there are many different topologies one can define on $\mathcal{B}(\mathcal{H})$, the bounded linear operators on $\mathcal{H}$. The topologies we are interested in are the norm, strong, and weak operator topologies. To define these topologies we consider a sequence $\{T_n\} \subset \mathcal{B}(\mathcal{H})$ and specify in what manner these linear operators converge to some operator T.

Definition 2.3.1. Let $\{T_n\} \subset \mathcal{B}(\mathcal{H})$ be a sequence. If $\|T - T_n\| \to 0$ then we say that $T_n \to T$ in the **operator norm topology** or **uniform operator topology**, or that T_n converges to T in norm.

The uniform topology is the strongest topology on $\mathcal{B}(\mathcal{H})$, and is the topology under which $\mathcal{B}(\mathcal{H})$ is a C^*-algebra.

Definition 2.3.2. Let $\{T_n\} \subset \mathcal{B}(\mathcal{H})$ be a sequence. If $T_n x \to Tx$ for all $x \in \mathcal{H}$, we say that $T_n \to T$ in the **strong operator topology**, or that T_n converges to T strongly.

Note that the definition of the strong operator topology can be thought of as pointwise convergence in the underlying Hilbert space $\mathcal{H}$.

Definition 2.3.3. Let $\{T_n\} \subset \mathcal{B}(\mathcal{H})$ be a sequence. If $\phi(T_n x) \to \phi(Tx)$ for all $x \in \mathcal{H}$ and for all $\phi \in \mathcal{H}^*$ then we say that $T_n \to T$ in the **weak operator topology**, or that T_n converges to T weakly.

We are now able to introduce a special class of C^*-algebras called von Neumann algebras, or W^*-algebras. These algebras have various equivalent ways of defining them, however we will use a definition which makes it apparent that von Neumann algebras really are just a special class of C^*-algebras.

Definition 2.3.4. A **von Neumann algebra**, $\mathcal{M}$ on a Hilbert space $\mathcal{H}$, is a $*$-subalgebra of $\mathcal{B}(\mathcal{H})$ containing the identity which is closed in the weak operator topology.

Remark 2.3.5. If $T_n \to T$ in norm, then $T_n \to T$ weakly, so a von Neumann algebra is also norm closed.

Example 2.3.6. Let $\mathcal{H} = L^2(\mathbb{R})$, the space of square integrable functions on $\mathbb{R}$. Then $\mathcal{M} = L^\infty(\mathbb{R})$, the space of essentially bounded measurable functions on $\mathbb{R}$, forms a commutative von Neumann algebra by acting on $\mathcal{H}$ via pointwise multiplication[5].

2.3.2 Double commutant theorem

The analytic definition for von Neumann algebras we have given is most useful for our purposes because it follows immediately from Remark 2.3.5 that von Neumann algebras are also C^*-algebras. Furthermore, weak convergence of operators has physical significance in the mathematical framework of quantum mechanics [60]. Von Neumann's celebrated bicommutant theorem asserts that the analytic definition is equivalent to a purely algebraic definition, and that the exact topology used in the analytic definition is somewhat flexible. We need an algebraic definition before we state the theorem.

Definition 2.3.7. Let $\mathcal{M}$ be a von Neumann algebra. The **commutant** of a subset $S \subseteq \mathcal{M}$ in $\mathcal{M}$ is defined to be the set S' of elements in $\mathcal{M}$ which commute with all elements from S. That is,

$$S' = \{x \in \mathcal{M} : xs = sx \text{ for all } s \in S\}.$$

We define the **double commutant** S'' of S (in $\mathcal{M}$) to be the commutant (in $\mathcal{M}$) of the commutant (in $\mathcal{M}$), i.e. $S'' = (S')'$.

Although similar to the notion of the centre, the commutant is not the same. For clarity, we include the definition of centre.

[5]There is some subtlety here. Functions in $L^2(\mathbb{R})$ and $L^\infty(\mathbb{R})$ are actually equivalence classes of functions, so multiplication is defined pointwise except possibly on a set of measure zero.

Definition 2.3.8. Let $\mathcal{M}$ be a von Neumann algebra. The **centre** of a subset $S \subseteq \mathcal{M}$ is defined to be the set $Z(S)$ of elements in S which commute with all elements from S. That is,

$$Z(S) = \{x \in S : xs = sx \text{ for all } s \in S\}.$$

As we can see, the definition of the centre of S consists of only those elements within the subset S which commute with every element of S, while the commutant consists of all elements in the entire von Neumann algebra which commute with every element of S. We therefore have $Z(S) \subset S'$, and in general, $Z(S) = S \cap S'$.

Theorem 2.3.9 (von Neumann's double commutant Theorem)**.** *Let $\mathcal{M}$ be a subset of bounded linear operators on a Hilbert space $\mathcal{H}$ which contains the identity. Then the following conditions are equivalent:*

1. *$\mathcal{M}$ is equal to the double commutant $\mathcal{M}''$ in $\mathcal{B}(\mathcal{H})$, i.e. $\mathcal{M} = \mathcal{M}''$.*
2. *$\mathcal{M}$ is a von Neumann algebra on $\mathcal{H}$ with $1_{\mathcal{B}(\mathcal{H})} = 1_{\mathcal{M}}$.*

If either of these conditions hold, then $\mathcal{M}$ is closed in the strong topology.

2.3.3 Unbounded operators

Not every operator we deal with in the context of quantum mechanics is bounded. Unbounded operators occur frequently in mathematical physics, and we don't need to think very hard to come up with examples of unbounded operators, as shown by Proposition 2.3.10. For a detailed introduction to the theory of unbounded operators, we refer the reader to [45, Section VIII].

Proposition 2.3.10. *Let x, p be linear operators acting on a Hilbert space $\mathcal{H}$, and suppose these operators satisfy the canonical commutation relation, namely*

$$xp - px = i\hbar 1, \tag{2.7}$$

where $\hbar$ is a positive constant. Then at least one of x, p is not a bounded operator.

Proof. We first prove, by induction, that $[x^n, p] = i\hbar n x^{n-1}$ for all $n \in \mathbb{N}$. Clearly this statement is true for $n = 1$. Assume that the statement is true for $n = k$. That is, suppose

$$[x^k, p] = i\hbar k x^{k-1}$$

To show that the statement is true for $n = k + 1$, we calculate

$$\begin{aligned}
[x^{k+1}, p] &= x^{k+1}p - px^{k+1} = x^k xp - px^{k+1} = x^k(i\hbar 1 + px) - px^{k+1} \\
&= i\hbar x^k + x^k px - px^k x \qquad \text{from Equation 2.7} \\
&= i\hbar x^k + [x^k, p]x \\
&= i\hbar x^k + i\hbar k x^{k-1} x \qquad \text{by hypothesis} \\
&= i\hbar(k+1)x^k.
\end{aligned}$$

Thus the statement is true for $n = k + 1$, and therefore all $n \in \mathbb{N}$. Now given $[x^n, p] = i\hbar n x^{n-1}$, we suppose for contradiction that both x and p are bounded[6]. Then we have

$$\begin{aligned}
\hbar n\|x\|^{n-1} = \hbar n\|x^{n-1}\| = \|i\hbar n x^{n-1}\| &= \|x^n p + (-px^n)\| \\
&\leq \|x^n p\| + \|px^n\| \leq \|x^n\|\,\|p\| + \|p\|\,\|x^n\| \\
&\leq 2\|x\|^n\|p\|,
\end{aligned}$$

so that

$$\|x\|\,\|p\| \geq \frac{\hbar}{2}n$$

for all $n \in \mathbb{N}$. This gives a contradiction since we supposed that x and p were both bounded. It follows that at least one of x, p is unbounded. □

Unlike bounded operators, unbounded operators are not, in general, defined on the whole Hilbert space.

Definition 2.3.11. Let $\mathcal{H}$ be a Hilbert space. An **unbounded operator** T with domain $\mathcal{D}(T)$ is a linear map $T : \mathcal{D}(T) \subset \mathcal{H} \to \mathcal{H}$. Two unbounded operators are equal if they have the same domain and agree on that domain.

Remark 2.3.12. We are defining an unbounded operator as a 'not necessarily bounded' operator. Thus a bounded operator $T \in \mathcal{B}(\mathcal{H})$ is an unbounded operator with $\mathcal{D}(T) = \mathcal{H}$.

Definition 2.3.13. Let T be an unbounded operator on a Hilbert space $\mathcal{H}$ which is densely defined, i.e. $\mathcal{D}(T)$ is dense in $\mathcal{H}$. Define a new operator T^*, called the **adjoint** of T, by defining the domain of T^* as

$$\mathcal{D}(T^*) = \{y \in \mathcal{H} : \exists z \in \mathcal{H} \text{ with } \langle z|x\rangle = \langle y|Tx\rangle\,, \forall x \in \mathcal{D}(T)\}.$$

We then define $T^* y = z$.

[6] If x and p are bounded linear operators on a Hilbert space, and are therefore elements of the C^*-algebra $\mathcal{B}(\mathcal{H})$, they satisfy the C^*-identity. In particular, $\|x\|^n = \|x^n\|$

We wish to define a self-adjoint operator as one which is equal to its adjoint.

Definition 2.3.14. Let $\mathcal{H}$ be a Hilbert space. A densely defined unbounded operator T is **symmetric** if

$$\langle Ty|x\rangle = \langle y|Tx\rangle$$

for all $x, y \in \mathcal{D}(T)$. An unbounded operator is **self-adjoint** if it is symmetric and $\mathcal{D}(T) = \mathcal{D}(T^*)$.

A symmetric operator clearly has $\mathcal{D}(T) \subset \mathcal{D}(T^*)$, but the domain of a symmetric operator is not, in general, the same as the domain of its adjoint. For a bounded operator A, $\mathcal{D}(A) = \mathcal{D}(A^*) = \mathcal{H}$, so a bounded symmetric operator is self-adjoint.

Unbounded[7] operators are not continuous and therefore much harder to work with. A closed operator is not necesarily continuous, but is, in some sense, the 'minimal' replacement for a continuous operator. Many operators we deal with in mathematical physics turn out to be either closed or closable.

Definition 2.3.15. Let T be an operator on a Hilbert space $\mathcal{H}$. The **graph** of T is the set of pairs

$$\Gamma(T) = \{(\xi, T\xi) : \xi \in \mathcal{D}(T)\}.$$

Definition 2.3.16. An operator T on a Hilbert space $\mathcal{H}$ is called **closed** if its graph $\Gamma(T)$ is a closed subset of $\mathcal{H} \times \mathcal{H}$.

Definition 2.3.17. Let T and T' be operators on a Hilbert space $\mathcal{H}$. If $\Gamma(T) \subset \Gamma(T')$ then T' is said to be an **extension** of T.

Definition 2.3.18. An operator T on a Hilbert space $\mathcal{H}$ is said to be **closable** if it has a closed extension. Every closable operator has a smallest closed extension, called its **closure**, which we denote by $\overline{T}$.

Proposition 2.3.19. *Let T be a densely defined operator on a Hilbert space $\mathcal{H}$. Then the adjoint T^* is a closed operator. Furthermore, T is closable if and only if $\mathcal{D}(T^*)$ is dense, in which case $\overline{T} = T^{**}$*

[7] Here we mean unbounded as in 'not bounded'.

Proof. We follow the proof of [45, Theorem VIII.1], and begin by defining a unitary operator V on $\mathcal{H} \times \mathcal{H}$ by

$$V(\phi, \psi) = (-\psi, \phi).$$

Since orthogonal complements are automatically closed, it suffices to show that $\Gamma(T^*) = [V\Gamma(T)]^\perp$. Let T be a linear operator on $\mathcal{H}$ and suppose $(\phi, \eta) \in \mathcal{H} \times \mathcal{H}$. Then, since V is unitary, $V[\Gamma(T)]^\perp = [V\Gamma(T)]^\perp$, and $(\phi, \eta) \in [V\Gamma(T)]^\perp$ if and only if

$$\langle (\phi, \eta), (-T\psi, \psi) \rangle = 0.$$

By the definition of the inner-product on $\mathcal{H} \times \mathcal{H}$, this is true if and only if

$$\langle \phi, T\psi \rangle = \langle \eta, \psi \rangle .$$

In other words, $(\phi, \eta) \in [V\Gamma(T)]^\perp$ if and only if $(\phi, \eta) = (\phi, T^*\phi) \in \Gamma(T^*)$, and therefore T^* is a closed operator. For the second part of the proposition, we note that since $\Gamma(T)$ is a linear subspace of $\mathcal{H} \times \mathcal{H}$, we have

$$\overline{\Gamma(T)} = \left(\Gamma(T)^\perp\right)^\perp = \left(V^2\Gamma(T)^\perp\right)^\perp = V(V\Gamma(T)^\perp)^\perp = V\Gamma(T^*)^\perp$$

If T^* is a densely defined operator, then the proof from the first part of the proposition says that

$$\overline{\Gamma(T)} = V\Gamma(T^*)^\perp = \Gamma(T^{**})$$

and therefore T^{**} is a closed extension for T. In particular, since $\Gamma(T^{**}) = \overline{\Gamma(T)}$, it is the smallest closed extension, and $\overline{T} = T^{**}$. We prove the converse by contrapositive, i.e. we suppose that $\mathcal{D}(T^*)$ is not dense and show that T is not closable. Suppose that $\mathcal{D}(T^*)$ is not dense and fix $\psi \in [\mathcal{D}(T^*)]^\perp$. For any $(\phi, T^*\phi) \in \Gamma(T^*)$, we have

$$\langle (\psi, 0), (\phi, T^*\phi) \rangle = \langle \psi, \phi \rangle + \langle 0, T^*\phi \rangle = \langle \psi, \phi \rangle = 0$$

where the last equality holds because $\psi \in [\mathcal{D}(T^*)]^\perp$. It follows that $(\psi, 0) \in [\Gamma(T^*)]^\perp$ and therefore $V[\Gamma(T^*)]^\perp$ is not the graph of a linear operator because it contains $(0, \psi)$. Since $\overline{\Gamma(T)} = [V\Gamma(T^*)]^\perp$, we see that T is not closable. □

Proposition 2.3.19 implies that every symmetric operator is necessarily closable, since its adjoint is a closed extension.

Definition 2.3.20. A symmetric operator T on a Hilbert space $\mathcal{H}$ is called **essentially self-adjoint** if its closure $\overline{T}$ is self-adjoint. If T is closed, a subset $\mathcal{C} \subset \mathcal{D}(T)$ is called a **core** of T if $\overline{T|_\mathcal{C}} = T$.

2.3.4 Tomita-Takesaki theory

This section is based largely on material covered in [7, Section 2.5].

Definition 2.3.21. Let $\mathcal{M}$ be a von Neumann algebra, and ϕ be a positive linear functional on $\mathcal{M}$. We say that ϕ is **normal** if

$$\phi(\text{l.u.b.}_\alpha A_\alpha) = \sup_\alpha \phi(A_\alpha)$$

for all increasing nets $\{A_\alpha\}$ in $\mathcal{M}_+$ with an upper bound.

Remark 2.3.22. If $\mathcal{M}$ is finite dimensional, then each state is a normal state.

Theorem 2.3.23. *Let ϕ be a state on a von Neumann algebra $\mathcal{M}$ acting on a Hilbert space $\mathcal{H}$. Then ϕ is normal if and only if there exists a density matrix ρ, i.e. a positive trace-class operator ρ on $\mathcal{H}$ with $\mathrm{Tr}(\rho) = 1$, such that*

$$\phi(A) = \mathrm{Tr}(\rho A) \qquad \forall A \in \mathcal{M}.$$

In order to state the Tomita-Takesaki theorem, we need to define the notion of a modular operator.

Definition 2.3.24. Let $\mathcal{M}$ be a von Neumann algebra on a Hilbert space $\mathcal{H}$. A vector $\Omega \in \mathcal{M}$ is **separating** if, for any $A \in \mathcal{M}$, $A\Omega = 0$ implies $A = 0$.

Definition 2.3.25. Let $\mathcal{M}$ be a von Neumann algebra on a Hilbert space $\mathcal{H}$, and $\Omega \in \mathcal{H}$ a separating and cyclic vector. We define operators[8] S_0 and F_0 by first specifying their domains:

$$\mathcal{D}(S_0) = \mathcal{M}\Omega = \{m\Omega : m \in \mathcal{M}\}$$
$$\mathcal{D}(F_0) = \mathcal{M}'\Omega = \{m\Omega : m \in \mathcal{M}'\},$$

where $\mathcal{M}'$ is the commutant of $\mathcal{M}$. The operators S_0 and F_0 are then defined by

$$S_0(m\Omega) = m^*\Omega$$
$$F_0(m\Omega) = m^*\Omega.$$

[8]These operators are unbounded operators, and therefore not in $\mathcal{B}(\mathcal{H})$. In particular, these operators are not defined on the whole Hilbert space $\mathcal{H}$.

The operators occurring in Definition 2.3.25 are unbounded, anti-linear operators defined on dense subspaces of $\mathcal{M}$. These operators are not closed, but are closable. For a proof, see [7, Proposition 2.5.9].

Proposition 2.3.26. *The operators S_0 and F_0 are closable.*

We will denote the closures by S and F, i.e.

$$S = \overline{S_0}, \qquad F = \overline{F_0}.$$

The following proposition is a particular case of a more general result known as polar decomposition. Polar decomposition is a generalisation of the polar form of a complex number to operators on a Hilbert space.. In our case, we are using [45, Proposition before Theorem VIII.33] which guarantees the existence of a polar decomposition for closed operators.

Proposition 2.3.27. *Let S be the closed operator defined above. Then there exists a unique, positive, self-adjoint operator Δ, and a unique anti-unitary operator J such that*

$$S = J\Delta^{1/2}.$$

We call Δ the ***modular operator associated to the pair*** $(\mathcal{M}, \Omega)$*, and J the* ***modular conjugation****.*

For a proof of the following proposition, see [7, Proposition 2.5.11].

Proposition 2.3.28. *The following relations are valid:*

$$\Delta = FS, \qquad \Delta^{-1} = SF, \qquad S = J\Delta^{1/2},$$
$$F = J\Delta^{-1/2}, \qquad J = J^*, \qquad J^2 = 1,$$
$$\Delta^{-1/2} = J\Delta^{1/2}J.$$

We are now in a position to state the Tomita-Takesaki theorem, sometimes called Tomita's theorem. For a proof, see [7, Theorem 2.5.14] or [26, Theorem 9.2.9].

Theorem 2.3.29 (Tomita-Takesaki theorem)**.** *Let $\mathcal{M}$ be a von Neumann algebra with cyclic and separating vector Ω, and let Δ be the associated modular operator and J the associated modular conjugation. It follows that*

$$J\mathcal{M}J = \mathcal{M}'$$

and, moreover,

$$\Delta^{it}\mathcal{M}\Delta^{-it} = \mathcal{M}.$$

Our primary interest in the Tomita-Takesaki theorem lies in the fact that we can use it to construct automorphisms of a von Neumann algebra.

Definition 2.3.30. A state ϕ on a von Neumann algebra $\mathcal{M}$ is **faithful** if $\phi(A) > 0$ for all non-zero $A \in \mathcal{M}_+$.

Lemma 2.3.31. *Let $\mathcal{M}$ be a von Neumann algebra, and ϕ a faithful, normal state on $\mathcal{M}$. Consider $(\mathcal{H}_\phi, \pi_\phi, \Omega_\phi)$, the GNS representation of $\mathcal{M}$ associated to ϕ. Then the cyclic vector Ω_ϕ is separating for $\pi_\phi(\mathcal{M})$.*

Proof. Fix $\pi_\phi(A) \in \pi_\phi(\mathcal{M})$ and suppose that $\pi_\phi(A)\Omega_\phi = 0$. Then

$$\begin{aligned} 0 = \|\pi_\phi(A)\Omega_\phi\|^2 &= \langle \pi_\phi(A)\Omega_\phi | \pi_\phi(A)\Omega_\phi \rangle \\ &= \langle \Omega_\phi | \pi_\phi(A)^*\pi_\phi(A)\Omega_\phi \rangle = \langle \Omega_\phi | \pi_\phi(A^*A)\Omega_\phi \rangle \\ &= \phi(A^*A). \end{aligned}$$

Since ϕ is faithful, this implies that A^*A must be zero, and hence $A = 0$. The GNS representation π_ϕ is a homomorphism, so $\pi(0) = 0$, and thus Ω_ϕ is separating. □

Definition 2.3.32. Let $\mathcal{M}$ be a von Neumann algebra and ϕ a faithful, normal state on $\mathcal{M}$. Let $(\mathcal{H}_\phi, \pi_\phi, \Omega_\phi)$ be the GNS representation of $\mathcal{M}$ associated to ϕ, and Δ the modular operator associated to the pair $(\pi_\phi(\mathcal{M}), \Omega_\phi)$. Then Theorem 2.3.29 defines a one-parameter group $t \mapsto \tau_t^\phi$ of automorphisms of $\mathcal{M}$ by the definition

$$\tau_t^\phi(A) = \pi_\phi^{-1}(\Delta^{it}\pi_\phi(A)\Delta^{-it}).$$

The group $t \mapsto \tau_t^\phi$ is called the **modular automorphism group associated with the pair** $(\mathcal{M}, \phi)$.

