Linear Operators for Quantum Mechanics

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Abstract

This report describes the mathematics of Linear Operators used in Quantum Mechanics. The first two chapters discuss Linear Spaces followed by Linear Functions and different types of Linear Operators. Further, the third and fourth chapters briefly introduce Daigonilising Operators and the need to use Operator Algebras to describe the general function properties of non-commuting operators. Lastly, the fifth and sixth chapters overview States and how the Equation of motion determines the probabilities change in time.

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Chapter 1

Linear Spaces and Linear Functionals

Understanding the concepts of *Linear Space*, we need to build the generalized concept of vectors in three-dimensional position space to vectors in a space of arbitrary dimension.

1.1 Linear Spaces

Definition 1.1.1. *A linear space is a set of elements, called vectors, with an operation of addition, which for each pair of vectors ψ and ϕ specifies a vector $\psi + \phi$, and an operation of scalar multiplication, having following properties-*

1. $\psi + \phi = \phi + \psi$
2. $\psi + (\phi + \chi) = (\psi + \phi) + \chi$
3. $\psi + 0 = \psi$
4. $a(\psi + \phi) = a\psi + a\psi$
5. $(a + b)\psi = a\psi + b\psi$
6. $a(b\psi) = (ab)\psi$
7. $1.\psi = \psi$
8. $0 \cdot \psi = 0.$

The vector space is called complex or real depending on whether complex numbers or real numbers are used as scalars. A set of vectors ψ_1, ψ_2...,ψ_n is **linearly dependent** if there are scalars $a_1, a_2..., a_n$, not all zero, such that a_1 ψ_1+a_2 ψ_2+...a_n ψ_n=0 or it is **linearly independent** if $\sum_{k=1}^{n} a_k$ ψ_k=0 is possible only for $a_1 = a_2 = ..., a_n$=0. A set of vectors ψ_1, ψ_2,...,ψ_k spans a linear space of each vector in the space is a linear combination a_1 ψ_1+a_2 ψ_2+...a_k ψ_k of the vectors ψ_1, ψ_2,..ψ_k with scalars $a_1, a_2..., a_k$.

Theorem 1.1.2. *A Linear space is n-dimensional if and only if it has a basis of n vectors.*

Proof. To show that the space is n-dimensional, we show that no set of *n+1* vectors ψ_1+ψ_2,...,ψ_{n+1} is linear independent. If ψ_1+ψ_2,...,ψ_{n+1} were linearly independent, there would be no scalars $c_1, c_2...c_{n+1}$ other than zeroes which satisfy-

$$\sum_{k=1}^{n}\sum_{j=1}^{n+1} a_{kj}c_j\phi_k = \sum_{j=1}^{n+1} c_j\psi_j = 0$$

If the space is n-dimensional, there are n linearly independent vectors φ_1, φ_2,..., φ_n. For any vector ψ the set of *n+1* vectors φ_1, φ_2,..., φ_n, ψ must be linearly dependent, so there must be scalars $a_1, a_2..., a_n$, not all zero, such that a_1 φ_1+a_2 φ_2+...a_n φ_n=0

Thus the set of vectors φ_1, φ_2,..., φ_n spans the space and is a basis. □

[1, Theorem 1.1.2]

1.1.1 Results

- Euclidean space is n-dimensional. It has a basis of n vectors,

$$\psi_1 = (1, 0, 0, ..0), \psi_2 = (0, 1, 0, ..0), \cdots, \psi_n = (0, 0, ..1).$$

- The space of the oscillating function is two-dimensional. It has a basis of two vectors, $\psi_1(x) = \sin(\omega x)$ and $\psi_2(x) = \cos(\omega x)$.

1.2 Inner Product

Definition 1.2.1. *An inner product or scalar product for a linear space is an assignment to each pair of vectors ψ and φ of a scalar (ψ,φ) called the inner product, with the following properties-*

1. (ψ,φ+χ)=(ψ,φ)+(ψ, χ)
2. (ψ, aφ)=a(ψ, φ)
3. $(\psi, \varphi) = (\varphi, \psi)^*$
4. $(\psi, \psi) \geq 0$ with the equality holding only if ψ=0

The non-negative number $\|\psi\|$=$\sqrt{(\psi, \psi)}$ is called the **norm** or **length** of the vector ψ. Two vectors are **orthogonal** if their inner product is zero.