Chapter 3

Algebraic quantum mechanics

3.1 Basic theory

In this section we describe the standard mathematical structure of physical systems and provide some physical motivation for why this structure generalises naturally to an algebraic description in terms of C^*-algebras. The content from this section is based largely on the material covered in [60]

When we describe a physical system, we often talk about the state of the system, and the observables of the system. The state of the system is a result of the way that system has been prepared - it is a particular arrangement of the physical system. An observable is a quantity that we can experimentally measure. When we perform an experiment, we are measuring an observable on a particular state. One can think of the state as possessing all the information possible about the system, and the observables as ways of accessing that information.

3.1.1 Classical mechanics

The Hamiltonian formulation of classical mechanics describes the state of a physical system by a point $P = \{p, q\} \in \Gamma$ in the phase space manifold, Γ, which we usually regard as being locally compact[1]. Observables of the physical system include the canonical variables, i.e. the position q and momentum p, and generally (real) continuous functions $f(q, p) \in C_{\mathbb{R}}(\Gamma)$.

We specify the dynamics of the system by a time evolution of the canonical variables,

[1]The phase space is usually the cotangent space T^*M for a possibly non-compact manifold M.

which induces a time evolution of the observables of the system

$$q \to q_t = q(t, q, p)$$
$$p \to p_t = p(t, q, p)$$
$$f(q, p) \to f_t(q, p) = f(q_t, p_t).$$

This time evolution of the system is usually assumed to be smooth in the time parameter, t, and is governed by an observable, $H(q, p, t)$, known as the Hamiltonian, which frequently corresponds to the total energy of the system. The time evolution of the canonical variables satisfy Hamilton's equations:

$$\dot{q} = \frac{\partial H}{\partial p} \qquad\qquad \dot{p} = -\frac{\partial H}{\partial q},$$

There is an equivalent way of writing Hamilton's equations which generalise more naturally to quantum mechanics. For two (smooth) functions $f(q, p)$ and $g(q, p)$, we define the **Poisson bracket** $\{f, g\}_{PB}$ of f and g to be

$$\{f, g\}_{PB} := \frac{\partial f}{\partial q}\frac{\partial g}{\partial p} - \frac{\partial f}{\partial p}\frac{\partial g}{\partial q}.$$

With this notation, Hamilton's equations become

$$\dot{q} = \{q, H\}_{PB} \qquad\qquad \dot{p} = \{p, H\}_{PB},$$

and more generally the time evolution of any observable $f(q, p)$ is given by

$$\dot{f} = \{f, H\}_{PB}.$$

Describing a physical system usually amounts to finding (or being given) the Hamiltonian and initial conditions for the system, and then integrating Hamilton's equations to obtain an explicit formula for how the canonical variables (and hence the observables of the system) change over time.

The Gelfand-Naimark theorem (2.2.12) suggests that it is possible to rephrase this formulation of classical physics into an algebraic framework. The classical observables form an algebra of real (or more generally complex) continuous functions on the phase space manifold, which we will denote $\mathcal{A}$. This is an abelian $*$-algebra, which becomes a Banach $*$-algebra under the sup-norm:

$$\|f\| = \sup_{x \in \Gamma} |f(x)|.$$

For any $a \in \mathbb{C}$, we have

$$a^* a = |a|^2,$$

and hence for any observable f we have

$$\|f^* f\| = \|f\|^2.$$

Since these observables also satisfy the C^*-identity, they therefore form an abelian C^*-algebra.

According to our current formulation, physical states correspond to exact points in our phase space Γ. This suggests that we are able to measure the values of the observables, in particular the position and momentum, to infinite precision. In reality, there is always some kind of systematic error in measurement, so that the configuration of the system of the system at the initial time t_0 is known to within a certain error, and this error then propagates through time.

The physical method for measuring an observable f on a state ϕ is to perform replicated measurements $f_1(\phi), f_2(\phi), ..., f_n(\phi)$ of f on ϕ and then take the average of these results:

$$\langle f \rangle_n^\phi = \frac{f_1(\phi) + f_2(\phi) + ... + f_n(\phi)}{n}.$$

The expectation value of the observable f on ϕ is defined to be the limit $n \to \infty$, written

$$\phi(f) = \lim_{n \to \infty} \langle f \rangle_n^\phi .$$

Each state, ϕ, therefore determines a functional on the observables, $\phi : f \mapsto \phi(f)$. From the definition of the expectation value as the average of the results of measurements, it is clear that these are linear functionals, and furthermore, that they satisfy the following condition

$$\phi(f^* f) \geq 0 \qquad \forall f \in \mathcal{A}.$$

To see this, simply note that $(f^* f)(x) = \overline{f(x)} f(x) = |f(x)|^2 \geq 0$, and then apply the definition of the expectation value to $f^* f$. This condition is known as the positivity condition, and functionals which satisfy it are known as positive functionals. The set of functionals on a normed vector space V over $\mathbb{C}$ form a Banach space with norm given by

$$\|\phi\| := \sup\{|\phi(a)| : \|a\| = 1\}.$$

Given a non-zero functional ϕ with finite norm, we can always normalise it: $\phi \to \phi_{norm} = \frac{\phi}{\phi(1)}$, so that $\phi_{norm}(1) = 1$. Thus, quite generally, we identify physical states of our system with positive, normalised, linear functionals on $\mathcal{A}$.

The following theorem[2] allows us to connect this view of our physical system with our notion that the canonical coordinates of the system are not known to infinite precision.

Theorem 3.1.1 (Riesz-Markov theorem)**.** *Let Γ be a compact Hausdorff space. For any positive linear functional, ϕ, on $C(\Gamma)$, there is a unique Baire measure μ_ϕ on Γ with*

$$\phi(f) = \int_\Gamma f \, d\mu_\phi \quad \textit{and} \quad \mu_\phi(\Gamma) = \phi(1) = 1.$$

Thus the expectation value is interpreted probabilistically: states are probability measures and observables are random variables. We are still able to describe a situation in which the canonical coordinates are known to infinite precision using this framework. We suppose that μ_x is a probability measure[3] such that $\mu_x(S) = 1$ if S is a measurable set containing x, and $\mu_x(S) = 0$ if S is a measurable set not containing x. Then the state corresponding to this probability measure is

$$\phi_x(f) = \int_\Gamma f \, d\mu_x = f(x).$$

We can calculate the variance for this state, or generally for any state, from the formula:

$$(\Delta_\phi f)^2 = \phi((f - \phi(f))^2).$$

For the Dirac state, ϕ_x, above, the variance is identically zero. States in which the variance vanishes are called dispersion free states.

The time evolution of the canonical coordinates, $\{q, p\} \to \{q_t, p_t\}$, determines a one-parameter family of continuous invertible mappings, $\tau_t : f(q,p) \to f(q_t, p_t)$, from the algebra of observables into itself which preserves the algebraic structure, i.e. $\tau_t(fg) = \tau_t(f)\tau_t(g)$ and $\tau_t(f^*) = (\tau_t(f))^*$. These mappings have a group structure, with the group operation being composition, $\tau_t \circ \tau_s = \tau_{t+s}$, and inverses given by $(\tau_t)^{-1} = \tau_{-t}$. Thus, according to Definition 2.1.8, the time evolution is given by a one-parameter group of automorphisms of our algebra of observables. We can define, if we like, the evolution of the states rather than the observables[4], by defining

$$\phi_t(a) := \phi(\tau_t(a)) \quad \forall a \in \mathcal{A}.$$

[2]The statement of this theorem is taken from [45, Theorem IV.14]

[3]The measure μ_x is actually the Dirac δ function, $\delta(x)$

[4]This idea occurs in section 3.1.2 where we mention the different formulations of quantum mechanics

3.1.2 Quantum mechanics

In the standard description of quantum mechanics, the state of a physical system is represented by a vector[5] in some Hilbert space, and that the physical observables of the system are represented by self-adjoint[6] operators acting on this Hilbert space. In particular, observables don't, in general, commute. Time evolution is specified in one of two ways: evolution of the observables, known as the Heisenberg picture, or evolution of the states, known as the Schrödinger picture.

Algebraic quantum mechanics abstracts the standard formalism of quantum mechanics, forgoing the Hilbert space of states. In parallel with the algebraic formulation of classical mechanics, the algebraic formalism focuses on the observables, which generate a $*$-algebra. We refer to this algebra as the algebra of observables, and the states become linear functionals on this algebra. The dynamics of the system is given by one-parameter group of $*$-automorphisms. This algebraic approach is suggested by an analogy with classical mechanics, the GNS-Theorem, and the physical method of measuring observables.

Algebra of observables

A physical system in a particular state has a variety of physical properties which we can experimentally measure. We call these properties observables, and denote the set of observables by $\mathcal{A}$. The observables which we are interested in frequently include the position, momentum and total energy. Each observable is intrinsically linked to an experimental apparatus, i.e. the method of measuring that observable. Given an observable $a \in \mathcal{A}$, we may define the scalar $\lambda a \in \mathcal{A}$ as the observable corresponding to the experimental apparatus obtained by scaling the apparatus associated to a. We could do this physically or by simply scaling the results of experiments of a by λ. Similarly, we can argue that powers of observables, a^n, should be included in our set of observables as the observable corresponding to raising the result of any experiment of a to the power of n. With this notion of observables, we define a^0 to be the observable whose results of measurements always take the value 1, independent of the state being measured. Quite

[5]Technically states in quantum mechanics are rays, since the two states $\vec{v}$ and $c\vec{v}$ are considered to be equivalent states for all $c \neq 0$. For this reason, we usually require states to be normalised, i.e. $\|\vec{v}\| = 1$, and the two states $e^{i\phi}\vec{v}$ and $\vec{v}$ are considered equivalent.

[6]Self-adjointness guarantees that expectation values, which are measurable quantities, are real.

generally, each observable $a \in \mathcal{A}$, generates an abelian algebra $\mathcal{A}_a$. In analogy with classical mechanics, we posit that the total set of observables form a unital C^*-algebra.

States as states

A physical state is a given way of preparing a physical system. For each observable a and each state ϕ, there is a corresponding quantity $\phi(a)$ called the expectation value. We have come across this notion already with classical systems, and the algebraic extension of quantum mechanics runs parallel to that discussion.

States associate a given observable to an expectation value - the 'average' value of the measurements of that observable when the system is in that particular state. It follows from the definition of the expectation value that a state defines a linear functional on the algebra of observables $\mathcal{A}$. This linear functional is assumed to be positive by analogy with classical mechanics, and from the way we have defined the identity observable 1, we know that $\phi(1) = 1$. By Corollary 2.2.7, this implies that a physical state is precisely a state in the C^*-algebraic sense of the word. This is not just a happy coincidence - much of the theory of C^*-algebras was created in order to study physical systems and in particular, quantum mechanics.

Algebraic dynamics

Our current description of a physical system involves an algebra of observables and states on that algebra which represents the information obtainable from the system by experiments. The system is implicitly static, since neither the algebra of observables nor the states have any notion of time evolution yet. To introduce a time evolution, we assume that the algebra of observables defines the observables at some time, say $t = 0$, and then define an evolution of the observables by $\tau_t : a \mapsto a_t$. This time evolution should behave well under compositions, i.e. $\tau_t(\tau_s(a)) = \tau_{t+s}(a)$, and be reversible, i.e. $(\tau_t)^{-1}(a) = \tau_{-t}(a)$. This evolution is thus a group, and in analogy with classical mechanics, a one-parameter group of $*$-automorphisms. A definition from the theory of C^*-algebras is relevant here.

Definition 3.1.2. Let $\mathcal{A}$ be a C^*-algebra and let G be a locally compact group. Suppose that $\tau : G \to \mathrm{Aut}(\mathcal{A})$ is a strongly continuous homomorphism. Then we call the tuple $(\mathcal{A}, G, \tau)$ a **C^*-dynamical system**.

Dynamical systems are ideal for modelling physical systems which have some notion of time evolution. In practice, we often deal with continuous (rather than discrete) time evolution parameterised by $t \in \mathbb{R}$, so that our group G is simply $\mathbb{R}$ under addition, and we write $\tau_t := \tau(t)$. This is a one parameter group of strongly continuous automorphisms, which 'shuffle around' the elements of our algebra as time changes. Like classical mechanics, the time evolution in qauntum mechanics is determined by a quantity called the Hamiltonian. The Hamiltonian in quantum mechanics is an observable, which usually corresponds to the total energy of the system, and so is represented by a self-adjoint operator H acting on a Hilbert space $\mathcal{H}$. One method of obtaining the quantum mechanical equations of motion is to formally 'qauntise' classical mechanics. This is done by replacing the classical observables with operators, and replacing the Poisson bracket of classical mechanics with the commutator (multiplied by some constant factor). The time evolution of an observable a then becomes

$$\dot{a} = -\frac{i}{\hbar}[a, H], \tag{3.1}$$

where $\hbar$ is the reduced Planck constant, which has an approximate value (in S.I. units) of 1.055×10^{-34} J·s. If the observable $a(t)$ at time $t = 0$ is a, then Equation (3.1) has the solution

$$a(t) = \tau_t(a) = e^{\frac{itH}{\hbar}} a e^{-\frac{itH}{\hbar}}.$$

This is known as the evolution generated by the Hamiltonian, and is the standard time evolution of a quantum mechanical system.

Theorem 3.1.3 (Stone's theorem)**.** *Let U_t be a strongly continuous one-parameter unitary group on a Hilbert space $\mathcal{H}$. Then there exists a unique self-adjoint operator A such that*

$$U_t = e^{itA}$$

for all $t \in \mathbb{R}$. Conversely, if A is a self-adjoint operator acting on a Hilbert space $\mathcal{H}$, then

$$U_t := e^{itA}$$

is a strongly continuous one-parameter family of unitary operators.

Since the Hamiltonian is self-adjoint, Stone's theorem guarentees that the time evolution generated by H is strongly continuous. The algebraic formulation of quantum

mechanics assumes that the time evolution of the algebra of observables is a strongly continuous group of automorphisms. As with classical mechanics, we define a time evolution of the states rather than the observables by defining

$$\phi_t(a) := \phi(\tau_t(a)) = \phi(a_t) \quad \forall a \in \mathcal{A}.$$

The mathematical description of a physical system can be summarised by the following:

A physical system is defined by its C^*-algebra of observables $\mathcal{A}$. The states of the physical system correspond to positive linear functionals of norm 1 whose value on an observable gives the expectation value of that observable in the given state. The dynamics of the system is determined by a strongly continuous one-parameter group of automorphisms of the algebra of observables (in the Heisenberg picture), or the states (in the Schrödinger picture). In particular, the system defines a C^*-dynamical system.

3.2 An exploration into $\mathcal{B}(\mathcal{H})$

This section deals with some techniques and ideas from the theory of bounded linear operators on a Hilbert space which are useful in a physical context. Many of these concepts come from the traditional formulation of quantum mechanics. We begin by describing explicitly a notation in common usage among physicists called bra-ket notation.

3.2.1 Bra-ket notation

Bra-ket notation was invented by Paul Dirac in 1939, and is also known as Dirac notation. Bra-ket notation is used to describe vectors and linear functionals in the context of Hilbert spaces.

Kets are just vectors

There are many common notations used to denote a vector, such as $\vec{\psi}, \bar{\psi}, \hat{\psi}$ or $\underline{\psi}$. In Dirac notation, we write vectors with vertical lines and angle brackets, $|\psi\rangle$, and say "ket-psi". Like other vector notation, the symbol inside the ket is simply a label for the vector. We are free to label our vectors however we like, so we often choose labels which are relevant to our particular problem. As an example, a vector $\vec{v} = (x, y) \in \mathbb{R}^2$ can be written, in

standard notation, as

$$\vec{v} = x\hat{e}_1 + y\hat{e}_2.$$

In Dirac notation, we would write

$$|v\rangle = x\,|e_1\rangle + y\,|e_2\rangle\,.$$

Bras are just linear functionals

Linear functionals on a vector space, V, are linear maps from V to the underlying scalar field (usually $\mathbb{C}$). The set of all linear functionals over V is a vector space called the dual space of V, written[7] V^*. In Dirac notation, functionals are written using angle brackets and vertical lines, $\langle\phi|$, and read "bra-phi". Thus a linear functional in standard notation looks like

$$\phi : V \to \mathbb{C},$$

while in Dirac notation, we would write

$$\langle\phi| : V \to \mathbb{C}.$$

So far all we have done is change the notation trivially. At the moment, the action of a bra, $\langle\phi|$, on a ket, $|\psi\rangle$, is written $\langle\phi|\,(|\psi\rangle)$. The reason for this notation change will hopefully become apparent in the next section.

Now it gets a bit trickier

The power of the bra-ket notation relies on the duality of vectors and functionals. The Riesz-representation theorem says that every vector (ket) in a Hilbert space defines a linear functional (bra) in a unique and unambigous way, via the inner product. Furthermore, every bra is defined in this way by some ket.

To state the theorem, we consider a Hilbert space, $\mathcal{H}$, with inner product $\langle\cdot,\cdot\rangle$ which is linear in the second variable. If x is an element of $\mathcal{H}$, then define

$$\phi_x(y) := \langle x, y\rangle \quad \forall y \in \mathcal{H}.$$

For each $x \in \mathcal{H}$, ϕ_x defines a linear functional, $\phi_x : \mathcal{H} \to \mathbb{C}$, so $\phi_x \in \mathcal{H}^*$.

[7] This notation should not be confused with C^*, W^*, or any other $*$-notation we have used.

Theorem 3.2.1 (Riesz Representation Theorem)**.** *The map* $\hat{\Phi} : x \mapsto \phi_x$ *is an isometric anti-isomorphism from* $\mathcal{H}$ *to* $\mathcal{H}^*$*.*

In terms of Dirac notation, our vectors are kets, $|x\rangle$, and since vectors correspond, in a one-to-one way, to linear functionals, we can define $\hat{\Phi}(|x\rangle) = \langle x|$. This notation is consistent with our previous definition of bras as linear functionals, and the action of a bra $\langle x|$ on a ket $|y\rangle$, now written compactly as $\langle x|y\rangle$, is given by the Riesz representation theorem as

$$\langle x|y\rangle := \langle x| \left(|y\rangle\right) = \langle x, y\rangle .$$

Thus a braket $\langle \cdot|\cdot\rangle$ defines an inner product which is linear in its second variable. Dirac notation emphasises that although a braket defines an inner product, bras and kets make sense individually.

Operators in the bra-ket notation

An operator, A, acting on a ket, $|x\rangle$, gives us another ket, simply written as $A|x\rangle$ or sometimes $|Ax\rangle$. We can also view operators as acting on bras by defining $\langle y| A$ to be the linear functional

$$\langle y| A \left(|x\rangle\right) := \langle y| \left(A|x\rangle\right) = \langle y, Ax\rangle$$

We thus unambiguously define $\langle y|A|x\rangle$ as the functional $\langle y|$ acting on the ket $A|x\rangle$. Since an operator acting on a vector gives another vector, it is natural to ask what is the linear functional associated (via the Riesz representation theorem) to the vector $A|x\rangle$. The associated linear functional is $\langle Ax| = \langle x| A^*$, where A^* is the adjoint of the operator A.

The rank one operators we defined in Example 2.1.7 can be written nicely in bra-ket notation. Recall that $\theta_{x,y}$ is the operator defined by

$$\theta_{x,y}(z) = \langle y, z\rangle\, x.$$

In bra-ket notation, we have

$$\theta_{x,y} = |x\rangle \langle y| .$$

Then the action of this operator on a vector $|z\rangle$ is simply

$$\begin{aligned} \theta_{x,y}(z) &= |x\rangle \langle y| \left(|z\rangle\right) \\ &= \langle y|z\rangle \ |x\rangle . \end{aligned}$$

3.2.2 Trace-class operators

If we choose a Hilbert space, $\mathcal{H}$, of finite dimension, n, then the bounded linear operators on $\mathcal{H}$ are simply the $n \times n$ matrices. For infinite dimensional Hilbert spaces this is no longer true, but we expect that some properties, such as the trace of a matrix, could have an analogue for $\mathcal{B}(\mathcal{H})$, where $\mathcal{H}$ is no longer finite dimensional. It turns out we do have such a notion, provided the Hilbert space is not 'too' infinite.

Definition 3.2.2. Let X be a topological space. We say that X is **separable** if it contains a countable dense subset.

For Hilbert Spaces, this topological definition is equivalent to the existence of a countable orthonormal basis.

Lemma 3.2.3. *Let $\mathcal{H}$ be a Hilbert Space. It follows that $\mathcal{H}$ is separable (in the sense defined above) if and only if it has a countable orthonormal basis.*

Proof. If $\mathcal{H}$ has a countable orthonormal basis, $\{e_n\}$, then

$$\left\{ \sum_n (a_n + ib_n)e_n : a_n,\, b_n \in \mathbb{Q} \right\}$$

forms a countable dense subset, and so $\mathcal{H}$ is separable. For the reverse implication, we show the contrapositive, i.e. we show that if $\mathcal{H}$ has an uncountable orthonormal basis, then it is not separable.

Let $\{e_\alpha\}_{\alpha \in I}$ be an orthonormal basis for $\mathcal{H}$ and suppose that I is uncountable. Let $\mathcal{E}$ be a dense subset of $\mathcal{H}$. For any two elements in our basis, e_α and e_β, orthonormality implies that

$$\begin{aligned} \|e_\alpha - e_\beta\|^2 &= \langle e_\alpha - e_\beta | e_\alpha - e_\beta \rangle \\ &= \langle e_\alpha | e_\alpha \rangle + \langle e_\beta | e_\beta \rangle \\ &= \|e_\alpha\|^2 + \|e_\beta\|^2 \\ &= 2. \end{aligned}$$

Thus the open balls, $B_{\sqrt{2}/2}(e_\alpha)$ are disjoint. Since $\mathcal{E}$ is dense in $\mathcal{H}$, each ball, being an open set, intersects $\mathcal{E}$ non-trivially. Thus for each $\alpha \in I$, we can find an element $x_\alpha \in \mathcal{E}$ such that $x_\alpha \in B_{\sqrt{2}/2}(e_\alpha)$ and $\alpha \neq \beta \implies x_\alpha \neq x_\beta$. Since I is uncountable, this implies that $\mathcal{E}$ is also uncountable, so $\mathcal{H}$ cannot be separable. □

The trace for linear operators acting on finite dimensional inner-product spaces is simply the sum of the diagonal elements in any matrix representation of the operator. That is, given any orthonormal basis, $(e_1, e_2, \ldots, e_n)$, of the vector space, the trace of a linear operator, A, is defined by

$$\mathrm{Tr}(A) = \sum_{i=1}^{n} \langle e_i \,|\, Ae_i \rangle \,.$$

This definition of the trace is what we generalise to bounded linear operators on a Hilbert space. In order for this extension to make sense, we need to make sure that we are able to sum over an orthonormal basis of the Hilbert space, and we need to make sure this sum converges and is independent of the basis we have chosen.

Definition 3.2.4. Let $\mathcal{H}$ be a separable Hilbert space. A bounded linear operator, $A \in \mathcal{B}(\mathcal{H})$, is **trace class** if for some (and hence all) orthonormal bases, $\{e_j\}_j$, of $\mathcal{H}$, the following sum of positive terms

$$\mathrm{Tr}\ (|A|) := \sum_j \left\langle e_j \,\middle|\, (A^*A)^{\frac{1}{2}} e_j \right\rangle$$

is finite.
If that is the case, then we define the **trace** to be

$$\mathrm{Tr}\ (A) := \sum_j \langle e_j \,|\, Ae_j \rangle \,.$$

The family of trace class operators on a Hilbert space, $\mathcal{H}$, is denoted $\mathcal{T}(\mathcal{H})$.

The trace has some nice properties, some of which matrix traces satisfy, as well as some that have no finite dimensional analogue.

Proposition 3.2.5. *The family of trace class operators, $\mathcal{T}(\mathcal{H})$, is an ideal of $\mathcal{B}(\mathcal{H})$, and the trace is a linear functional on $\mathcal{T}(\mathcal{H})$.*

We will not prove this result, but will refer the interested reader to [45, Theorem VI.19]

Proposition 3.2.6. *The trace is independent of the choice of orthonormal basis used to compute it.*

Proof. Let $\{|e_i\rangle\}_{i=1}^{\infty}$ and $\{|f_j\rangle\}_{j=1}^{\infty}$ be two orthonormal bases for $\mathcal{H}$, and suppose that A is a trace class operator. For each $|e_i\rangle$, we have

$$|e_i\rangle = \sum_{j=1}^{\infty} |f_j\rangle \langle f_j|e_i\rangle ,$$

so the trace of A is given by

$$\begin{aligned}\mathrm{Tr}(A) &= \sum_{i=1}^{\infty} \langle e_i|Ae_i\rangle = \sum_{i=1}^{\infty} \langle e_i| A |e_i\rangle = \sum_{i,j=1}^{\infty} \langle e_i| A |f_j\rangle \langle f_j|e_i\rangle \\ &= \sum_{i,j=1}^{\infty} \langle f_j|e_i\rangle \langle e_i|Af_j\rangle = \sum_{j=1}^{\infty} \langle f_j|Af_j\rangle .\end{aligned}$$

□

Proposition 3.2.7. *If $A \in \mathcal{T}(\mathcal{H})$ and $B \in \mathcal{B}(\mathcal{H})$, then* $\mathrm{Tr}(AB) = \mathrm{Tr}(BA)$.

Again, we will not prove this result, but the proof is not especially hard. One first shows that every $B \in \mathcal{B}(\mathcal{H})$ can be written as the sum of unitaries[8], and so it is sufficient to show that the equality holds for B unitary. Then one has

$$\begin{aligned}\mathrm{Tr}(AB) &= \sum_j \langle e_j|ABe_j\rangle = \sum_j \langle B^*Be_j|ABe_j\rangle \\ &= \sum_j \langle B^*\psi_j|A\psi_j\rangle = \sum_j \langle \psi_j|BA\psi_j\rangle = \mathrm{Tr}(BA).\end{aligned}$$

The last equality holds because the trace is independent of the basis which is used to calculate it. More generally, the trace is invariant under cyclic permutations of its arguments. Thus $\mathrm{Tr}(ABC) = \mathrm{Tr}(BCA) = \mathrm{Tr}(CAB)$ and so on.

Proposition 3.2.8. *The trace defines an inner product on $\mathcal{T}(\mathcal{H})$ by* $\mathrm{Tr}(A^*B) = \langle A \,|\, B\rangle$. *The associated norm is known as the Hilbert-Schmidt norm.*

One of the most important results in linear algebra says that the trace of a matrix is the sum of the eigenvalues. Lidskii's Theorem says this is also true for trace class operators. For a proof of Lidskii's theorem, see [46, Corollary to Theorem XIII.106].

Theorem 3.2.9 (Lidskii's theorem)**.** *Let A be a trace class operator over a separable Hilbert space $\mathcal{H}$, and let $\{\lambda_n\}_{n=1}^{N}$ with $N \leq \infty$ be the eigenvalues of A, repeated according to multiplicity. Then*

$$\mathrm{Tr}\,(A) = \sum_{n=1}^{N} \lambda_n.$$

[8] See [45, Lemma preceding Theorem IV.20]

3.3 Quantum statistical mechanics

Statistical mechanics is a branch of physics which studies physical systems composed of large numbers of particles. Such systems commonly include macroscopic volumes of gas, or the arrangement of magnetic spins on a lattice. Because of the large number of particles involved in a standard statistical mechanics problem, solving the standard equations of motion typically becomes intractable[9], and other methods are sought. The main idea of statistical mechanics is to use probability theory and statistical methods to study the bulk, or macroscopic, properties of the system - properties such as heat, pressure, entropy and work. Quantum statistical mechanics is a particular form of statistical mechanics in which the quantum nature of the constituent particles is taken into account.

3.3.1 Introduction

Following the lead of [7] and [8], a primary goal of this project is to describe quantum statistical systems using the algebraic framework of quantum mechanics. This framework turns out to be well suited to describing quantum statistical systems. In the algebraic formulation of quantum mechanics, physical states are represented by positive linear functionals of norm 1. We expect, or rather hope, that there exist states which are natural candidates for what we call equilibrium states.

3.3.2 Equilibrium states

Statistical mechanics often deals with system in thermodynamic equilibrium because they are simpler to solve and tell us the long term behaviour of the system. A system is in thermodynamic equilibrium if there is no net flow of matter or energy, no phase changes and no unbalanced potentials or external forces on the system. Rather than attempt to define these concepts in a precise mathematical framework, we will instead list some physically motivated properties we expect equilibrium states to have.

- **Time invariance:** The properties of an equilbrium state shouldn't vary over time.
- **Stability:** If the system is perturbed slightly, then the system should evolve towards the equilibrium state. Stability is an important property of any physical

[9]The number of particles in ideal gas calculations is typically of the order 10^{23}.

system in equilibrium.

- **Maximal entropy:** A consequence of the second law of thermodynamics is that the entropy is maximised for a system in equilibrium.

Classically, there are three main descriptions of equilibrium states. These are the microcanonical ensemble, the canonical ensemble, and the grand canonical ensemble. The first describes a state in which the energy and particle number are fixed. In the second, the number of particles is still fixed but the energy may change. In the third, both the energy and the number of particles may change. We will describe equilibrium states using the grand canonical ensemble. In the traditional study of statistical mechanics, the Gibbs state is an equilibrium state of the system. We now discuss the traditional Gibbs view within the algebraic framework.

Example 3.3.1. If $\mathcal{H}$ is the Hilbert space of states for all possible energies and particle numbers of the system and H the self-adjoint Hamiltonian, then the Gibbs equilibrium state at inverse temperature β is

$$\phi_\beta(A) = \frac{\mathrm{Tr}(e^{-\beta H}A)}{\mathrm{Tr}(e^{-\beta H})},$$

where $e^{-\beta H}$ is assumed to be trace class.

It is not immediately obvious that the Gibbs state is an equilibrium state. For instance, it is not apparent that the Gibbs state is independent of time. We will show that this is the case, but will first attempt to justify the characterisation of the Gibbs state as an equilibrium state through a consideration of the principle of maximum entropy. For concreteness, we will consider a finite-dimensional Hilbert space $\mathcal{H}$ of dimension n.

Remark 3.3.2. Let $\mathcal{H}$ be a finite dimensional Hilbert space of dimension n, and let $M_n(\mathbb{C})$ be the C^*-algebra of $n \times n$ matrices acting on $\mathcal{H}$. The Gibbs state can then be written as

$$\phi_\beta(A) = \mathrm{Tr}(\rho_G A)$$

where

$$\rho_G = \frac{e^{-\beta H}}{\mathrm{Tr}(e^{-\beta H})}.$$

This ρ_G is a density matrix as introduced in Theorem 2.3.23. Here, as before, H is the self-adjoint Hamiltonian and β is the inverse temperature. Note that since $\mathcal{H}$ is finite

dimensional, $e^{-\beta H}$ is automatically trace class. We now define what we mean by the entropy of a state. Given a state $\phi \in \mathcal{S}(M_n(\mathbb{C}))$ with density matrix[10] ρ, the entropy function $S : \mathcal{S}(M_n(\mathbb{C})) \to [0, \log(n)]$ is defined to be $S(\phi) = -\operatorname{Tr}(\rho \log(\rho))$. We now show that the Gibbs state is the unique state which maximises this entropy, but in order to do so we will need the following lemma, the proof of which may be found in [8, Lemma 6.2.21].

Lemma 3.3.3. *Let A be a positive $n \times n$ matrix and B a strictly positive $n \times n$ matrix. It follows that*

$$-\operatorname{Tr}(A \log A - A \log B) \leq \operatorname{Tr}(A - B)$$

with equality if, and only if, $A = B$.

Given a state ϕ with density matrix ρ, and the Gibbs state ϕ_β with density matrix ρ_G, we define the entropy of ϕ relative to ϕ_β by

$$S(\phi|\phi_\beta) = -\operatorname{Tr}(\rho \log \rho - \rho \log \rho_G).$$

Computing this by inserting the expression for the density matrix ρ_G, one obtains

$$S(\phi|\phi_\beta) = S(\phi) - \beta\phi(H) - \log \operatorname{Tr}\left(e^{-\beta H}\right) \tag{3.2}$$

It follows from Lemma 3.3.3 that the entropy of any state ϕ relative to ϕ_β is less than or equal to zero, and $S(\phi|\phi_\beta) = 0$ if and only if $\phi = \phi_\beta$. Therefore the Gibbs state is the unique state which maximises the entropy (for a fixed temperature).

The power of the algebraic formulation of quantum mechanics is that it allows us to generalise classical notions using results from the theory of C^*-algebras. For instance, in more abstract situations it's not always clear how to define the Gibbs state, or even whether such a state exists. It turns out that there is a special type of state on a C^*-algebra which generalises the notion of a Gibbs state. Such states are called KMS states, and are the main focus of the next subsection.

3.3.3 KMS-states

Kubo-Martin-Schwinger (KMS) states are generalisations of the Gibbs states and provide excellent candidates for equilibrium states on a C^*-dynamical system. Although there

[10]Each state ϕ over $M_n(\mathbb{C})$ is a normal state, and therefore by Theorem 2.3.23 there exists a density matrix ρ such that $\phi(A) = \operatorname{Tr}(\rho A)$

are different, equivalent characterisations of KMS states, we will focus on a definition which emphasises a particular algebraic property of the KMS state.

Definition 3.3.4. Let $\mathcal{A}$ be a C^*-algebra and $t \mapsto \tau_t$ a strongly continuous group of automorphisms of $\mathcal{A}$, i.e. suppose $(\mathcal{A}, \tau, \mathbb{R})$ is a C^*-dynamical system. An element $A \in \mathcal{A}$ is said to be **analytic** if there exists a strip

$$I_\lambda = \{z \in \mathbb{C} : |\Im(z)| < \lambda\}$$

and a function $f : I_\lambda \to \mathcal{A}$ which satisfies the conditions:

1. $f(t) = \tau_t(A)$ for all $t \in \mathbb{R}$.
2. $z \mapsto f(z)$ is analytic for $z \in I_\lambda$

If A is analytic and $\lambda = \infty$, we say that A is an **entire analytic** element. We denote the set of entire analytic elements of $\mathcal{A}$ by $\mathcal{A}_\tau$.

The following proposition is a consequence of [7, Corollary 2.5.23].

Proposition 3.3.5. *Let $(\mathcal{A}, \tau, \mathbb{R})$ be a C^*-dynamical system. It follows that $\mathcal{A}_\tau$ is a norm-dense, τ-invariant $*$-subalgebra of $\mathcal{A}$.*

Definition 3.3.6. Let $(\mathcal{A}, \tau, \mathbb{R})$ be a C^*-dynamical system. A state ϕ over $\mathcal{A}$ is defined to be a τ-KMS state at value $\beta \in \mathbb{R}$, or a (τ, β)-KMS state, if

$$\phi(A\tau_{i\beta}(B)) = \phi(BA)$$

for all A, B in a norm-dense, τ-invariant $*$-subalgebra of $\mathcal{A}_\tau$.

Remark 3.3.7. It's important to be careful with units here if we wish to do any numerical calculations and interpret these in a physical context. Strictly speaking, the β used in Definition 3.3.6, which we shall refer to as $\tilde{\beta}$ for the present discussion, is not the same as the inverse temperature. The inverse temperature β has units of inverse energy, while $\tilde{\beta}$ has units of time. As we shall see in Proposition 3.3.8, the Gibbs state is technically a $(\tau, \beta\hbar)$-KMS state. This follows from the fact that the standard quantum mechanical time evolution is given by

$$\tau_t(A) = e^{\frac{iHt}{\hbar}} A e^{\frac{-iHt}{\hbar}}.$$

Since $\hbar$ has units of energy·time, $\tilde{\beta} = \beta\hbar$ has units of time as expected.

To justify our claim that KMS states generalise Gibbs states, we first show that the Gibbs state is a KMS state for the standard time evolution.

Proposition 3.3.8. *Let A be an arbitrary bounded operator on a Hilbert space $\mathcal{H}$, H a self-adjoint operator with $e^{-\beta H}$ trace class, and let ϕ_β be the Gibbs equilibrium state defined by*

$$\phi_\beta(A) := \frac{\mathrm{Tr}(e^{-\beta H}A)}{\mathrm{Tr}(e^{-\beta H})}.$$

Consider the time evolution generated by $\frac{H}{\hbar}$,

$$\tau_t(A) = e^{\frac{itH}{\hbar}} A e^{\frac{-itH}{\hbar}}.$$

It follows that ϕ_β is a $(\tau, \beta\hbar)$-KMS state.

Proof. We calculate, using the cyclicity of the trace,

$$\begin{aligned}\phi_\beta(A\tau_{i\beta\hbar}(B)) &= \frac{\mathrm{Tr}(e^{-\beta H}A\tau_{i\beta\hbar}(B))}{\mathrm{Tr}(e^{-\beta H})} = \frac{\mathrm{Tr}(e^{-\beta H}Ae^{-\beta H}Be^{\beta H})}{\mathrm{Tr}(e^{-\beta H})} = \frac{\mathrm{Tr}(e^{-\beta H}BA)}{\mathrm{Tr}(e^{-\beta H})} \\ &= \phi_\beta(BA).\end{aligned}$$

□

Since the Gibbs state is a KMS-state, it will satisfy the properties of KMS states that we prove in the next section. In particular, Proposition 3.3.9 guarantees the time invariance of the Gibbs state.

Properties and alternative characterisation

The most relevant property of KMS states is that they are invariant under the time evolution - a property we definitely want for equilibrium states. We show a slightly weaker proposition, namely the invariance under time evolution if the algebra of observables is unital. The proof for this proposition was adapted from the proof given in [8, Proposition 5.3.3].

Proposition 3.3.9. *Let ϕ be a (τ, β)-KMS state over the unital C^*-algebra $\mathcal{A}$ with $\beta \neq 0$. Then ϕ is τ-invariant, i.e.*

$$\phi(A) = \phi(\tau_t(A))$$

for all $A \in \mathcal{A}$ and all $t \in \mathbb{R}$.

Proof. Suppose that B is an entire analytic element from the norm-dense, τ-invariant, $*$-subalgebra $\mathcal{B}_\tau \subseteq \mathcal{A}_\tau$ for which the KMS conditions holds. Define a function $F : \mathbb{C} \to \mathbb{C}$ by

$$F(z) = \phi(\tau_z(B)).$$

This function is analytic by the analyticity of B. Then for $z = x + iy$, we have

$$|F(z)| \leq \|\tau_z(B)\| = \|\tau_{x+iy}(B)\| = \|\tau_x(\tau_{iy}(B))\| = \|\tau_{iy}(B)\|.$$

Thus F is bounded on the strip

$$\mathcal{I} = \{z \in \mathbb{C} : 0 \leq \Im(z) \leq \beta\}$$

by

$$M = \sup\{\|\tau_{iy(B)}\| : y \in [0, \beta]\}.$$

Since $\mathcal{A}$ is unital, the KMS condition implies

$$\begin{aligned} F(i\beta + z) &= \phi(\tau_{i\beta+z}(B)) = \phi(1\tau_{i\beta}(\tau_z(B))) \\ &= \phi(\tau_z(B)1) = F(z), \end{aligned}$$

and therefore F is periodic with period $i\beta$. It follows that F is bounded everywhere, and therefore constant by Liouville's theorem. In particular, $F(z) = F(0)$ for all $z \in \mathbb{C}$. It follows that the KMS state is then τ-invariant for the dense subalgebra $\mathcal{B}_\tau$ of $\mathcal{A}$, and therefore all of $\mathcal{A}$. □

There is an equivalent characterisation of the KMS condition which was originally taken to be the definition. The statement of this characterisation comes from [8, Proposition 5.3.7].

Proposition 3.3.10. *Let $(\mathcal{A}, \mathbb{R}, \tau)$ be a C^*-dynamical system, and ϕ be a (τ, β)-KMS state. Then for all A, $B \in \mathcal{A}$, there exists a function $F_{A,B}(z)$ which is holomorphic on the strip*

$$I_\beta = \{z \in \mathbb{C} : 0 < \Im(z) < \beta\},$$

continuous on the boundary ∂I_β and bounded, with the property that for all $t \in \mathbb{R}$,

$$F_{A,B}(t) = \phi(A\tau_t(B)) \quad \textit{and} \quad F_{A,B}(t + i\beta) = \phi(\tau_t(B)A).$$

In Section 2.3.4 we introduced the concept of a modular automorphism group associated to the pair $(\mathcal{M}, \phi)$, where $\mathcal{M}$ is a von Neumann algebra and ϕ is a faithful, normal state on $\mathcal{M}$. Recall that the modular automorphism group associated to $(\mathcal{M}, \phi)$ is the one-parameter group of automorphisms of $\mathcal{M}$ given by

$$\tau_t^\phi(A) = \pi_\phi^{-1}(\Delta^{it}\pi_\phi(A)\Delta^{-it}),$$

where $\pi_\phi : \mathcal{M} \to \mathcal{B}(\mathcal{H}_\phi)$ is the GNS representation of $\mathcal{M}$ associated to ϕ. We now show that the state ϕ satisfies the KMS condition with respect to the modular automorphism group.