Theorem 1.2.2. *(Schwarz's Inequality)- An inner product for a linear space has the property that any two vectors φ, ψ*

$$|(\varphi, \psi)| \leq ||\varphi|| \cdot ||\psi||$$

Proof. If let a=-$(\varphi, \psi)(\varphi\varphi)$ in the equality, then

$$0 \leq (\psi + a\varphi, \psi + a\varphi) = (\psi, \psi) + a(\psi, \varphi) + a^*(\varphi, \psi) + |a|^2(\varphi, \varphi) \tag{1.1}$$

and then multiply by (φ, φ), we get the required result. $0 \leq |(\varphi, \psi)| - \|\varphi\| \cdot |\psi\|$ □

[1, Theorem 1.2.1]

1.2.1 Gram Schmidt Orthogonalization Process

This algorithm makes it possible to construct a corresponding orthonormal basis for each list of linearly independent vectors (respectively basis). [1, 1.2.1]

1.2.2 Results

- If $(v_1, ..., v_m)$ is a set of linearly independent vectors in V, then $\exists$ an orthonormal basis $(e_1, ..., e_m)$ such that

  span$(v_1, ..., v_k)$=span $(e_1, ..., e_k)$ $\forall$ k=1,...,m.

- All vectors have positive lengths except the zero vector with zero length.
- When a vector is multiplied by a scalar, the length of the vector is multiplied by the magnitude of the scalar.
- The length of the third side is less than the sum of the lengths of the other two sides.

1.3 Hilbert Space

Definition 1.3.1. *If a linear space with an inner product is complete is complete is called Hilbert space.*

A Hilbert space is separable if it has an orthonormal basis that consists of a countable (finite or infinite) number of vectors, say ψ_1, ψ_2, ψ_3.

An example of an infinite-dimensional Hilbert space is the space l^2 of infinite sequences $(x_1, x_2, ..., x_k, ..)$ such that $\sum_{k=1}^{\infty} |x_k|^2$ is finite.

The space l^2 is a separable Hilbert space. It has an orthonormal basis consisting of the vectors $\varphi_1 = (1, 0, 0...), \varphi_2 = (0, 1, 0, ...)$ and so forth. Each vector $\psi = (x_1, x_2, ..., x_k, ..)$ in l^2 is a linear combination $\psi = \sum_{k=1}^{\infty} x_k \varphi_k$; the sequence of partial sums $\psi_n = \psi = \sum_{k=1}^{\infty} x_k \varphi_k$ converges to $\psi_n = (x_1, x_2, ...x_n, 0, 0, ...)$ So,

$$\|\psi - \psi_n\|^2 = \sum_{k=n+1}^{\infty} |x_k|^2$$

must converge to zero as $n \to \infty$.

1.3.1 Examples

1. L^2 space

$$\langle f, g \rangle = \int_X f g d\mu \tag{1.2}$$

2. Fock space

$$\|f\|_F^2 = \frac{1}{\pi} \int_{\mathbb{C}} |f(z)|^2 \exp\left(-|z|^2\right) dA(z). \tag{1.3}$$

3. Function space of Generalized Gaussian Radial Basis Measure [3, Example- 3]

$$d\mu_{\sigma,\sigma_0,d}(z) \coloneqq e^{-\sigma^2|z|^2} e^{e^{-\sigma_0^2|z|^2}-1} dV_{\mathbf{C}^d}(z). \tag{1.4}$$

Here,'$dV_{\mathbf{C}^d}(z)$' is the usual Lebesgue measure on entire $\mathbf{C}^d$. For $d = 1$, we write simply $d\mu_{\sigma,\sigma_0}(z)$

$$\langle f, g\rangle_{\sigma,\sigma_0,\mathbf{C}^d} \coloneqq \mathcal{N}_{\sigma,\sigma_0,d} \int_{\mathbf{C}^d} f(z)\overline{g(z)} d\mu_{\sigma,\sigma_0,d}(z). \tag{1.5}$$

Here, '$\mathcal{N}_{\sigma,\sigma_0,d}$' is the normalization constant whose value is explicitly given as $\left(\frac{e\sigma^2}{2\pi}\right)^d$.

$$\|f\|^2_{\sigma,\sigma_0,\mathbf{C}^d} \coloneqq \left(\frac{e\sigma^2}{2\pi}\right)^d \int_{\mathbf{C}^d} |f(z)|^2 d\mu_{\sigma,\sigma_0,d}(z). \tag{1.6}$$

1.3.2 Orthogonal Complement

Definition 1.3.2. *Let $\mathcal{M}$ be a subspace of a separable Hilbert space. The set of all vectors that are orthogonal to every vector in $\mathcal{M}$ is called the orthogonal complement $\mathcal{M}^\perp$ of $\mathcal{M}$.*

If ψ and φ are vectors in $\mathcal{M}^\perp$ and a is a scalar, then for any vector x in $\mathcal{M}$
$(\chi, \psi + \varphi) = (\chi, \psi) + (\chi, \varphi) = 0$ and $(\chi, a\psi) = a(\chi, \psi) = 0$
Two subspaces $\mathcal{M}$ and $\mathcal{N}$ are called *orthogonal* if every vector in $\mathcal{M}$ is orthogonal to every vector in $\mathcal{N}$.