Proposition 3.3.11. *Let $\mathcal{M}$ be a von Neumann algebra, ϕ a faithful, normal state on $\mathcal{M}$. Then ϕ is a KMS state at temperature $\beta = -1$ with respect to the modular automorphism group associated with $(\mathcal{M}, \phi)$.*

Proof. To increase transparency in the following calculation, we will drop the subscript ϕ for the representation π_ϕ and the cyclic vector Ω_ϕ. Using the relations in Proposition 2.3.28, we calculate, for any A, $B \in \mathcal{M}_{\tau^\phi}$,

$$\begin{aligned}
\phi(A\tau_{-i}^\phi(B)) &= \langle\Omega|\pi(A)\pi(\pi^{-1}(\Delta\pi(B)\Delta^{-1})\Omega\rangle \\
&= \langle\Delta^{1/2}\pi(A^*)\Omega|\Delta^{1/2}\pi(B)\Delta^{-1/2}\Delta^{-1/2}\Omega\rangle \\
&= \langle\Delta^{1/2}\pi(A^*)\Omega|\Delta^{1/2}\pi(B)J\Delta^{1/2}\Delta^{1/2}J\Omega\rangle \\
&= \langle\Delta^{1/2}\pi(A^*)\Omega|\Delta^{1/2}\pi(B)\Omega\rangle \\
&= \langle J\Delta^{1/2}\pi(B)\Omega|J\Delta^{1/2}\pi(A^*)\Omega\rangle \\
&= \langle\pi(B^*)\Omega|\pi(A)\Omega\rangle = \langle\Omega|\pi(BA)\Omega\rangle = \phi(BA).
\end{aligned}$$

□

3.3.4 The thermal time hypothesis

Proposition 3.3.11, together with the Tomita-Takesaki theorem, says that each (normal, faithful) state of a von Neumann algebra determines a time flow of the algebra, under which the original state is a KMS state.

Remark 3.3.12. This conclusion also applies to an arbitrary C^*-algebra $\mathcal{A}$, since the GNS construction defines a representation, and therefore a $*$-subalgebra $\pi_\phi(\mathcal{A})$ of $\mathcal{B}(\mathcal{H})$. The

double commutant, $\pi_\phi(\mathcal{A})''$ of this $*$-subalgebra is necessarily a von Neumann algebra to which we may apply the Tomita-Takesaki theorem.

The time flow defined by the modular group of automorphisms depends on the state chosen, although we shall see that the time flows determined by two different states are related.

Definition 3.3.13. An automorphism τ of a C^*-algebra $\mathcal{A}$ is called an **inner automorphism** if there is a unitary element U such that

$$\tau(A) = U^* A U.$$

Not all automorphisms are inner, but we may define an equivalence relation between automorphisms of a C^*-algebra whenever they are related by an inner automorphism. We say that two automorphisms τ_1 and τ_2 are equivalent if there exists an inner automorphism τ_{inner}, such that

$$\tau_1 = \tau_{inner} \circ \tau_2.$$

The resulting equivalence classes of automorphisms are denoted outer automorphisms, and the space of all outer automorphisms of $\mathcal{A}$ is denoted $\mathrm{Out}(\mathcal{A}) = \mathrm{Aut}(\mathcal{A})/\mathrm{Inn}(\mathcal{A})$.

Theorem 3.3.14 (Connes cocycle Radon-Nikodym theorem)**.** *Let $\mathcal{M}$ be a von Neumann algebra, and let ϕ, ψ be two faithful, normal states over $\mathcal{M}$. Then the modular automorphisms associated to ϕ and ψ are related by an inner automorphism, i.e. τ^ϕ and τ^ψ are equivalent in Out($\mathcal{M}$).*

The Connes cocycle Radon-Nikodym theorem [10] says that all the modular automorphisms of a von Neumann algebra $\mathcal{M}$ are inner-equivalent, and therefore determine the same 1-parameter group in $\mathrm{Out}(\mathcal{M})$. It follows that a von Neumann algebra has a canonically determined 1-parameter group of outer automorphisms of the algebra. In the algebraic formulation of quantum mechanics, this result forms the structural motivation of the "thermal time hypothesis" developed in [49]:

> *"we propose a unifying perspective on these problems, based on the hypothesis that in a generally covariant quantum theory the physical time-flow is not a universal property of the mechanical theory, but rather it is determined by the thermodynamical state of the system".*

The thermal time hypothesis assumes that the time evolution of a physical system is determined by the modular automorphism group associated to a state of the system, referred to as the thermal time. In [48], [49] and [12], it is shown that the thermal time hypothesis has a number of interesting consequences:

1. **Non-relativistic limit** - In a non-relativistic setting, the thermal time is proportional to the standard non-relativistic time determined by the Hamiltonian, where the constant of proportionality is the inverse temperature β. One then interprets the temperature as 'the rate at which time is flowing'.

2. **Statistical Mechanics of gravity** - In the classical limit of the thermal time hypothesis, one is able to define a theoretical framework for the statistical mechanics of the gravitational field

3. **Cosmological time** - The time flow determined by the cosmological background radiation thermal state in a covariantly formulated cosmological model is precisely the usual Friedman-Robertson-Walker time.

4. **Unruh and Hawking effects** - The authors derive the Unruh effect, which states that the ground state for an intertial observer has a non-zero temperature as measured by a uniformly accelerating observer. Using this, one can calculate the Hawking temperature of a black hole.

The thermal time hypothesis is an extraordinary connection between theoretical physics and pure mathematics which provides further justification for the validity of the algebraic formulation of quantum mechanics. The consequences of the thermal time hypothesis, such as the derivation of the Hawking and Unruh effects, are analysed in detail in [43].

Chapter 4

Examples of quantum systems

4.1 Some simple quantum systems

In this chapter we introduce some simple quantum systems which we will describe using the algebraic formulation of quantum mechanics. The first of these is the quantum harmonic oscillator, the quantum analogue of the classical harmonic oscillator. Since any potential can be approximated by a harmonic potential in the vicinity of a stable equilibrium point, the quantum harmonic oscillator is one of the most important models in quantum mechanics. We calculate some quantities of interest for the one-dimensional quantum harmonic oscillator, then perform the same calculations for the N-dimensional version.

The second system we will look at is a non-interacting system of fermions, known as an ideal Fermi gas. The Pauli exclusion principle states that, unlike bosons, no two fermions can co-exist in the same quantum state. This implies that even at a temperature of absolute zero, the pressure of the ideal Fermi gas is non-zero[1]. This so-called degeneracy pressure is a purely quantum effect that is not present in classical ideal gases. The ideal Fermi gas is an idealisation, but can still be used to approximate the behaviour of conduction electrons in a metal and fermions in a white dwarf star [27, 4].

[1] See [27, Page 182]

4.1.1 Quantum harmonic oscillator

1-dimensional harmonic oscillator

The time-independent Schrödinger equation,

$$H\psi = E\psi,$$

determines the allowed (time independent) states of a quantum mechanical system with a given Hamiltonian H. For the harmonic oscillator, the Hamiltonian H is a self-adjoint operator on the Hilbert space $\mathcal{H} = L^2(\mathbb{R})$, given by

$$H = \frac{p^2}{2m} + \frac{m\omega^2 x^2}{2}.$$

Here p is the momentum operator

$$p = -i\hbar\frac{\partial}{\partial x}$$

and x is the position operator which acts on a vector ψ by multiplication. Note that both x and p are self-adjoint. The time-independent Schrödinger equation is then a second order, ordinary differential equation

$$\frac{-\hbar^2}{2m}\frac{d^2\psi}{dx^2} + \frac{1}{2}m\omega^2 x^2\psi = E\psi, \tag{4.1}$$

the solutions of which correspond to energy eigenstates of the harmonic oscillator. It is possible to solve Equation 4.1 for the wavefunction ψ. Doing so, we obtain[2] a family of solutions:

$$\psi_n(x) = \frac{e^{\frac{-m\omega^2 x^2}{2\hbar}}}{\sqrt{2^n n!}}\left(\frac{m\omega}{\pi\hbar}\right)^{1/4}\mathcal{H}_n\left(x\sqrt{\frac{m\omega}{\hbar}}\right) \tag{4.2}$$

where $\mathcal{H}_n(x)$ are the Hermite polynomials. These wavefunctions are eigenfunctions (also called eigenkets) of the Hamiltonian, with corresponding eigenvalues

$$E_n = \hbar\omega\left(n + \frac{1}{2}\right)$$

. There is an alternate way to solve the harmonic oscillator using operators known as ladder operators[3], which relies on the fact that $L^2(\mathbb{R})$ is separable, and therefore

[2] For a derivation of these solutions, see [1, Pages 73-74]

[3] For a more detailed discussion of the use of ladder operators to solve the harmonic oscillator, consult [1, 50, 18].

isomorphic to $\ell^2(\mathbb{N})$. Originally developed by Dirac [14], the ladder operator method is similar to the method used to investigate the ideal Fermi gas, which we will discuss in the next section. For real numbers, we can factorise a sum of squares as

$$u^2 + v^2 = (u + iv)(u - iv).$$

Since the harmonic oscillator Hamiltonian is the sum of squares of operators, we can naïvely try to factorise the Hamiltonian in a similar way. We don't expect our Hamiltonian to factor perfectly since x and p don't commute, but we nevertheless define ladder operators a and $a^\dagger$ by:

$$a = \sqrt{\tfrac{m\omega}{2\hbar}}\left(x + \tfrac{ip}{m\omega}\right), \quad a^\dagger = \sqrt{\tfrac{m\omega}{2\hbar}}\left(x - \tfrac{ip}{m\omega}\right) \tag{4.3}$$

With these operators[4] our Hamiltonian can be written in the form

$$H = \hbar\omega\left(a^\dagger a + \frac{1}{2}\right),$$

and we define the **number operator**, $\mathcal{N}$, by

$$\mathcal{N} := a^\dagger a.$$

Thus H is a linear function of $\mathcal{N}$, and so both H and $\mathcal{N}$ can be simultaneously diagonalised. This means that eigenfunctions of the Hamiltonian are also eigenfunctions of the number operator. We denote an eigenfunction of the number operator $\mathcal{N}$ by the eignenvalue n, giving

$$\mathcal{N}\left|n\right\rangle = n\left|n\right\rangle.$$

Associating the number eigenket $|n\rangle$ with the sequence $(0, \dots, 0, 1, 0, \dots) \in \ell^2(\mathbb{N}_0)$ defines an isomorphism from $L^2(\mathbb{R})$ to $\ell^2(\mathbb{N}_0)$. We can write each of the operators we are interested in as the sum of rank one operators on this Hilbert space $\mathcal{H} = \ell^2(\mathbb{N}_0)$ for which the eigenkets $\{|n\rangle\}_{n\in\mathbb{N}_0}$ form a complete orthonormal basis. The operators are given by:

$$H = \sum_{n=0}^{\infty}\left(n + \frac{1}{2}\right)\hbar\omega\left|n\right\rangle\left\langle n\right|$$

$$\mathcal{N} = \sum_{n=0}^{\infty} n\left|n\right\rangle\left\langle n\right|$$

[4]Note that $a^\dagger$ is the adjoint of a, and in particular, neither a nor $a^\dagger$ are self-adjoint.

$$a = \sum_{n=0}^{\infty} \sqrt{n}\,|n-1\rangle\,\langle n|$$

$$a^\dagger = \sum_{n=0}^{\infty} \sqrt{n+1}\,|n+1\rangle\,\langle n|$$

$$x = \sqrt{\frac{\hbar}{2m\omega}} \sum_{n=0}^{\infty} \left(\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle\right)\langle n| = \sqrt{\frac{\hbar}{2m\omega}}(a^\dagger + a)$$

$$p = i\sqrt{\frac{m\hbar\omega}{2}} \sum_{n=0}^{\infty} \left(-\sqrt{n}\,|n-1\rangle + \sqrt{n+1}\,|n+1\rangle\right)\langle n| = i\sqrt{\frac{m\hbar\omega}{2}}(a^\dagger - a).$$

The form of $\mathcal{N}$ and H follow from the basis we are using. The ladder operators a and $a^\dagger$ are derived in this form in [50, Pages 90-91]. Finally, the x and p are just combinations of the annihilation and creation operators obtained by rearranging Equation 4.3. We now investigate the Gibbs state for this system. For any A in our algebra of observables, the Gibbs state at inverse temperature β is given by

$$\phi_\beta(A) = \frac{\mathrm{Tr}\left(e^{-\beta H}A\right)}{\mathrm{Tr}\left(e^{-\beta H}\right)}$$

whenever this is defined. To simplify calculations later, we evaluate

$$\begin{aligned}
\mathrm{Tr}\left(e^{-\beta H}\right) &= \sum_{n=0}^{\infty} \left\langle n \,\middle|\, e^{-\beta H} \,\middle|\, n \right\rangle \\
&= \sum_{n=0}^{\infty} e^{-\beta\left(n+\frac{1}{2}\right)\hbar\omega} \langle n \,|\, n\rangle \\
&= e^{\frac{-\beta\hbar\omega}{2}} \sum_{n=0}^{\infty} e^{-\beta\hbar\omega n}.
\end{aligned}$$

This infinite sum is a geometric series and converges provided $\hbar\omega\beta > 0$. We then obtain

$$\mathrm{Tr}\left(e^{-\beta H}\right) = \frac{e^{\frac{\beta\hbar\omega}{2}}}{e^{\beta\hbar\omega} - 1}. \tag{4.4}$$

Remark 4.1.1. Physical arguments allow us to predict the results of calculating the average value for the observables we are interested in, and make sure that our results coincide with experimental evidence. For the Hamiltonian calculation, we expect that as the temperature of the system increases the expectation value of the Hamiltonian should also increase. Indeed, when the thermal energy is large enough that the system is able to explore many of its possible quantum states then we expect that we should obtain the classical result from the equipartition theorem: $E = k_B T$. Since the Hamiltonian operator is just a linear function of the number operator, we should see similar results with

the number operator. The physical system we are considering has a reflection symmetry about the origin. Mathematically, this means that the Hamiltonian is invariant under the transformations $x \to -x$ and $p \to -p$. As a result of this, we expect that both the position and momentum averages should be zero, since the particle is equally likely to be on either side of the origin. The ladder operators are not observables in the physical sense since they are not self-adjoint, however there is no mathematical reason we cannot evaluate the Gibbs state on these operators.

We evaluate the Gibbs state at the Hamiltonian

$$\begin{aligned}
\langle H \rangle = \phi_\beta(H) &= \frac{\operatorname{Tr}\left(e^{-\beta H} H\right)}{\operatorname{Tr}\left(e^{-\beta H}\right)} \\
&= \frac{e^{\beta\hbar\omega} - 1}{e^{\frac{\beta\hbar\omega}{2}}} \sum_{n=0}^{\infty} \left\langle n \,\middle|\, e^{-\beta H} H \,\middle|\, n \right\rangle \\
&= \frac{e^{\beta\hbar\omega} - 1}{e^{\frac{\beta\hbar\omega}{2}}} \sum_{n=0}^{\infty} \left(n + \frac{1}{2}\right) \hbar\omega e^{-\beta\left(n+\frac{1}{2}\right)\hbar\omega} \left\langle n \,\middle|\, n \right\rangle \\
&= \hbar\omega \frac{e^{\beta\hbar\omega} - 1}{e^{\beta\hbar\omega}} \sum_{n=0}^{\infty} \left(n + \frac{1}{2}\right) e^{-\beta\hbar\omega n} \\
&= \hbar\omega \frac{e^{\beta\hbar\omega} - 1}{e^{\beta\hbar\omega}} \left(\frac{e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega} - 1\right)^2} + \frac{1}{2} \frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega} - 1} \right) \\
&= \hbar\omega \left(\frac{1}{e^{\beta\hbar\omega} - 1} + \frac{1}{2} \right).
\end{aligned}$$

There are two things we note about this result. The first is the limit as the temperature goes to zero ($\beta \to \infty$), which is

$$\lim_{\beta\to\infty} \langle H \rangle = \frac{\hbar\omega}{2}.$$

This is known as the zero-point energy of the system. This is a purely quantum mechanical property of the system, since classically the energy of the system at zero temperature is zero. The second is what happens as the temperature becomes large ($\beta \to 0$, and in particular, when $k_B T$ is much larger then $\hbar\omega$). When β is close to 0, we can expand the exponential $e^{\beta\hbar\omega}$ in terms of its power series $e^{\beta\hbar\omega} = 1 + \beta\hbar\omega + \mathcal{O}((\beta\hbar\omega)^2)$. Ignoring the quadratic terms, we obtain

$$\langle H \rangle = \frac{1}{\beta} = k_B T.$$

As $k_B T$ is the average energy of the classical harmonic oscillator obtained from the equipartition theorem, there is good agreement between our calculations and physical arguments.

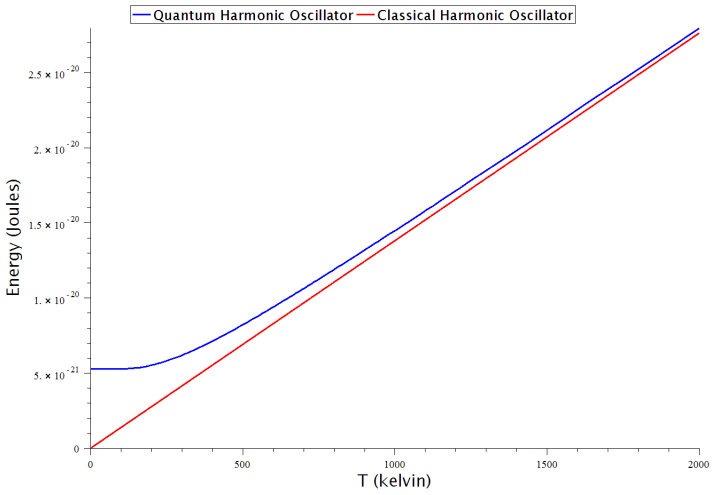

Figure 4.1: The average energy for the quantum and classical harmonic oscillators at oscillation frequency $\omega = 10^{14}$ rad/s.

What about the average occupancy level? From the computations for H we have

$$\langle \mathcal{N} \rangle = \phi_\beta(\mathcal{N}) = \frac{1}{e^{\beta\hbar\omega} - 1},$$

by direct calculation, a result which follows rather straightforwardly from the expression of H as a linear function of $\mathcal{N}$. The average position and momentum of the oscillator in the Gibbs state is calculated in the same way. As mentioned in Remark 4.1.1, the symmetry of the system leads us to suspect that the average position and momentum should be zero. We calculate

$$\begin{aligned}
\langle x \rangle = \phi_\beta(x) &= \frac{\operatorname{Tr}\left(e^{-\beta H} x\right)}{\operatorname{Tr}(e^{-\beta H})} = \frac{e^{\beta\hbar\omega} - 1}{e^{\frac{\beta\hbar\omega}{2}}} \sum_{n=0}^{\infty} \langle n \,|\, e^{-\beta H} x \,|\, n \rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}} \frac{e^{\beta\hbar\omega} - 1}{e^{\frac{\beta\hbar\omega}{2}}} \sum_{n=0}^{\infty} \langle n \,|\, e^{-\beta H} (a + a^\dagger) \,|\, n \rangle \\
&= \sqrt{\frac{\hbar}{2m\omega}} \frac{e^{\beta\hbar\omega} - 1}{e^{\frac{\beta\hbar\omega}{2}}} \sum_{n=0}^{\infty} \left\{ \sqrt{n} \langle n \,|\, e^{-\beta H} \,|\, n-1 \rangle + \sqrt{n-1} \langle n \,|\, e^{-\beta H} \,|\, n+1 \rangle \right\} \\
&= 0.
\end{aligned}$$

This is consistent with our expectations. The last equality holds because the eigenkets $\{|n\rangle\}_{n \in \mathbb{N}_0}$ are orthonormal. Performing a similar calculation with the momentum operator we obtain

$$\langle p \rangle = \phi_\beta(p) = 0.$$

N-dimensional harmonic oscillator

We now consider an N-dimensional harmonic oscillator in thermal equilibrium with a reservoir at inverse temperature β. The time independent schrödinger equation for this model is given by:

$$\frac{-\hbar^2}{2m}\left(\sum_{j=1}^{N}\frac{\partial^2}{\partial x_j^2}\right)\psi(x_1,\ldots,x_N)+m\omega^2\left(\sum_{j=1}^{N}x_j^2\right)\psi(x_1,\ldots,x_N)=E\psi(x_1,\ldots,x_N).$$

In analogy to the one dimensional case, we define ladder operators by

$$a_j=\sqrt{\frac{m\omega}{2\hbar}}\left(x_j+\frac{i}{m\omega}p_j\right)$$
$$a_j^\dagger=\sqrt{\frac{m\omega}{2\hbar}}\left(x_j-\frac{i}{m\omega}p_j\right)$$

and number operators $\mathcal{N}_j := a_j^\dagger a_j$. The Hilbert space of this system is $\mathcal{H}=\bigotimes_{i=1}^{N}\mathcal{H}_i$, where $\mathcal{H}_i=\ell^2(\mathbb{N}_0)$ is the one-particle subspace. We write a simple tensor in this space as $|n_1,n_2,\ldots n_N\rangle := |n_1\rangle\otimes|n_2\rangle\otimes\cdots\otimes|n_N\rangle$, and the action of the ladder operators on these vectors is more accurately written as

$$a_j\left|n_1,n_2,\ldots,n_N\right\rangle=\sum_{n_j=0}^{\infty}\sqrt{n_j}\left|n_1,\ldots,n_j-1,\ldots n_N\right\rangle\left\langle n_1,n_2,\ldots,n_j,\ldots,n_N\right|$$

$$a_j^\dagger\left|n_1,n_2,\ldots,n_N\right\rangle=\sum_{n_j=0}^{\infty}\sqrt{n_j+1}\left|n_1,\ldots,n_j+1,\ldots n_N\right\rangle\left\langle n_1,n_2,\ldots,n_j,\ldots,n_N\right|.$$

One easily verifies that the Hamiltonian can be expressed as

$$H=\hbar\omega\sum_{j=0}^{N}\left(\mathcal{N}_j+\frac{1}{2}\right)$$

and that the action of H and $\mathcal{N}_j$ on $|n_1,n_2,\ldots,n_N\rangle$ is given by

$$\mathcal{N}_j\left|n_1,n_2,\ldots,n_N\right\rangle=n_j\left|n_1,n_2,\ldots,n_N\right\rangle$$
$$H\left|n_1,n_2,\ldots,n_N\right\rangle=\hbar\omega\left(n_1+n_2+\cdots+n_N+\frac{N}{2}\right)\left|n_1,n_2,\ldots,n_N\right\rangle.$$

To simplify the calculations, we split the Gibbs state calculation and first evaluate

$$\begin{aligned}\operatorname{Tr}\left(e^{-\beta H}\right)&=\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_N=0}^{\infty}\left\langle n_1,n_2,\ldots,n_N\right|e^{-\beta H}\left|n_1,n_2,\ldots,n_N\right\rangle\\&=e^{\frac{-\beta\hbar\omega N}{2}}\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_N=0}^{\infty}e^{-\beta\hbar\omega n_1}e^{-\beta\hbar\omega n_2}\cdots e^{-\beta\hbar\omega n_N}\\&=\frac{e^{\frac{\beta\hbar\omega N}{2}}}{\left(e^{\beta\hbar\omega}-1\right)^N}.\end{aligned}$$

Then calculating $\mathrm{Tr}(e^{-\beta H}H)$:

$$\begin{aligned}
&\mathrm{Tr}(e^{-\beta H}H)\\
&= \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_N=0}^{\infty}\left\langle n_1, n_2, \ldots, n_N \,\middle|\, e^{-\beta H}H \,\middle|\, n_1, n_2, \ldots, n_N\right\rangle\\
&= \sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_N=0}^{\infty}\hbar\omega\left(n_1+n_2+\cdots+n_N+\frac{N}{2}\right)e^{-\beta\hbar\omega\left(n_1+n_2+\cdots+n_N+\frac{N}{2}\right)}\\
&= \hbar\omega e^{\frac{-\beta\hbar\omega N}{2}}\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_N=0}^{\infty}\left(n_1+n_2+\cdots+n_N+\frac{N}{2}\right)e^{-\beta\hbar\omega n_1}e^{-\beta\hbar\omega n_2}\cdots e^{-\beta\hbar\omega n_N}\\
&= \hbar\omega e^{\frac{-\beta\hbar\omega N}{2}}\left\{\sum_{i=1}^{N}\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_N=0}^{\infty}n_i e^{-\beta\hbar\omega n_1}e^{-\beta\hbar\omega n_2}\cdots e^{-\beta\hbar\omega n_N}\right.\\
&\qquad\left.+\frac{N}{2}\sum_{n_1=0}^{\infty}\sum_{n_2=0}^{\infty}\cdots\sum_{n_N=0}^{\infty}e^{-\beta\hbar\omega n_1}e^{-\beta\hbar\omega n_2}\cdots e^{-\beta\hbar\omega n_N}\right\}\\
&= \hbar\omega e^{\frac{-\beta\hbar\omega N}{2}}\left\{\left(\frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega}-1}\right)^{N-1}\sum_{i=1}^{N}\sum_{n_i=0}^{\infty}n_i e^{-\beta\hbar\omega n_i}+\frac{N}{2}\left(\frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega}-1}\right)^{N}\right\}\\
&= \hbar\omega e^{\frac{-\beta\hbar\omega N}{2}}\left\{N\left(\frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega}-1}\right)^{N-1}\left(\frac{e^{\beta\hbar\omega}}{\left(e^{\beta\hbar\omega}-1\right)^{2}}\right)+\frac{N}{2}\left(\frac{e^{\beta\hbar\omega}}{e^{\beta\hbar\omega}-1}\right)^{N}\right\}\\
&= N\hbar\omega\frac{e^{\frac{N\beta\hbar\omega}{2}}}{\left(e^{\beta\hbar\omega}-1\right)^{N}}\left\{\frac{1}{e^{\beta\hbar\omega}-1}+\frac{1}{2}\right\}.
\end{aligned}$$

So that the average energy for the N-dimensional harmonic oscillator is

$$\langle H\rangle = \phi_\beta(H) = \frac{\mathrm{Tr}(e^{-\beta H}H)}{\mathrm{Tr}(e^{-\beta H})} = N\hbar\omega\left(\frac{1}{e^{\beta\hbar\omega}-1}+\frac{1}{2}\right).$$

This result says that the average energy of the N-dimensional harmonic oscillator is simply N times the average energy of the one-dimensional harmonic oscillator. The straightforwardness of this result arises because there are no interaction terms in the Hamiltonian.

Remark 4.1.2. The astute reader would have noticed that the Hamiltonian for the harmonic oscillator is not a bounded operator. If we wish to phrase the harmonic oscillator problem in terms of the algebraic formulation of quantum mechanics, we immediately run into the problem that the Hamiltonian is not in our algebra of observables. Since the Hamiltonian frequently represents the total energy of the system, and is therefore an observable we are very interested in, this is problematic. Indeed, none of the observables we introduced in the harmonic oscillator problem are bounded. To fix this, we consider projections P_m which project onto the first m eigenvectors, i.e. $P_m = \sum_{n=0}^{m}|n\rangle\langle n|$. We then

define, for each m, $H_m = P_m H P_m$. Note that each H_m is bounded and self-adjoint. One sees that for each m, $\phi_\beta(H_m) \leq \phi_\beta(H)$. Indeed, since $\phi_\beta(H_m) \leq \phi_\beta(H_{m+1})$, the expectation values of the H_m form a bounded, non-decreasing sequence in $\mathbb{R}$, and therefore the monotone convergence theorem implies the limit $\lim_{m\to\infty} \phi_\beta(H_m)$ exists and is finite. For this system, one computes

$$\lim_{m\to\infty} \phi_\beta(H_m) = \phi_\beta(H),$$

which is finite, even though ϕ was not *a priori* defined on H.

4.1.2 Ideal Fermi gas

In this section we introduce a system of non-interacting fermions, the ideal Fermi gas. Our description of the ideal Fermi gas follows [8], and is closely related to a procedure in quantum field theory known as second quantization.

In order to describe the ideal Fermi gas we introduce a special type of Hilbert space called a Fock space.

Building a Fock space

In the standard construction of quantum mechanics, the state of a particle is described by a vector in a complex Hilbert space. To describe systems in which the number of particles is not fixed, it is necessary to introduce the notion of a Fock space.

Assume that the states of each particle form a complex Hilbert space $\mathcal{H}$ and let $\mathcal{H}^{\otimes n} = \mathcal{H} \otimes \cdots \otimes \mathcal{H}$ denote the n-fold tensor product of $\mathcal{H}$ with itself. Vectors in $\mathcal{H}^{\otimes n}$ describe states of a system of n particles, and by definition we set $\mathcal{H}^{\otimes 0} = \mathbb{C}$. Note that $\mathcal{H}^{\otimes n}$ is the closure of the span of finite linear combinations of pure tensors of the form $f_1 \otimes f_2 \otimes \cdots \otimes f_n$, with each $f_i \in \mathcal{H}$.

The **Fock space**, $\mathcal{F}(\mathcal{H})$, which describes the quantum mechanics of a variable number of particles is given by

$$\mathcal{F}(\mathcal{H}) = \bigoplus_{n=0}^{\infty} \mathcal{H}^{\otimes n}.$$

To describe bosons and fermions in the Fock space, we introduce operators P_+ and P_- which project onto the subspaces describing bosons and fermions respectively. The

action of the operators on pure tensors are given by

$$P_+(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = \frac{1}{n!}\sum_\pi (f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_n})$$
$$P_-(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = \frac{1}{n!}\sum_\pi \epsilon_\pi (f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_n}),$$

where the sum ranges over all the permutations of the indices, and ϵ_π is the sign of the permutation. The operators extend by linearity to each $\mathcal{H}^{\otimes n}$, and are thus defined on a dense subset of the Fock space.

Lemma 4.1.3. *The operators $P_\pm$ are projections with $\|P_\pm\| = 1$.*

Proof. To show that the operators $P_\pm$ are projections we show that $P_\pm^2 = P_\pm$ and $P_\pm^* = P_\pm$. For the first part, we calculate

$$\begin{aligned} P_+^2(f_1 \otimes f_2 \otimes \cdots \otimes f_n) &= P_+\left(\frac{1}{n!}\sum_\pi (f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_n})\right) \\ &= \frac{1}{n!}\sum_\pi P_+(f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_n}) \\ &= \frac{1}{n!}\sum_\pi (f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_n}) \\ &= P_+(f_1 \otimes f_2 \otimes \cdots \otimes f_n). \end{aligned}$$

And similarly for P_-. Thus $P_\pm^2 = P_\pm$. To see that $P_\pm^* = P_\pm$, we have to see what the projection does inside the inner product. We calculate

$$\begin{aligned} &\langle g_1 \otimes g_2 \otimes \cdots \otimes g_n \,|\, P_\pm(f_1 \otimes f_2 \otimes \cdots \otimes f_n)\rangle \\ &= \left\langle g_1 \otimes g_2 \otimes \cdots \otimes g_n \,\middle|\, \frac{1}{n!}\sum_\pi (f_{\pi_1} \otimes f_{\pi_2} \otimes \cdots \otimes f_{\pi_n})\right\rangle \\ &= \frac{1}{n!}\sum_\pi \prod_{i,j} \langle g_i \,|\, f_{\pi_j}\rangle = \frac{1}{n!}\sum_\pi \prod_{i,j} \langle g_{\pi_i} \,|\, f_j\rangle \qquad \text{by relabelling} \\ &= \langle P_\pm(g_1 \otimes g_2 \otimes \cdots \otimes g_n) \,|\, f_1 \otimes f_2 \otimes \cdots \otimes f_n\rangle\,, \end{aligned}$$

and similarly for P_-. Thus $P_\pm^* = P_\pm$, and the operators $P_\pm$ are projections. It follows that $\|P_\pm\| = \|P_\pm^2\| = \|P_\pm\|^2$ so that $\|P_\pm\| = 1$. □

Since the operators $P_\pm$ are bounded, and hence continuous on simple tensors, they extend by continuity to bounded operators on the entire Fock space. We then define the **Bose-Fock space**, $\mathcal{F}_+(\mathcal{H})$, and the **Fermi-Fock Space**, $\mathcal{F}_-(\mathcal{H})$, to be the subspaces

$$\mathcal{F}_\pm(\mathcal{H}) = P_\pm \mathcal{F}(\mathcal{H}).$$

The Fermi-Fock space describes a system containing an arbitrary number of fermions, and is sometimes known as the anti-symmetric Fock space. Tensors in the Fermi-Fock space are antisymmetric by construction. While this seems like an arbitrary decision, it turns out that this condition is exactly what is required in order to give us observed properties of fermions such as the Pauli exclusion principle. In contrast, the Bose-Fock space is symmetric by construction, and is sometimes referred to as the symmetric Fock space.

Remark 4.1.4 (The Pauli exclusion principle). The Pauli exclusion principle states that no two identical fermions may occupy the same state. The definitions of the Fermi and Bose Fock spaces have been designed to reflect this physical principle. To see this, consider a two particle system in which both particles are in the state f. We can write the state of this system as $f \otimes f \in \mathcal{H}^{\otimes 2}$. The projection of this state onto the Fermi-Fock space is

$$P_-(f \otimes f) = \frac{1}{2}(f \otimes f - f \otimes f) = 0.$$

It follows that no two fermions can occupy the same quantum state, in accordance with the Pauli exclusion principle. On the other hand, the projection of $f \otimes f \in \mathcal{H}^{\otimes 2}$ onto the Bose-Fock space gives

$$P_+(f \otimes f) = \frac{1}{2}(f \otimes f + f \otimes f) = f \otimes f.$$

Since there is no reason why this cannot be a physical state, particles described using the Bose-Fock space (i.e. bosons) do not obey the Pauli exclusion principle.

CAR and CCR algebras

We now give an abstract characterisation of a C^*-algebra which is commonly studied in the context of quantum statistical mechanics. This algebra is the canonical anticommutation relation (CAR) algebra. Related to this algebra is the canonical commutation relation algebra (CCR), which we will mention later.

The CCR and CAR Algebras arise from the study of canonical commutation and anticommutation relations in bosonic and fermionic quantum mechanics. Because of our interest in the ideal Fermi gas, we are primarily interested in the CAR algebra. Before we define the CAR algebra, we first introduce some notation.

Remark 4.1.5. Recall that if A, B are elements of an algebra, we define the commutator of A and B to be

$$[A, B] := AB - BA.$$

Similarly, we define the anti-commutator of A and B to be

$$\{A, B\} := AB + BA.$$

Definition 4.1.6. Let $\mathcal{H}$ be a Hilbert space. A **CAR algebra** over $\mathcal{H}$ is a C^*-algebra generated by operators

$$\{a(f) : f \in \mathcal{H}\}$$

where the $a(f)$ satisfy the following relations:

1. $f \mapsto a(f)$ is antilinear.
2. $\{a(f), a(g)\} = 0 \qquad \forall f,\, g \in \mathcal{H}.$
3. $\{a(f), a(g)^*\} = \langle f|g\rangle\, 1 \qquad \forall f,\, g \in \mathcal{H}.$

These conditions are known as the canonical anticommutation relations (CAR).

Remark 4.1.7. The corresponding conditions for the commutator are known as the canonical commutation relations (CCR). These are

1. $f \mapsto a(f)$ is antilinear.
2. $[a(f), a(g)] = 0 \qquad \forall f,\, g \in \mathcal{H}.$
3. $[a(f), a(g)^*] = \langle f|g\rangle\, 1 \qquad \forall f,\, g \in \mathcal{H}.$

Although these conditions look remarkably similar to the conditions for the CAR algebra, we cannot define a C^*-algebra using the canonical commutation relations in the same way we did with the CAR algebra. The reason for this will become apparent when we discuss the CAR algebra over the Fermi-Fock space.

The following proposition says that CAR algebras over finite dimensional Hilbert spaces are simply matrix algebras.

Proposition 4.1.8. *Let $\mathcal{H}$ be a Hilbert space, and $\mathcal{A}$ be a CAR algebra over $\mathcal{H}$. If $\mathcal{H}$ is n dimensional with $n \in \mathbb{N}$, then $\mathcal{A}$ is isomorphic to the C^*-algebra of $2^n \times 2^n$ complex matrices.*

Proof. We will not prove[5] Proposition 4.1.8 in general, but only for the simplest case $n = 1$. In this case, the proposition states that any CAR algebra over a one-dimensional Hilbert space is isomorphic to $M_2(\mathbb{C})$. To prove this, let $\mathcal{A}$ be a CAR algebra over a one-dimensional Hilbert space $\mathcal{H}$. Let $f \in \mathcal{H}$ be a unit vector (which is an orthonormal basis for $\mathcal{H}$ since $\mathcal{H}$ is one-dimensional), and $a(f)$, $a^*(f)$ be the corresponding elements in $\mathcal{A}$ satisfying the canonical anticommutation relations. For any $g \in \mathcal{H}$, $g = \lambda f$ for some $\lambda \in \mathbb{C}$, and therefore the anticommutation relation $a(f)a(g) + a(g)a(f) = 0$ implies $a^2(f) = 0$. Furthermore, the anticommutation relation $a(f)a^*(g) + a^*(g)a(f) = \langle f|g\rangle \, 1_{\mathcal{A}}$ implies $a(f)a^*(f)+a^*(f)a(f) = 1_{\mathcal{A}}$. For simplicity we drop the f and write these relations as

$$aa^* + a^*a = 1_{\mathcal{A}} \qquad\qquad a^2 = 0 \tag{4.5}$$

We now wish to define a map $\Phi : M_2(\mathbb{C}) \to \mathcal{A}$ which is an isomorphism. Let $(e_{ij})_{mn} = \delta_{im}\delta_{jn}$ be the standard basis for $M_2(\mathbb{C})$, and define a map Φ on the basis elements by

$$\Phi(e_{11}) = aa^* \qquad\qquad \Phi(e_{12}) = a$$
$$\Phi(e_{21}) = a^* \qquad\qquad \Phi(e_{22}) = a^*a$$

and extending by linearity. This map preserves the adjoint since a^*a and aa^* are self-adjoint (as are e_{11} and e_{22}), and we have $\Phi(e_{12}^*) = \Phi(e_{21}) = a^*$ and $\Phi(e_{21}^*) = \Phi(e_{12}) = a = (a^*)^*$. To see that multiplication is preserved, we need to verify that the multiplication relations of the (e_{ij}) are preserved. This is apparent by noting that a^*a and aa^* are orthogonal projections, and a and a^* are partial isometries between them. Finally since the operators a, a^*, a^*a and aa^* form a basis for the algebra $\mathcal{A}$, Φ is bijective, and therefore an isomorphism. □

Proposition 4.1.9. *Let $\mathcal{H}$ be a Hilbert space, and $\mathcal{A}_1$, $\mathcal{A}_2$ be two CAR algebras over $\mathcal{H}$. Then $\mathcal{A}_1$ and $\mathcal{A}_2$ are isomorphic.*

Remark 4.1.10. Proposition 4.1.9 says that there is a unique (up to isomorphism) CAR algebra associated to each Hilbert space $\mathcal{H}$. We will not prove this proposition. For a

[5] A more detailed version of this proposition, as well as a full proof may be found in [8, Theorem 5.2.5]

proof, see [8, Proposition 5.2.5]. Note that if $\mathcal{H}$ is finite dimensional the result follows immediately from Proposition 4.1.8.

The CAR algebra on Fock space

We have defined the CAR algebra as an abstract C^*-algebra associated to a Hilbert space $\mathcal{H}$. We now investigate the CAR algebra associated to the Fock space, or more specifically, the Fermi-Fock space.

Definition 4.1.11. Let $\mathcal{H}$ be a Hilbert space and $\mathcal{F}(\mathcal{H})$ the Fock space over $\mathcal{H}$. For each $f \in \mathcal{H}$, we define a **creation operator** $a^*(f)$ acting on pure tensors by

$$a^*(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = (n+1)^{1/2}(f \otimes f_1 \otimes f_2 \otimes \cdots \otimes f_n).$$

We similarly define an **annihilation operator** $a(f)$ by

$$a(f)(f_1 \otimes f_2 \otimes \cdots \otimes f_n) = n^{1/2} \langle f|f_1\rangle (f_2 \otimes f_3 \otimes \cdots \otimes f_n).$$

These operators extend by linearity to each $\mathcal{H}^{\otimes n}$, and are therefore defined on a dense subset of $\mathcal{F}(\mathcal{H})$. We define the annihilation and creation operators on the Fermi Fock space by

$$a_-(f) = P_- \, a(f) \, P_-$$

and

$$a_-^*(f) = P_- \, a^*(f) \, P_-.$$

We claim that the creation and annihilation operators satisfy the canonical anticommutation relations, and therefore generate the[6] CAR algebra over the Fermi-Fock space. The following lemma guarentees the notation we are using is consistent: creation and annihilation operators really are each others adjoints.

Lemma 4.1.12. *Let $\mathcal{H}$ be a Hilbert space and $\mathcal{F}(\mathcal{H})$ be the Fock space over $\mathcal{H}$. For each $f \in \mathcal{H}$, the creation operator $a^*(f)$ is the adjoint of the annihilation operator $a(f)$. That is*

$$a(f)^* = a^*(f).$$

[6]Note that by Proposition 4.1.9, all CAR algebras over $\mathcal{F}_-(\mathcal{H})$ are isomorphic, and therefore it makes sense to talk about *the* CAR algebra over $\mathcal{F}_-(\mathcal{H})$.