1.4 Linear Functionals

Definition 1.4.1. *Linear scalar-valued functions of vectors are called linear functionals. A linear functional F assigns a scalar $F(\varphi)$ to each vector φ such that for any vectors φ and ψ and scalar a*

1. $F(\varphi + \psi) = F(\varphi) + F(\psi)$
2. $F(a\varphi) = aF(\varphi)$

For a space with an inner product, a linear functional F_ψ is defined for each vector ψ by letting $F_\psi(\varphi) = (\psi, \varphi)$ for every vector φ. For any vector ψ and χ and a scalar a

1. $F_\psi + F_\chi = F(\psi + \chi)$
2. $aF_\psi = F_{a^*\psi}$

1.4.1 Dirac's Notation

In Dirac's notation, a vector ψ is written as $|x\rangle$ and inner product (x, y) as $\langle x|y\rangle$. Linear functional F_x is defined by

$$F_x(y) = (x, y)$$

is denoted by $\langle x|$ and $F_x(y)$ by $\langle x|y\rangle$

Chapter 2

Linear Operators

In quantum mechanics, the state vectors span a n-dimensional Hilbert space. and operators representing the dynamical variables when operating on a particular state transform it to a different state.

2.1 Operators

Definition 2.1.1. *A linear operator A on a vector space assigns to each vector ψ a vector $A\psi$ such that*

1. $A(\psi + \varphi) = A\psi + A\varphi$
2. $A(ax) = aAx$

The product AB of two linear operators of A and B is defined as- $(AB)\psi = A(B\psi)$

2.1.1 Bounded Operators

Definition 2.1.2. *A linear operator A is bounded if there is a positive number b such that $\|A\psi\| \leq b\,\|\psi\|$ for every vector ψ; the smallest number b with this property is called the norm of A and is denoted by $\|A\|$.*

Theorem 2.1.3. *A liner operator is continuous if and only if it is bounded.*

Proof. Let A be a bounded linear operator. If a sequence of vectors ψ_n converges to a limit vector ψ, then

$$\|A\psi - A\psi_n\| = \|A(\psi - \psi_n)\| \leq \|A\|\,\|\psi - \psi_n\| \to 0 \tag{2.1}$$

so $A\psi_n \to A\psi$ as $n \to \infty$. Thus A is continuous. Suppose A is not bounded. For each positive integer n must be a vector ψ_n such that $\|A\psi_n\| \geq n\,\|\psi_n\|$
Let

$$\chi_n = (\frac{1}{n}\,\|\psi_n\|\,\psi_n)$$

Then $\|\chi_n\| = \frac{1}{n}$ so, $\chi_n \to 0$ as $n \to \infty$
Thus A is not continuous. This completes the proof of the theorem. □

[1, Theorem 2.1.2]

2.1.2 Properties

Sums, scalars, multiples, and products of bounded operators are bounded.

1. $\|A + B\| \leq \|A\| + \|B\|$
2. $\|aA\| = |a| \, \|A\|$
3. $\|AB\| \leq \|A\| \, \|B\|$

2.2 Inverses

A linear operator A has an inverse if there is a linear operator B such that $BA = 1 = AB$. No operator has more than one inverse; if B and C are inverses of A, then $BA = 1$ and $AB = 1 = AC$ so,

$$B - C = BA(B - C) = B(AB - AC) = 0 \tag{2.2}$$

Thus if A has inverse, we denote it by A^{-1}

Theorem 2.2.1. *A linear operator A has an inverse if and only if for each vector ψ there is one and only one vector φ such that $\psi = A\varphi$*

If linear operators A and B have inverses A^{-1} and B^{-1}, then AB has an inverse $(AB)^{-1} = B^{-1}A^{-1}$ [1, Theorem 2.2.1]

2.3 Unitary Operators

A linear operator U is unitary if it has an inverse and if $\|U\psi\| = \|\psi\|$ for every vector ψ.

- For a finite-dimensional space the condition that $\|U\psi\| = \|\psi\|$ for every vector ψ implies that U has an inverse.
- For an infinite-dimensional space this condition does not imply that U has an inverse.