Proof. It is enough to show that, for simple tensors $f_1 \otimes \cdots \otimes f_{n+1}$ and $g_1 \otimes \cdots \otimes g_n$, we have

$$\langle a^*(f)(g_1 \otimes \cdots \otimes g_n)|f_1 \otimes \cdots \otimes f_{n+1}\rangle = \langle g_1 \otimes \cdots \otimes g_n \,|\, a(f)(f_1 \otimes \cdots \otimes f_{n+1})\rangle\,.$$

This is a straightforward calculation. We have

$$\begin{aligned}
\langle a^*(f)(g_1 \otimes \cdots \otimes g_n)|f_1 \otimes \cdots \otimes f_{n+1}\rangle &= \left\langle \sqrt{n+1}(f \otimes g_1 \otimes \cdots \otimes g_n) \,\middle|\, f_1 \otimes \cdots \otimes f_{n+1} \right\rangle \\
&= \sqrt{n+1}\,\langle f|f_1\rangle\,\langle g_1 \otimes \cdots \otimes g_n|f_2 \otimes \cdots \otimes f_{n+1}\rangle \\
&= \langle g_1 \otimes \cdots \otimes g_n|\sqrt{n+1}\,\langle f|f_1\rangle\,(f_2 \otimes \cdots \otimes f_{n+1})\rangle \\
&= \langle g_1 \otimes \cdots \otimes g_n|a(f)(f_1 \otimes \cdots \otimes f_{n+1})\rangle
\end{aligned}$$

□

Proposition 4.1.13. *Let $\mathcal{H}$ be a Hilbert space and $\mathcal{F}_-(\mathcal{H})$ be the Fermi-Fock space. For each $f \in \mathcal{H}$, let $a_-(f)$ and $a_-^*(f)$ be the creation and annihilation operators on the Fermi-Fock space. The creation and annihilation operators satisfy the canonical anticommutation relations, and therefore generate the CAR algebra over $\mathcal{F}_-(\mathcal{H})$.*

Proof. Fix $f, g \in \mathcal{H}$. For simplicity we will omit the subscript on the creation and annihilation operators for the remainder of the proof. The creation operator is anti-linear because the inner-product on $\mathcal{H}$ is anti-linear in the first variable. To see that $\{a(f), a(g)\} = 0$, we calculate

$$\begin{aligned}
a(f)a(g)\,(f_1 \otimes \cdots \otimes f_n) &= a(f)\left(\sqrt{n}\,\langle g|f_1\rangle\,(f_2 \otimes \cdots \otimes f_n)\right) \\
&= \sqrt{n}\sqrt{n-1}\,\langle g|f_1\rangle\,\langle f|f_2\rangle\,(f_3 \otimes \cdots \otimes f_n) \\
&= \sqrt{n}\sqrt{n-1}\,\langle g \otimes f|f_1 \otimes f_2\rangle\,(f_3 \otimes \cdots \otimes f_n) \\
&= -\sqrt{n}\sqrt{n-1}\,\langle f \otimes g|f_1 \otimes f_2\rangle\,(f_3 \otimes \cdots \otimes f_n) \\
&= -\sqrt{n}\sqrt{n-1}\,\langle f|f_1\rangle\,\langle g|f_2\rangle\,(f_3 \otimes \cdots \otimes f_n) \\
&= -a(g)a(f)\,(f_1 \otimes \cdots \otimes f_n)
\end{aligned}$$

Therefore $a(f)a(g) + a(g)a(f) = 0$ on all simple tensors, and hence all of $\mathcal{F}_-(\mathcal{H})$. To

show that $\{a(f), a^*(g)\} = \langle f|g\rangle\, 1$, we first calculate

$$\begin{aligned} a^*(g)a(f)\,(f_1 \otimes \cdots \otimes f_n) &= a^*(g)\sqrt{n}\,\langle f|f_1\rangle\,(f_2 \otimes \cdots \otimes f_n) \\ &= \sqrt{n}\sqrt{n}\,\langle f|f_1\rangle\,(g \otimes f_1 \otimes \cdots \otimes f_n) \\ &= \sqrt{n}\,a(f)\,(f_1 \otimes g \otimes f_2 \otimes \cdots \otimes f_n) \\ &= -\sqrt{n}\,a(f)\,(g \otimes f_1 \otimes \cdots \otimes f_n) \\ &= -n\,\langle f|g\rangle\,(f_1 \otimes \cdots \otimes f_n)\,. \end{aligned}$$

Then we calculate

$$\begin{aligned} a(f)a^*(g)(f_1 \otimes \cdots \otimes f_n) &= a(f)\sqrt{n+1}(g \otimes f_1 \otimes \cdots \otimes f_n) \\ &= (n+1)\,\langle f|g\rangle\,(f_1 \otimes \cdots \otimes f_n), \end{aligned}$$

which says

$$(a(f)a^*(g) + a^*(g)a(f))\,(f_1 \otimes \cdots \otimes f_n) = \langle f|g\rangle\,(f_1 \otimes \cdots \otimes f_n).$$

It follows that $\{a(f), a^*(g)\} = \langle f|g\rangle\, 1$ on all simple tensors, and therefore all of $\mathcal{F}_-(\mathcal{H})$. Since the creation operators $a(f)$ satisfy the canonical anticommutation relations, Proposition 4.1.9 says that the C^*-algebra generated by these elements is the unique CAR algebra over the Fermi-Fock space $\mathcal{F}_-(\mathcal{H})$. □

Remark 4.1.14. The material of this section was originally created in order to study physical systems, so the fact that these objects should have physical interpretation is not surprising. As we have mentioned, the Fock space is the Hilbert space used when describing an arbitrary number of particles. If the particles we are describing are fermions or bosons, then we use the corresponding Fermi and Bose Fock spaces. The creation and annihilation operators then correspond to the creation and annihilation of particles. If $\Omega = (1, 0, \dots)$ is the zero particle state (i.e. the vacuum), then the vector given by $a^*_\pm(f)\Omega$ is an element of the one particle subspace, and hence the creation operator 'creates' a particle in the state f. In a similar way, the annihilation operator 'annihilates' a particle. As noted in Remark 4.1.4, the Pauli exclusion principle is built into the structure of the Fermi-Fock space, and is succinctly expressed by the condition $a^*_-(f)a^*_-(f) = 0$.

A proof of the following lemme is found in [8, Proposition 5.2.2]

Lemma 4.1.15. *Let $\mathcal{H}$ be a Hilbert space and $\mathcal{F}_-(\mathcal{H})$ be the Fermi-Fock space. For each $f \in \mathcal{H}$, let $a_-(f)$ and $a_-^*(f)$ be the creation and annihilation operators on the Fermi-Fock space. It follows that*

$$\|a_-^*(f)\| = \|a_-(f)\| = \|f\|$$

Note that this lemma implies that the creation operators on the Fermi-Fock space have bounded extensions.

Lemma 4.1.16. *Let $\mathcal{H}$ be a Hilbert space and $\mathcal{F}_+(\mathcal{H})$ be the Bose-Fock space. The annihilation operator on $\mathcal{F}_+(\mathcal{H})$ is an unbounded operator.*

Proof. Suppose $f \in \mathcal{H}$ and consider the n-fold tensor product of f with itself,

$$\psi^{(n)} = \underbrace{f \otimes \cdots \otimes f}_{n \text{ times}}.$$

The action of $a(f)$ on $\psi^{(n)}$ is

$$a(f)\psi^{(n)} = \sqrt{n}\,\langle f|f\rangle \underbrace{f \otimes \cdots \otimes f}_{n-1 \text{ times}}.$$

Taking the norm of this gives

$$\|a(f)\psi^{(n)}\| = \sqrt{n}\,\|f\|^2\,\|f \otimes \cdots \otimes f\| = \sqrt{n}\,\|f\|^{n+1}$$

It follows that the norm of $\|a(f)\|$ can be arbitrarily large, and therefore $a(f)$ cannot be a bounded operator. □

Remark 4.1.17. Lemma 4.1.16 justifies our assertion in Remark 4.1.7 that defining a CCR algebra in the same manner as we defined the CAR algebra isn't possible - the reason it fails is because operators satisfying the canonical commutation relations are necessarily unbounded. We shouldn't be surprised by this, since we saw exactly this result in Proposition 2.3.10. The unboundedness of the creation and annihilation operators for the Bose-Fock space make the analysis much more difficult. On the other hand, there are interesting features of the ideal Bose gas which occur as a direct result of this unboundedness, and are therefore not present in the ideal Fermi gas. A good example of this is Bose-Einstein condensation, a particularly special type of phase transition. A Bose-Einstein condensate is a collection of bosons in which a finite proportion of the

collection occupy the lowest energy state. For a detailed discussion of the ideal Bose gas and Bose Einstein condensation see [8, Section 5.2.5]. We will content ourselves here to the study of fermions in the ideal Fermi gas.

So far, we have set up the Hilbert space required to talk about the ideal Fermi gas. We still need to describe operators on this space and in particular, the Hamiltonian. To do this, we take operators defined on the one dimensional subspaces, and extend them to the entire Fock space.

Definition 4.1.18. Let $\mathcal{H}$ be a Hilbert space, and $\mathcal{F}_\pm(\mathcal{H})$ be the Bose/Fermi-Fock space associated to $\mathcal{H}$. Suppose that H is a self-adjoint operator on $\mathcal{H}$. Let $H_0 = 0$ and for each $n \in \mathbb{N}$, define

$$H_n(P_\pm((f_1 \otimes \cdots \otimes f_n)) = P_\pm \left(\sum_{i=1}^{n} f_1 \otimes \cdots \otimes Hf_i \otimes \cdots \otimes f_n \right)$$

for all $f_i \in \mathcal{D}(H)$. Extending by continuity leads to operators $H_n : \mathcal{H}_\pm^{\otimes n} \to \mathcal{H}_\pm^{\otimes n}$ defined on the n-particle subspaces. The direct sum of these operators is essentially self-adjoint[7], and its closure

$$d\Gamma(H) := \overline{\bigoplus_{n=0}^{\infty} H_n}$$

is therefore self-adjoint. We call $d\Gamma(H)$ the **second quantization** of H.

Example 4.1.19. We consider the simplest example of second quantisation, $d\Gamma(1)$. The operator $1 : \mathcal{H} \to \mathcal{H}$ is defined by $1(f) = f$ for all $f \in \mathcal{H}$. Then

$$1_n(f_1 \otimes \cdots \otimes f_n) = \sum_{i=1}^{n} (f_1 \otimes \cdots \otimes f_i \otimes \cdots \otimes f_n) = n(f_1 \otimes \cdots \otimes f_n).$$

The closure of the direct sum of these operators is called the **number operator**, written $N := d\Gamma(1)$. The action on each n-particle subspace $N : \mathcal{H}^{\otimes n} \to \mathcal{H}^{\otimes n}$ is

$$N\psi = n\psi,$$

and the domain[8] of N is

$$\mathcal{D}(N) = \left\{ \psi = (\psi^{(0)}, \psi^{(1)}, \psi^{(2)}, \dots) \in \mathcal{F}(\mathcal{H}) : \sum_{n=0}^{\infty} n^2 \|\psi^{(n)}\|^2 < \infty \right\}.$$

[7] See [45, Example 2 following Theorem VIII.33]

[8] in $\mathcal{F}(\mathcal{H})$

If U is a unitary operator on the one-particle Hilbert space $\mathcal{H}$, then the second quantisation of U has a slightly different definition.

Definition 4.1.20. Let U be a unitary operator on a Hilbert space $\mathcal{H}$, and let $\mathcal{F}_{\pm}(\mathcal{H})$ be the Bose/Fermi-Fock space associated with $\mathcal{H}$. Let $U_0 = 1$ and define, for each $n \in \mathbb{N}$,

$$U_n(P_{\pm}(f_1 \otimes \cdots \otimes f_n)) = P_{\pm}(Uf_1 \otimes \cdots \otimes Uf_n).$$

The **second quantisation** of U, denoted $\Gamma(U)$, is defined by

$$\Gamma(U) := \bigoplus_{n=0}^{\infty} U_n.$$

Note that $\Gamma(U)$ is unitary.

Remark 4.1.21. The notation $\Gamma(U)$ for the second quantisation of a unitary element U is chosen in a suggestive way to reflect the fact that if $U_t = e^{itH}$ is a strongly continuous one-parameter group of unitaries, then

$$\Gamma(U_t) = e^{itd\Gamma(H)}.$$

This follows from the Trotter product formula [45, Theorem VIII.31] and the definition of the second quantisation.

Quantum description of the ideal Fermi gas

In this section we give the quantum mechanical description of an ideal gas of fermions. We suppose that $\mathcal{H}$ is the Hilbert space of a single fermion, that $\mathcal{F}_{-}(\mathcal{H})$ is the anti-symmetric Fock space over $\mathcal{H}$ and that $\mathcal{A}$ is the CAR algebra over $\mathcal{F}_{-}(\mathcal{H})$. Let H be a self-adjoint Hamiltonian for the one-particle space. For the ideal Fermi gas, we are interested in an operator known as the **generalised Hamiltonian**, K_μ, defined by

$$K_\mu = d\Gamma(H - \mu 1) = d\Gamma(H) - \mu N,$$

where $\mu \in \mathbb{R}$ is a quantity known as the chemical potential. This determines a time evolution, $\tau_t : \mathcal{A} \to \mathcal{A}$ of the system, given by

$$\tau_t(A) = \Gamma(e^{itK_\mu})A\Gamma(e^{-itK_\mu}).$$

To see what this evolution does to the creation and annihilation operators, we calculate

$$\begin{aligned}\tau_t(a(f))(f_1 \otimes \cdots \otimes f_n) &= \Gamma(e^{itK_\mu})a(f)\Gamma(e^{-itK_\mu})(f_1 \otimes \cdots \otimes f_n) \\ &= \Gamma(e^{itK_\mu})a(f)(e^{-it(H-\mu 1)}f_1 \otimes \cdots \otimes e^{-it(H-\mu 1)}f_n) \\ &= \Gamma(e^{itK_\mu})\sqrt{n}\,\langle f|e^{-it(H-\mu 1)}f_1\rangle\,(e^{-it(H-\mu 1)}f_2 \otimes \cdots \otimes e^{-it(H-\mu 1)}f_n) \\ &= \sqrt{n}\,\langle e^{it(H-\mu 1)}f|f_1\rangle\,(f_2 \otimes \cdots \otimes f_n) \\ &= a(e^{it(H-\mu 1)}f)(f_1 \otimes \cdots \otimes f_n).\end{aligned}$$

Therefore $\tau_t(a(f)) = a(e^{it(H-\mu 1)}f)$, and similarly, we have $\tau_t(a^*(f)) = a^*(e^{it(H-\mu 1)}f)$. We now define the Gibbs state at inverse temperature β, on $\mathcal{F}_-(\mathcal{H})$, by

$$\phi_\beta(A) = \frac{\operatorname{Tr}\left(e^{-\beta K_\mu}A\right)}{\operatorname{Tr}\left(e^{-\beta K_\mu}\right)},$$

where $A \in \mathcal{A}$ and the trace is over $\mathcal{F}_-(\mathcal{H})$, provided it is finite. The time evolution is strongly continuous because

$$\|\tau_t(a(f)) - a(f)\| = \|a(e^{it(H-\mu 1)}f) - a(f)\| = \|a(e^{it(H-\mu 1)}f - f)\| = \|e^{it(H-\mu 1)}f - f\|.$$

For later use, we define the quantity $z := e^{\beta\mu}$ to be the **activity**. The condition that $\phi_\beta(A)$ be finite is automatically satisfied when $e^{-\beta K_\mu}$ is trace-class. Fortunately, the following proposition asserts that we only need to check this for the one-particle Hamiltonian.

Proposition 4.1.22. *Let H be a self-adjoint operator on a Hilbert space $\mathcal{H}$ and $\beta \in \mathbb{R}$. Let K_μ be the generalised Hamiltonian on the Fermi-Fock space $\mathcal{F}_-(\mathcal{H})$. Then the following conditions are equivalent:*

1. *$e^{-\beta H}$ is trace class on $\mathcal{H}$.*
2. *$e^{-\beta K_\mu}$ is trace class on $\mathcal{F}_-(\mathcal{H})$ for all $\mu \in \mathbb{R}$.*

Proof. Suppose that $e^{-\beta H}$ is trace class on $\mathcal{H}$, and denote the eigenvalues of H in increasing order by $\{\lambda_n\}_{n\geq 0}$, repeated according to multiplicity. To calculate the trace of $e^{-\beta K_\mu}$ in $\mathcal{H}_-^{\otimes m}$, we simply sum the elements $\langle n|e^{-\beta K_\mu}|n\rangle$ over an orthonormal basis $\{|n\rangle\}_{n\geq 0}$ of $\mathcal{H}_-^{\otimes m}$. The eigenvectors $\{|n\rangle\}_{n\geq 0}$ corresponding to the eigenvalues $\{\lambda_n\}_{n\geq 0}$ of H form an orthonormal basis for $\mathcal{H}$, and therefore an orthonormal basis for $\mathcal{H}^{\otimes m}$ is given by

$\{|n_1, n_2, \ldots, n_m\rangle\}$. We then calculate

$$\begin{aligned}\mathrm{Tr}_{\mathcal{H}^{\otimes m}}(e^{-\beta K_\mu}) &= \sum_{n_1}\sum_{n_2}\cdots\sum_{n_m}\left\langle n_1, n_2, \ldots, n_m \,\middle|\, e^{-\beta K_\mu} \,\middle|\, n_1, n_2, \ldots, n_m\right\rangle \\ &= (e^{\beta\mu})^m \sum_{n_1}\sum_{n_2}\cdots\sum_{n_m}\left\langle n_1, n_2, \ldots, n_m \,\middle|\, e^{-\beta H_m} \,\middle|\, n_1, n_2, \ldots, n_m\right\rangle \\ &= z^m \sum_{n_1}\sum_{n_2}\cdots\sum_{n_m} e^{-\beta(\lambda_{n_1}+\lambda_{n_2}+\cdots+\lambda_{n_m})}.\end{aligned}$$

Since $\mathcal{F}_-(\mathcal{H})$ is a direct sum, the trace over $\mathcal{F}_-(\mathcal{H})$ is the sum of the traces over the m particle subspaces. That is,

$$\begin{aligned}\mathrm{Tr}_{\mathcal{F}_-(\mathcal{H})}(e^{-\beta K_\mu}) &= \sum_{m=0}^{\infty}\mathrm{Tr}_{\mathcal{H}^{\otimes m}}(e^{-\beta K_\mu}) \\ &= \sum_{m=0}^{\infty} z^m \sum_{n_1}\sum_{n_2}\cdots\sum_{n_m} e^{-\beta(\lambda_{n_1}+\lambda_{n_2}+\cdots+\lambda_{n_m})} \\ &= \prod_{m=0}^{\infty}(1+ze^{-\beta\lambda_m}).\end{aligned}$$

We note that for all $x \geq 0$, we have $1 + x \leq e^x$. Since $ze^{-\beta\lambda_m} \geq 0$ for all m, we therefore have

$$\prod_{m=0}^{\infty}(1+ze^{-\beta\lambda_m}) \leq \prod_{m=0}^{\infty}\exp\{ze^{-\beta\lambda_m}\}.$$

This finally gives us

$$\mathrm{Tr}_{\mathcal{F}_-(\mathcal{H})}(e^{-\beta K_\mu}) \leq \prod_{m=0}^{\infty}\exp\left\{ze^{-\beta\lambda_m}\right\} = \exp\left\{z\sum_{m=0}^{\infty}e^{-\beta\lambda_m}\right\} = \exp\{z\,\mathrm{Tr}_{\mathcal{H}}\,e^{-\beta H}\},$$

which is finite by hypothesis. To prove the converse, simply note that

$$\mathrm{Tr}_{\mathcal{F}_-(\mathcal{H})}(e^{-\beta K_\mu}) = \sum_{m=0}^{\infty}\mathrm{Tr}_{\mathcal{H}^{\otimes m}}(e^{-\beta K_\mu}) = z\,\mathrm{Tr}_{\mathcal{H}}\,e^{-\beta H} + \sum_{m\neq 1}^{\infty}\mathrm{Tr}_{\mathcal{H}^{\otimes m}}(e^{-\beta K_\mu}).$$

An infinite sum of positive terms can only be finite if each term is finite, and therefore $e^{-\beta H}$ is trace class over $\mathcal{H}$ if $e^{-\beta K_\mu}$ is trace class over $\mathcal{F}_-(\mathcal{H})$.

□

We now calculate a quantity known as the two-point function of the Gibbs state. This function gives an explicit method of calculating the value of the Gibbs state on operators of the form $a^*(f)a(g)$, and will be used in the calculation of various physical properties of the ideal Fermi gas. The results of this calculation are summarised in the following lemma.

Lemma 4.1.23. *Let $\mathcal{F}_-(\mathcal{H})$ be the Fermi-Fock space over a Hilbert space $\mathcal{H}$. Let H be a self-adjoint operator on $\mathcal{H}$ and assume that $e^{-\beta H}$ is trace-class. Let*

$$\phi_\beta(A) = \frac{\operatorname{Tr}\left(e^{-\beta K_\mu} A\right)}{\operatorname{Tr}\left(e^{-\beta K_\mu}\right)}$$

denote the Gibbs grand canonical equilibrium state at inverse temperature β over the CAR algebra $\mathcal{A}$, with the generalised Hamiltonian $K_\mu = d\Gamma(H - \mu 1)$. It follows that ϕ_β satisfies the following identity:

$$\phi_\beta(a^*(f)a(g)) = \left\langle g \,\middle|\, ze^{-\beta H}(1 + ze^{-\beta H})^{-1} f \right\rangle.$$

Proof. We begin by calculating, on simple tensors,

$$\begin{aligned}
e^{-\beta K_\mu} a^*(f)(f_1 \otimes \cdots \otimes f_n) &= \sqrt{n+1}\, e^{-\beta d\Gamma(H)} e^{\beta\mu N}(f \otimes f_1 \otimes \cdots \otimes f_n) \\
&= e^{\beta\mu(n+1)} \sqrt{n+1}\, e^{-\beta d\Gamma(H)}(f \otimes f_1 \otimes \cdots \otimes f_n) \\
&= z e^{\beta\mu n} \sqrt{n+1}\, (e^{-\beta H} f \otimes e^{-\beta H} f_1 \otimes \cdots \otimes e^{-\beta H} f_n) \\
&= z a^*(e^{-\beta H} f) e^{\beta\mu n}(e^{-\beta H} f_1 \otimes \cdots \otimes e^{-\beta H} f_n) \\
&= z a^*(e^{-\beta H} f) e^{-\beta K_\mu}(f_1 \otimes \cdots \otimes f_n),
\end{aligned}$$

from which it follows that $e^{-\beta K_\mu} a^*(f) = z a^*(e^{-\beta H} f) e^{-\beta K_\mu}$. We then calculate

$$\phi_\beta(a^*(f)a(g)) = \frac{\operatorname{Tr}\left(e^{-\beta K_\mu} a^*(f)a(g)\right)}{\operatorname{Tr}\left(e^{-\beta K_\mu}\right)} = \frac{z \operatorname{Tr}\left(a^*(e^{-\beta H}) e^{-\beta K_\mu} a(g)\right)}{\operatorname{Tr}\left(e^{-\beta K_\mu}\right)}.$$

Cyclicity of the trace and the anticommutation relation

$$a(g)a^*(e^{-\beta H} f) + a^*(e^{-\beta H} f)a(g) = \langle g | e^{-\beta H} f \rangle$$

gives

$$\phi_\beta(a^*(f)a(g)) = z\phi_\beta(a(g)a^*(e^{-\beta H} f)) = z \langle g | e^{-\beta H} f \rangle - z\phi_\beta(a^*(e^{-\beta H} f)a(g)).$$

Rearranging this, we get

$$\begin{aligned}
\langle g | z e^{-\beta H} f \rangle &= \phi_\beta(a^*(f)a(g) + z a^*(e^{-\beta H} f)a(g)) \\
&= \phi_\beta(a^*((1 + ze^{-\beta H}) f)a(g)).
\end{aligned}$$

Replacing f with $(1 + ze^{-\beta H})^{-1} f$, we get the required result. □

When $f = g$, the previous lemma gives us an explicit method for constructing $\phi_\beta(a^*(f)a(f))$. Consistent with the definition of the annihilation and creation operators, the operator $a^*(f)a(f)$ counts the number of particles in the state f. We define a number functional, $\hat{N} : \mathcal{S}(\mathcal{A}) \to [0, \infty]$, by

$$\hat{N}(\phi) = \sup_F \sum_{\{f_i\} \subset F} \phi(a^*(f_i)a(f_i)),$$

where the supremum is taken over all finite orthonormal subsets of $\mathcal{H}$.

One of the main advantages of KMS states over Gibbs states is that the former survives the transition to the thermodynamic limit. In order to discuss the thermodynamic limit of the ideal Fermi gas, we choose an explicit Hilbert space $\mathcal{H} = L^2(\Lambda)$, where $\Lambda \subset \mathbb{R}^\nu$ is bounded and open. This choice coincides with the usual Schrödinger picture of quantum mechanics in a finite region of ν-dimensional space. We consider the laplacian operator $-\nabla^2$ which acts on $C_0^\infty(\Lambda)$, the smooth functions with support in Λ as our candidate for the one-particle Hamiltonian[9]. We have the following local picture: For each $\Lambda \subset \mathbb{R}^\nu$, we denote by $\mathcal{A}_\Lambda$ the CAR algebra over $L^2(\Lambda)$, H_Λ a[10] self-adjoint extension of the laplacian over $L^2(\Lambda)$, and τ^Λ the time evolution generated by H_Λ such that $\tau^\Lambda(a(f)) = a(e^{itH_\Lambda} f)$. Let ϕ_β^Λ be the (τ^Λ, β)-KMS state on $\mathcal{A}_\Lambda$ given by the two point function

$$\phi_\beta^\Lambda(a^*(f)a(g)) = \langle g | z e^{-\beta H_\Lambda} (1 + z e^{-\beta H_\Lambda})^{-1} f \rangle .$$

Globally, we have the CAR algebra $\mathcal{A}$ over $L^2(\mathbb{R}^\nu)$, the self-adjoint extension H of the laplacian over $L^2(\mathbb{R}^\nu)$, and the time evolution τ generated by H such that $\tau(a(f)) = a(e^{itH} f)$. Let ϕ_β be the (τ, β)-KMS state on $\mathcal{A}$ given by the two point function

$$\phi_\beta(a^*(f)a(g)) = \langle g | z e^{-\beta H} (1 + z e^{-\beta H})^{-1} f \rangle .$$

The action of H on $f \in L^2(\mathbb{R}^\nu)$ is given by

$$(Hf)(x) = \left(\frac{1}{\sqrt{2\pi}} \right)^\nu \int \hat{f}(p)\, p^2\, e^{ipx}\, d^\nu p,$$

[9] If we choose units such that $\frac{\hbar^2}{2m} = 1$, then this choice corresponds to the usual quantum mechanical Hamiltonian of a free particle

[10] The laplacian does not have a unique self-adjoint extension to $L^2(\Lambda)$, since different boundary conditions give rise to different extensions. It does, however, have a unique self-adjoint extension to $L^2(\mathbb{R}^\nu)$, where there is no ambiguity introduced by the boundary.

where $\hat{f}$ is the fourier transform of f, and the domain of H is given by

$$\mathcal{D}(H) = \left\{ f \in L^2(\mathbb{R}^\nu) : \int p^4 \, |\hat{f}(p)|^2 \, d^\nu p \, < \infty \right\}.$$

Although we will not prove it, it turns out that the thermodynamical limit of the finite volume states is uniquely defined and independent of the choice of boundary conditions for the H_Λ. That is,

$$\lim_{\Lambda' \to \infty} \phi_\beta^{\Lambda'}(A) = \phi_\beta(A)$$

where the $\Lambda' \to \infty$ in the sense that Λ' eventually contains any given $\Lambda \subset \mathbb{R}^\nu$. For a proof of this, see [8, Theorem 5.2.24]. With this picture, we can calculate some quantities of interest for the ideal Fermi gas. By restricting the state ϕ_β to the local algebras $\mathcal{A}_\Lambda$, one can define local number functionals $\hat{N}_\Lambda(\phi_\beta)$. This functional then gives the number of particles in Λ, and the local density, ρ_Λ is therefore given by

$$\rho_\Lambda(\beta, z) = \frac{\hat{N}(\phi_\beta)}{|\Lambda|},$$

where $|\Lambda|$ is the volume[11] of Λ. Doing this computation, we get

$$\begin{aligned}
\rho_\Lambda(\beta, z) &= |\Lambda|^{-1} \sum_{n \geq 0} \phi_\beta(a^*(f_n) a(f_n)) \\
&= |\Lambda|^{-1} \sum_{n \geq 0} \left\langle f_n \,\middle|\, z e^{-\beta H} (1 + z e^{-\beta H})^{-1} f_n \right\rangle = |\Lambda|^{-1} \operatorname{Tr}(z e^{-\beta H} (1 + z e^{-\beta H})^{-1}),
\end{aligned}$$

where the trace is over $L^2(\Lambda)$. To calculate this, we consider what the function $z e^{-\beta H}(1 + z e^{-\beta H})^{-1}$ does to a function $f \in L^2(\Lambda)$.

$$\begin{aligned}
\left(z e^{-\beta H} (1 + z e^{-\beta H})^{-1} f \right)(x) &= \left(\frac{1}{\sqrt{2\pi}} \right)^\nu \int \frac{z e^{-\beta p^2}}{(1 + z e^{-\beta p^2})} e^{ipx} \hat{f}(p) d^\nu p \\
&= (2\pi)^{-\nu} \int \frac{z e^{-\beta p^2}}{(1 + z e^{-\beta p^2})} e^{ipx} \int f(y) e^{-ipy} d^\nu y \, d^\nu p \\
&= (2\pi)^{-\nu} \int f(y) \int \frac{z e^{-\beta p^2}}{(1 + z e^{-\beta p^2})} e^{ip(x-y)} d^\nu p \, d^\nu y \\
&= (2\pi)^{-\nu} \int_\Lambda f(y) K(x, y) d^\nu y,
\end{aligned}$$

where the integral is over Λ since f has support in Λ, and

$$K(x, y) = \int \frac{z e^{-\beta p^2}}{(1 + z e^{-\beta p^2})} e^{ip(x-y)} d^\nu p.$$

[11] i.e. Lebesegue measure of Λ

Now for an operator T defined by

$$(Tf)(x) = \int_\Lambda f(y)K(x,y)dy,$$

the trace is given by[12]

$$\mathrm{Tr}(T) = \int_\Lambda K(x,x)dx.$$

It follows that

$$\begin{aligned}\rho_\Lambda(\beta,z) &= (2\pi)^{-\nu}|\Lambda|^{-1}\int_\Lambda\left(\int \frac{ze^{-\beta p^2}}{(1+ze^{-\beta p^2})}d^\nu p\right)d^\nu x \\ &= (2\pi)^{-\nu}\int \frac{ze^{-\beta p^2}}{(1+ze^{-\beta p^2})}d^\nu p.\end{aligned}$$

It can be shown (see [8, Section 5.2.4]) through the use of quadratic forms, that when the local regions Λ are given Neumann boundary conditions, the local energy of the state ϕ_β is given by

$$\sum_{n\geq 0}\phi_\beta(a^*(\nabla f_n)\cdot a(\nabla f_n))$$

where f_n is an orthonormal basis for $L^2(\Lambda)$. It follows that the local energy density $\varepsilon(\beta,z)$ is given by

$$\begin{aligned}\varepsilon(\beta,z) &= |\Lambda|^{-1}\sum_{n\geq 0}\phi_\beta(a^*(\nabla f_n)\cdot a(\nabla f_n)) \\ &= |\Lambda|^{-1}\sum_{n\geq 0}\left\langle \nabla f_n \,\middle|\, ze^{-\beta H}(1+ze^{-\beta J})^{-1}\nabla f_n\right\rangle \\ &= (2\pi)^{-\nu}\int p^2\,\frac{ze^{-\beta p^2}}{1+ze^{-\beta p^2}}\,d^\nu p.\end{aligned}$$

We can simplify this last integral through a ν-dimensional integration by parts. This is not overly difficult, although the notation can complicate the calculation. We will illustrate the integration by parts in two dimensions for simplicity of exposition. We choose cartesian coordinates (x,y), and calculate

$$\begin{aligned}&\iint (x^2+y^2)\,\frac{ze^{-\beta(x^2+y^2)}}{1+ze^{-\beta(x^2+y^2)}}\,dx\,dy \\ &= \iint \frac{zx^2e^{-\beta(x^2+y^2)}}{1+ze^{-\beta(x^2+y^2)}}\,dx\,dy + \iint \frac{zy^2e^{-\beta(x^2+y^2)}}{1+ze^{-\beta(x^2+y^2)}}\,dx\,dy \\ &= \left(\frac{-1}{2\beta}\right)\iint \frac{-2\beta zxe^{-\beta(x^2+y^2)}}{1+ze^{-\beta(x^2+y^2)}}\,xdx\,dy + \left(\frac{-1}{2\beta}\right)\iint \frac{-2\beta zy^2e^{-\beta(x^2+y^2)}}{1+ze^{-\beta(x^2+y^2)}}\,ydy\,dx.\end{aligned}$$

[12][47]

Performing integration by parts on each integral and using Neumann boundary conditions gives us

$$\left(\frac{1}{2\beta}\right)\iint \log(1+ze^{-\beta(x^2+y^2)})\,dx\,dy+\left(\frac{1}{2\beta}\right)\iint \log(1+ze^{-\beta(x^2+y^2)})\,dy\,dx.$$

For the ν-dimensional case, you simply split the integral up into the ν different parts, separately perform integration by parts, and then combine. The local energy density is therefore given by

$$\varepsilon(\beta,z)=\left(\frac{\nu}{2\beta}\right)(2\pi)^{-1}\int \log(1+ze^{-\beta p^2})d^\nu p.$$

The local energy density and particle density are independent of the region Λ chosen. Since the variable p conjugate to x is defined as the momentum, we interpret

$$(2\pi)^{-\nu}\frac{ze^{-\beta p^2}}{1+z^{-\beta p^2}}\,d^\nu p$$

as the momemtum distribution per unit volume. For high temperatures and low densities, i.e. for classical gases, we have

$$\rho(\beta,z)=(2\pi)^{-\nu}\int ze^{-\beta p^2}d^\nu p \qquad\qquad \varepsilon(\beta,z)=(2\pi)^{-\nu}\int zp^2e^{-\beta p^2}d^\nu p.$$

In this case, we have the usual classical Maxwellian form of the momentum distribution, $(2\pi)^{-\nu}ze^{-\beta p^2}d^\nu p$. With the identification of the pressure P as

$$P(\beta,z)=\frac{2}{\nu}\varepsilon(\beta,z),$$

one then calculates

$$\frac{P(\beta,z)}{\rho(\beta,z)}=\frac{2\varepsilon(\beta,z)}{\nu\rho(\beta,z)}=\frac{2\int p^2e^{-\beta p^2}d^\nu p}{\nu\int e^{-\beta p^2}d^\nu p}.$$

Splitting the top integral up into the ν separate integrals and performing integration by parts, we obtain

$$\frac{P(\beta,z)}{\rho(\beta,z)}=\frac{2\left(\frac{\nu}{2\beta}\right)\int e^{-\beta p^2}d^\nu p}{\nu\int e^{-\beta p^2}d^\nu p}=\frac{1}{\beta}.$$

Since the density is simply the amount of substance of the gas divided by the volume V, and β is the inverse temperature (in suitable units), we have just derived the ideal gas law

$$PV\propto T.$$

This is cited in [8] as the ultimate justification of the identification of β as the inverse temperature. We now consider the low temperature limit of the momentum distribution. This limit depends on the value of the activity z. Recall that $z = e^{\beta\mu}$, so the momentum distribution has the form

$$(2\pi)^{-\nu}\frac{e^{-\beta(p^2-\mu)}}{1+e^{-\beta(p^2-\mu)}} = (2\pi)^{-\nu}\left(1 - \frac{1}{1+e^{-\beta(p^2-\mu)}}\right)$$

The low temperature limit, $\beta \to \infty$, for this is given by

$$\lim_{\beta\to\infty}(2\pi)^{-\nu}\frac{e^{-\beta(p^2-\mu)}}{1+e^{-\beta(p^2-\mu)}} = \begin{cases}(2\pi)^{-\nu}, & \text{if } p^2 < \mu \\ 0, & \text{if } p^2 > \mu.\end{cases}$$

This result says that only particles whose energy is less than the chemical potential can exist in the low temperature limit. This is sometimes referred to as the Fermi sea, and the critical value of p, the surface $p^2 = \mu$ is referred to as the Fermi surface.

Remark 4.1.24. Although we have calculated the local particle and energy densities, we haven't shown that these densities are equal to the thermodynamic limit of their finite volume counterparts. To do so would require a deeper analysis of boundary conditions, and remains outside the scope of this report. The thermodynamic limit of the finite volume counterparts with classical boundary conditions (i.e. Dirichlet, Neumann and periodic) are analysed in [8, Example 5.2.26]. An important result of their analysis is[13] a bound obtained on the error occurring when one replaces the finite volume particle density ρ_{Λ_L} with its thermodynamic limit ρ. This bound is

$$0 \leq 1 - \frac{\rho_{\Lambda_L}(\beta, z)}{\rho(\beta, z)} \leq 12\frac{\lambda}{L},$$

where $\lambda = \sqrt{4\pi\beta}$ is the thermal wavelength of the fermions which, in some sense, is a measure of the 'size' of the fermions. Even if the system being considered is as small as 1 cm, the infinite-volume limit is an excellent approximation. For instance, helium at room temperature has a thermal wavelength of $\lambda \sim 2 \times 10^{-8}$ cm, so that the error is approximately 2 parts in 10^7.

[13] in the case of a parallelepiped shaped region Λ_L

Chapter 5

Interacting systems

In the previous chapter we described two simple quantum systems: the harmonic oscillator and the ideal Fermi gas. In this chapter, we will introduce an interacting system. We will study such an interacting system using perturbation theory. Perturbation theory for automorphisms of C^*-algebras provides further justification for the interpretation of KMS states as equilibrium states of the system. As a result, we will begin this chapter with an introduction to the perturbation theory of automorphisms of a C^*-algebra, and proceed to use perturbation theory to explore various criteria for stability and how the KMS condition is related to these criteria. We will conclude the chapter by describing an application of perturbation theory to the interacting Fermi oscillator.

5.1 Perturbation theory

The general idea of the perturbation theory we are considering is to introduce some kind of change in the dynamics of the system and study the change in the state of the system as a result. More specifically, we wish to introduce self-adjoint perturbations of the infinitesimal generators of the time evolution of the system, and study the equilibrium states under the associated evolution. To do this, we first discuss derivations and infinitesimal generators of the dynamics.

Definition 5.1.1. A **derivation** δ of a C^*-algebra $\mathcal{A}$ is a linear operator from a $*$-subalgebra $\mathcal{D}(\delta)$, the domain of δ, into $\mathcal{A}$ with the properties that

- $\delta(A)^* = \delta(A^*) \qquad \forall A \in \mathcal{D}(\delta)$.

- $\delta(AB) = \delta(A)B + A\delta(B) \qquad \forall A,\, B \in \mathcal{D}(\delta).$

We are interested in derivations because the infinitesimal generators of our one-parameter groups of automorphisms are derivations.

Definition 5.1.2. Let $\mathcal{A}$ be a C^*-algebra, and τ_t a strongly continuous one-parameter group of automorphisms of $\mathcal{A}$. The **infinitesimal generator** of τ_t is defined to be the linear operator δ, whose domain $\mathcal{D}(\delta)$ consists of those $A \in \mathcal{A}$ for which the limit

$$B := \lim_{t\to 0} \frac{\tau_t(A) - A}{t}$$

exists. For $A \in \mathcal{D}(\delta)$, the action of δ is then defined to be $\delta(A) = B$.

Example 5.1.3. Suppose $\mathcal{H}$ is a Hilbert space, and let H be the self-adjoint Hamiltonian acting on $\mathcal{H}$. By Stone's theorem, the Hamiltonian generates a strongly continuous one-parameter group of unitaries $U_t = e^{itH}$. The infinitesimal generator for this group is $\delta(A) = i[H, A]$.

Proposition 5.1.4. *Let $\mathcal{A}$ be a C^*-algebra, and τ_t a strongly continuous one-parameter group of automorphisms of $\mathcal{A}$. Then the infinitesimal generator δ of τ_t is a derivation of $\mathcal{A}$.*

Proof. Fix $A,\, B \in \mathcal{D}(\delta)$. Then

$$\delta(A)^* = \left(\lim_{t\to 0} \frac{\tau_t(A) - A}{t}\right)^* = \lim_{t\to 0} \frac{\tau_t(A^*) - A^*}{t} = \delta(A^*).$$

We also have

$$\begin{aligned}\delta(AB) &= \lim_{t\to 0} \frac{\tau_t(AB) - AB}{t} = \lim_{t\to 0} \frac{\tau_t(A)\tau_t(B) - \tau_t(A)B + \tau_t(A)B - AB}{t} \\ &= \lim_{t\to 0} \tau_t(A)\frac{\tau_t(B) - B}{t} + \lim_{t\to 0} \frac{\tau_t(A) - A}{t} B = \delta(A)B + A\delta(B).\end{aligned}$$

□

We now wish to perturb the dynamics of our system. To do this, we consider C^*-dynamical system $(\mathcal{A}, \tau, \mathbb{R})$ with infinitesimal generator δ. We then introduce a self-adjoint perturbation P, and define a bounded derivation δ_P by $\delta_P(A) = i[P, A]$. We are then interested in dynamics generated by $\delta + \delta_P$.

Remark 5.1.5. It helps to keep the physical interpretation in mind during this section. The generator of the time evolution in physics is the Hamiltonian H, which usually corresponds to the total energy of the system. Adding a perturbation then corresponds to the addition of 'energy' P to the Hamiltonian, and studying the resulting dynamics.

Proposition 5.1.6. *Let $(\mathcal{A}, \tau, \mathbb{R})$ be a C^*-dynamical system and let δ be the infinitesimal generator of τ. Furthermore, assume that $t \in \mathbb{R} \mapsto P_t = P_t^* \in \mathcal{A}$ is a norm-continuous one-parameter family of self-adjoint elements. It follows that there exists a unique one-parameter family of automorphisms τ^P of $\mathcal{A}$ given by*

$$\tau_t^P(A) = \tau_t(A) + \sum_{n=1}^{\infty} i^n \int_0^1 \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n [\tau_{t_n}(P_{t_n}), [\cdots [\tau_{t_1}(P_{t_1}), \tau_t(A)]]].$$

Moreover, one has

$$\tau_t^P(A) = \Gamma_t^P \tau_t(A) \Gamma_t^{P*},$$

where Γ_t^P is a one-parameter family of unitary elements, determined by

$$\Gamma_t^P = 1 + \sum_{n=1}^{\infty} i^n \int_0^t \mathrm{d}t_1 \int_0^{t_1} \mathrm{d}t_2 \cdots \int_0^{t_{n-1}} \mathrm{d}t_n \tau_{t_n}(P) \cdots \tau_{t_1}(P).$$

We will make no attempt to prove this proposition, but refer the reader to [8, Proposition 5.4.26], or to [8, Proposition 5.4.1] for a time independent version of Proposition 5.1.6. Our primary interest in Proposition 5.1.6 is as a calculational tool. The series in Proposition 5.1.6 can be approximated with finite sums in order to estimate the resulting perturbation. Estimates for the bounds of these sums can then provide justification for the approximation.

5.2 Ground states, passivity and stability

In this section we wish to provide further justification for the idea that the KMS condition provides an adequate characterisation for states of thermal equilibrium. This section is based on material from [44]. Proofs for the results in this section can be found in [44] and [8, Section 5.4.4].

Recall from Remark 3.3.2 the notion of the entropy of a state. We let $\mathcal{H}$ be a finite dimensional Hilbert space of dimension n, and consider $M_n(\mathbb{C})$, the C^*-algebra of $n \times n$ matrices acting on $\mathcal{H}$. For $\phi \in \mathcal{S}(M_n(\mathbb{C}))$ with density matrix ρ, we define the entropy of ϕ

to be $S(\phi) = -\operatorname{Tr}(\rho \log \rho)$. We have already seen that the Gibbs state is the unique state which maximises the entropy for a fixed temperature. Indeed, it follows from Equation 3.2 that the Gibbs state is the unique state which maximises the function

$$F(\phi) = \frac{S(\phi)}{\beta} - \phi(H) \qquad \text{for } \phi \in \mathcal{S}(M_n(\mathbb{C})),$$

and therefore $F(\phi_G) \geq F(\Sigma(\phi_G))$ for any map $\Sigma : \mathcal{S}(M_n(\mathbb{C})) \to \mathcal{S}(M_n(\mathbb{C}))$. If we consider the map $\Sigma(\phi(A)) = \phi(U^*AU)$, with U a unitary matrix, then $S(\Sigma(\phi)) = S(\phi)$, since the trace is invariant under conjugation by unitaries. We then have

$$-\phi_G(H) \geq -\phi_G(U^*HU),$$

or to put it another way,

$$\phi_G(U^*[H, U]) \geq 0.$$

Since the infinitesimal generator for the time evolution associated to the Gibbs state is $\delta(A) = i[H, A]$, we conclude that the Gibbs state ϕ_G satisfies the condition

$$-i\phi(U^*\delta(U)) \geq 0, \tag{5.1}$$

for each unitary U. This condition has no reference to the temperature, so we cannot expect that it is completely equivalent to the KMS condition. On the other hand, this condition is intimately related to the maximal entropy principle, so we expect that it, or another related property, is something that will be satisfied by general equilibrium states.

Definition 5.2.1. Let $(\mathcal{A}, \tau, \mathbb{R})$ be a C^*-dynamical system, and let δ be the infinitesimal generator of τ. A state ϕ over $\mathcal{A}$ is said to be a **ground state** if

$$-i\phi(A^*\delta(A)) \geq 0$$

for all $A \in \mathcal{D}(\delta)$. Similarly, ϕ is called a **ceiling state** if

$$i\phi(A^*\delta(A)) \geq 0$$

for all $A \in \mathcal{D}(\delta)$.

We informally refer to ground and ceiling states as "(τ, ∞)-KMS states". and "$(\tau, -\infty)$-KMS states" respectively. This convention is justified by the following proposition.

Proposition 5.2.2. *Let $(\mathcal{A}, \tau, \mathbb{R})$ be a C^*-dynamical system, and let ϕ be a ground state. Then for all A, $B \in \mathcal{A}_\tau$, the entire analytic function*

$$z \mapsto \phi(A\tau_z(B))$$

is uniformly bounded in the region $\{z \in \mathbb{C} : \Im(z) \geq 0\}$.

There exists a corresponding proposition for ceiling states which we omit. The following definition defines the notion of a passive state. We have chosen this definition because it is immediately clear that all ground states are passive. Indeed, passivity is a property that equilibrium states generally satisfy, and as we shall see, is intimately related to the second law of thermodynamics.

Definition 5.2.3. Let $(\mathcal{A}, \tau, \mathbb{R})$ be a C^*-dynamical system, where $\mathcal{A}$ is unital, and let δ be the infinitesimal generator of τ. A state ϕ on $\mathcal{A}$ is a **passive state** if

$$-i\phi(A^*\delta(A)) \geq 0$$

for any $A \in \mathcal{D}(\delta) \cap \mathcal{U}_0$, where $\mathcal{U}_0$ is the connected component of the identity of the group $\mathcal{U}(\mathcal{A})$ of all unitaries of $\mathcal{A}$ with the uniform topology. Moreover, ϕ is said to be **completely passive** if the state $\bigotimes_{i=1}^n \phi$ is a passive state of the C^*-dynamical system $(\bigotimes_{i=1}^n \mathcal{A}, \bigotimes_{j=1}^n \tau, \mathbb{R})$.

We now discuss the physical interpretation of passive states. To do this, we consider a C^*-dynamical system $(\mathcal{A}, \tau, \mathbb{R})$ with infinitesimal generator δ. We introduce a perturbation of the dynamics of the system by assuming that

$$\delta_t(A) = \delta(A) + i[P_t, A]$$

with $A \in \mathcal{D}(\delta)$ and $\{P_t\}_{t\in\mathbb{R}}$ a family of self-adjoint elements of $\mathcal{A}$. We will only consider perturbations for which there is some $T \in \mathbb{R}$ such that $P_t = 0$ for $t \leq 0$ and P_t is constant for $t \geq T$. We will also assume that P_t is continuous and differentiable (in the norm topology) for $0 \leq t \leq T$. The physical interpretation is that the family $\{P_t\}$ corresponds to a change in the external parameters of the system, and the perturbed dynamics are how the system responds to this change. The change in the external parameters could be arranged by moving the walls of the container confining the system or by switching on some external fields. From Remark 5.1.5, we note that the perturbation of the dynamics

corresponds to the addition (or removal) of some energy from the system. This makes sense physically, since changing the external parameters of the system generally involves work being done on or by the system. We now calculate the energy that is transferred to the system during the time interval $[0, T]$, by using the formula

$$L^P(\phi) = \int_0^T \phi\left(\tau_t^P\left(\frac{dP_t}{dt}\right)\right) dt. \tag{5.2}$$

To justify this formula, we split $[0, T]$ into small intervals of length Δt, such that the state is almost constant on each small interval. Then the Riemann sum

$$L^P(\phi) = \sum \phi(\tau_t^P(P_{t+\Delta t} - P_t))$$

approximates the energy transmitted to the system in the interval $[0, T]$, and in the limit $\Delta t \to 0$ we obtain Equation (5.2). The sign of $L^P(\phi)$ determines whether the system gains or loses energy during the time interval. If $L^P(\phi) \geq 0$ then positive work is done by the external forces, and the energy of the system increases. Conversely, if $L^P(\phi) < 0$, the system does positive work on its surroundings and the energy of the system decreases.

We now restrict to perturbations $\{P_t\}$ such that $P_t = 0$ for all $t \geq T$. This corresponds to a cyclic process. A statement of the second law of thermodynamics is that systems in equilibrium are unable to perform work in cyclic processes. The following proposition indicates that passivity is a necessary condition for an equilibrium state to be consistent with the second law of thermodynamics.

Proposition 5.2.4. *Let $(\mathcal{A}, \tau, \mathbb{R})$ be a C^*-dynamical system. A state ϕ on $\mathcal{A}$ is passive if and only if*

$$L^P(\phi) \geq 0$$

for any differentiable family $\{P_t\}_{t\in\mathbb{R}}$ of self-adjoint elements of $\mathcal{A}$ such that $P_t = 0$ for $t \leq 0$ and $t \geq T$.

This proposition says exactly that a passive state is one which is unable to perform work in a cyclic process. The relationship between the various characterisations of equilibrium introduced in this chapter are stated in the following theorem.

Theorem 5.2.5. *Let $(\mathcal{A}, \tau, \mathbb{R})$ be a C^*-dynamical system and δ be the generator of τ. A state ϕ is completely passive if and only if ϕ is a (τ, β)-KMS state[1] for some $\beta \in [0, \infty]$, and ϕ is τ-invariant.*

[1] i.e. ϕ is either a ground state or a (τ, β)-KMS state for some $\beta \in [0, \infty)$.

Remark 5.2.6. Since KMS states are automatically invariant under the time evolution by Proposition 3.3.9, Theorem 5.2.5 says that a completely passive state is either a KMS state or a τ-invariant ground state. Conversely, every KMS state or τ-invariant ground state is completely passive. Since a completely passive state is necessarily passive, it follows that KMS states are passive, and therefore they are unable to perform work in cyclic processes, in accordance with the second law of thermodynamics.

Before we apply this theory to the Fermi oscillator, we conclude this section with a small but interesting application of passive systems. We require the following lemma.

Lemma 5.2.7. *Let $(\mathcal{A}, \tau, \mathbb{R})$ be a C^*-dynamical system with infinitesimal generator δ. Furthermore, let $\{P_t\}_{t\in\mathbb{R}}$ be a norm-differentiable one-parameter family of self-adjoint elements with $P_t \in \mathcal{D}(\delta)$ for all t, and suppose $P_t = 0$ for all $t \leq 0$ and $t \geq T$, for some $T \in \mathbb{R}^+$. Let*

$$\frac{d(\delta(P_t))}{dt} = \delta\left(\frac{dP_t}{dt}\right),$$

and consider the one-parameter family of automorphisms τ^P determined by $\{P_t\}_{t\in\mathbb{R}}$ from Proposition 5.1.6. It follows that

$$L^P(\phi) = -i\phi(\Gamma_T^P\, \delta(\Gamma_T^{P*})),$$

where Γ_T^P is the unitary element relating τ_T^P and τ_T from Proposition 5.1.6.

Remark 5.2.8. Lemma 5.2.7 has an interesting application. We consider two C^*-dynamical systems $(\mathcal{A}_1, \tau^1, \mathbb{R})$ and $(\mathcal{A}_2, \tau^2, \mathbb{R})$. We wish to link these two systems by perturbing the system with some perturbation P_t. We write $\mathcal{A} = \mathcal{A}_1 \otimes \mathcal{A}_2$ and $\tau = \tau^1 \otimes \tau^2$, for the combined (but as yet unlinked) systems. If ϕ_1 and ϕ_2 are (τ^1, β_1)-KMS and (τ^2, β_2)-KMS states respectively, then we write $\phi = \phi_1 \otimes \phi_2$. The generator for the time evolution τ is $\delta = \delta^1 \otimes \iota + \iota \otimes \delta^2$, where δ^1 and δ^2 are the infinitesimal generators of τ^1 and τ^2 respectively,and $\iota : A \in \mathcal{A}_i \mapsto A \in \mathcal{A}_i$ is the identity map. We now introduce a family $\{P_t\}_{t\in\mathbb{R}}$ of self-adjoint perturbations which temporarily link the systems, and which satisfy the hypotheses of Lemma 5.2.7. It follows that the mechanical work performed on the combined system is the sum of the mechanical work performed on the individual subsystems. To see this, note

$$\begin{aligned} L^P(\phi) &= -i\phi(\Gamma_T^P \delta(\Gamma_T^{P*})) = -i\phi(\Gamma_T^P(\delta^1 \otimes \iota)(\Gamma_T^{P*})) - i\phi(\Gamma_T^P(\iota + \delta^2)(\Gamma_T^{P*})) \\ &= L_1^P(\phi) + L_2^P(\phi), \end{aligned}$$

where $L_1^P(\phi)$ is the work performed on the first system and $L_2^P(\phi)$ is the work performed on the second system. Furthermore, we note that the state $\phi = \phi_1 \otimes \phi_2$ is a $(\tilde{\tau}, 1)$-KMS state on $\mathcal{A}$ where $\tilde{\tau}_t = \tau^1_{\beta_1 t} \otimes \tau^2_{\beta_2 t}$. This time evolution has infinitesimal generator $\tilde{\delta} = \beta_1 \delta_1 \otimes \iota + \beta_2 \iota \otimes \delta_2$, and it follows from Proposition 5.2.4 and Theorem 5.2.5 that the work done on the system is positive, i.e.

$$\tilde{L}^P(\phi) = \beta_1 L_1^P(\phi) + \beta_2 L_2^P(\phi) \geq 0. \tag{5.3}$$

We now suppose that $0 < \beta_1 < \beta_2$, so that the system is not in equilibrium (with respect to the time evolution $\tau = \tau_1 \otimes \tau_2$). Then, using the fact the $\beta_i = \frac{1}{k_B T_i}$, we have

$$\frac{L_1^P(\phi)}{T_1} + \frac{L_2^P(\phi)}{T_2} \geq 0,$$

and therefore

$$L_1^P(\phi) + L_2^P(\phi) + \left(\frac{T_2}{T_1} - 1\right) L_1^P(\phi) \geq 0.$$

Rearranging this and noticing that $L^P(\phi) = L_1^P(\phi) + L_2^P(\phi)$, we get

$$\frac{-L^P(\phi)}{-L_2^P(\phi)} \leq 1 - \frac{T_2}{T_1}. \tag{5.4}$$

The inequality (5.4) is a statement of *Carnot's theorem*, which says that for any heat engine operating between two thermal reservoirs of temperature T_1 and T_2, with $T_1 > T_2$, the maximum efficiency is $1 - \frac{T_2}{T_1}$.

5.3 The Fermi oscillator

In this section we introduce a simple interacting system, the Fermi oscillator. The Fermi oscillator is a quantum harmonic oscillator (described in Section 4.1.1), coupled to an ideal Fermi gas (described in Section 4.1.2). To describe this interacting system, we consider two C^*-dynamical systems with associated KMS states: one describing the harmonic oscillator and the other describing the ideal Fermi gas. We shall label the harmonic oscillator system by the triple $(\mathcal{K}, \psi_{\beta_1}, \rho_t)$, where $\mathcal{K}$ is the algebra of observables for the harmonic oscillator, ρ_t is the time evolution for the harmonic oscillator, and ψ_{β_1} is a (ρ_t, β_1)-KMS state on $\mathcal{K}$. Similarly, we shall label the ideal Fermi gas system by the triple $(\mathcal{A}, \phi_{\beta_2}, \sigma_t)$, where $\mathcal{A}$ is the algebra of observables for the ideal Fermi gas, σ_t is the time evolution for the ideal Fermi gas, and ϕ_{β_2} is a (σ_t, β_2)-KMS state on $\mathcal{A}$. The algebra

of the combined system we wish to study is then $\mathcal{K} \bigotimes \mathcal{A}$, with time evolution $\tau_t = \rho_t \otimes \sigma_t$. Introducing a norm-continuous one parameter family of self-adjoint perturbations of the dynamics allows one to study the interacting system using the results of Section 5.1. In particular, we will give an example of a physically motivated perturbation and outline how one would calculate an expression for the work done by/on the combined system under this perturbation when the individual systems are linked.

In order to use Equation 5.2 to calculate the work done by/on the system, we need to introduce family of self-adjoint perturbations P_t. These perturbations are elements of the algebra of observables, and should therefore consist of elements from $\mathcal{K}$ and $\mathcal{A}$. When the two systems are linked, physically one expects the systems to interact by exchanging momentum, energy or particles. The following perturbation was created in order to capture that idea. Recall that the creation and annihilation operators for both the harmonic oscillator and the ideal Fermi gas generate our observables of interest. For this discussion, we denote by b^* and b the creation and annihilation operators for the harmonic oscillator, and H_0 the Hamiltonian for the harmonic oscillator. Similarly, we denote by $a^*(f)$ and $a(f)$ the creation and annihilation operators for the ideal Fermi gas, and H_F the Hamiltonian. We then have the following perturbation:

$$P_t = \left(e^{-h(\beta,t)H_0} \otimes 1\right) \left(b \otimes a^*(f) + b^* \otimes a(f)\right) \left(e^{-h(\beta,t)H_0} \otimes 1\right),$$

where $h(\beta, t)$ is a smooth function. The mixture of creation and annihilation operators of the harmonic oscillator and ideal Fermi gas simulates a momentum/particle transfer between the two systems. One then calculates $L^P(\psi \otimes \phi)$ using the results of Lemma 5.2.7 and Proposition 5.1.6. This is easier said than done, as the Γ_t^P is a complicated infinite series. One method would be to approximate Γ_t^P by finite sums, and then deduce convergence and other properties later. A second approximation[2] for Γ_t^P would be

$$\Gamma_t^P = 1 + i \int_0^t \tau_s(P_s) ds.$$

One then uses

$$\tau_t^P(A) = \Gamma_t^P \tau_t(A) \Gamma_t^{P*}$$

to calculate

$$L^P(\psi \otimes \phi) = \int (\psi \otimes \phi) \left(\tau_t^P \left(\frac{dP_t}{dt}\right)\right) dt.$$

[2]The first being $\Gamma_t^P = 1$

Unfortunately, results in this direction have been limited due to time constraints.

5.4 Concluding remarks

This study set out to explore the relationship between KMS states on C^*-algebras and equilibrium states in quantum statistical mechanics. This relationship is founded on the algebraic description of quantum mechanics, a generalised mathematical framework for studying quantum systems. Like the standard mathematical framework of quantum mechanics, the validity of the algebraic formulation depends on consistency with known experimental and theoretical results, some of which we have attempted to outline in this thesis.

The implications of the thermal time hypothesis of Connes and Rovelli, discussed in chapter 3, provides some theoretical justification of the algebraic framework. In chapter 4, the characterisation of KMS states as equilibrium states was examined through an analysis of the harmonic oscillator and ideal Fermi gas. For the harmonic oscillator, we obtained expressions for the average energy of the oscillator at inverse temperature β which was consistent, in the classical regime, with the equipartition theorem. For the ideal Fermi gas, the classical limit allowed a derivation of the ideal gas law, and the low temperature limit reproduced the Fermi sea of the degenerate Fermi gas. The theory of passive systems in chapter 5 provided another justification for the algebraic framework of quantum mechanics, and in particular the KMS condition as a condition for equilibrium, with the derivation of Carnot's theorem.

An underlying assumption throughout this thesis has been that all systems studied have been non-relativistic. The axiomatic approach to quantum field theory pioneered by Haag and Kastler extends the algebraic approach to a relativistic setting. The ideal Fermi gas in particular can be made relativistic, although for the situations where the ideal Fermi gas is used to model a physical system, the non-relativistic case is usually sufficient.

The Fermi oscillator example we introduced in chapter 5 is an interesting example of an interacting system. Exploration of the properties of the system could result from a more detailed analysis of the given perturbation expansion, or from analysis of a new, possibly simpler interaction perturbation. It is noted in [8] that the description of arbitrary

continuous quantum systems is incomplete, and that "it is doubtful that any complete understanding of these models will be obtained in the near future".

While interesting, the Fermi oscillator is by no means the only type of interacting system we may study using KMS states. Following [8], we also investigated KMS states in the context of quantum spin systems. In particular, we studied the classical Ising model in dimensions one and two. Although the application of the algebraic formulation of quantum mechanics to quantum spin systems is considered one of the most fruitful applications of the theory, we have omitted it from this thesis in favour of structural coherence.

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