Theorem 2.3.1. *If U is a unitary operator, then $(U\psi, U\varphi) = (\psi, \varphi)$ for any vectors ψ and φ.*

Proof. Let $\chi = \psi + \varphi$. Then

$$\|\chi\|^2 = \|\psi\|^2 + \|\varphi\|^2 + 2Re(\psi, \varphi)$$
$$\|U\chi\|^2 = \|U\psi\|^2 + \|U\varphi\|^2 + 2Re(U\psi, U\varphi).$$

Hence, we conclude that $Re(U\psi, U\varphi) = Re(\psi, \varphi)$. □

[1, Theorem 2.3.1]

2.3.1 Properties

1. Every unitary operator is bounded if U unitary operator, then $\|U\| = 1$
2. The eigenvalues must have magnitude one that is $\|\lambda^2\| = 1$
3. Rotation operators $\hat{R}(\theta)$, Translation operator $\hat{T}(\vec{a})$ and Time Evolution operator $\hat{U}(t)$ must be unitary operators, these transformations should conserve probability.

2.4 Adjoints and Hermitian Operators

The adjoint $A^\dagger$ of a bounded linear operator A is defined by letting $(\varphi, A^\dagger\psi) = (A\varphi, \psi)$
For each vector ψ a linear functional F is defined by $F(\varphi) = (\psi, A\varphi)$. This linear functional is continuous because A is bounded, if a sequence of vectors χ_n converges to a limit vector χ then,

$$|F(x) - F(x_n)| \leq \|\psi\| \, \|A\| \, \|x - x_n\| \to 0 \tag{2.3}$$

A bounded linear operator A is called *self-adjoint* or *Hermitian* if $A^\dagger = A$.

The equation characterizes a Hermitian operator A as- $(\varphi, A\psi) = (\psi, A\varphi)^*$
In particular, if A is Hermitian, then $(\psi, U\psi)$ is real for any vector ψ. For example, consider again the space $L^2(0,1)$ of square-integrable functions $\psi(x)$ on the interval $0 \leq x \leq 1$. Let A be the linear operator defined on $L^2(0,1)$ by $(A\psi)(x) = x\psi(x)$ for every vector ψ.

For any vector ψ,

$$||A\psi||^2 = \int_0^1 |(A\psi)(x)|^2 \, dx \leq \int_0^1 |\psi(x)|^2 \, dx = ||\psi||^2$$

If A is a bounded Hermitian operator which has a bounded inverse A^{-1}, then isA^{-1} Hermitian. Bounded linear operators on a complex vector space are related to bounded Hermitian operators. For each bounded operator A let

$$Re(A) = \frac{1}{2}(A + A^\dagger)$$

$$Im(A) = \frac{-\iota}{2}(A - A^\dagger)$$

If A is Hermitian, then $\mathrm{Re}(A) = A$ and $\mathrm{Im}(A) = 0$.

- Hermitian operators are the analogs of real numbers.
- Unitary operators are the analogs of complex numbers of absolute value one.

Theorem 2.4.1. *A linear operator U is unitary if and only if $U^\dagger U = 1 = U^\dagger U$*

2.4.1 Properties of Adjoints

1. $(A^\dagger)^\dagger = A$
2. $(A + B)^\dagger = A^\dagger + B^\dagger$
3. $(aA)^\dagger = a^* A^\dagger$
4. $(AB)^\dagger = B^\dagger A^\dagger$

2.4.2 Properties of Hermitian operator

1. Hermitian operators have real eigenvalues.
2. Eigenvectors of Hermitian operators are *orthogonal* if they have different eigenvalues.
3. Set of eigenvectors of Hermitian operator can be used as basis.

2.5 Projection Operator

The *Projection operator* $E_\mathcal{M}$ onto the subspace $\mathcal{M}$ is defined by letting $E_\mathcal{M}\psi = \psi_\mathcal{M}$. $E_\mathcal{M}$ is the bounded linear operator; $||E_\mathcal{M}|| = 1$ if $\mathcal{M}$ contains nonzero vectors.

- The *identity operator* is the projection operator onto the whole space.
- The *zero operator* is the projection operator onto the subspace which contains only the zero vector.

2.5.1 Properties

Let E_1 and E_2 be projection operators onto subspaces $\mathcal{M}_1$ and $\mathcal{M}_2$.

1. If $E_1E_2 = E_2E_1$ then E_1E_2 is a projection operator and the subspace onto which it projects is the intersection of$\mathcal{M}_1$ and$\mathcal{M}_2$.
2. If E_1 and E_2 are orthogonal, then $E_1 + E_2$ is the projection operator onto $\mathcal{M}_1 \oplus \mathcal{M}_2$.
3. If $E_1 \leq E_2$, then E_2–E_1 is a projection operator and the subspace onto which it projects is the orthogonal complement of $\mathcal{M}_1$ in $\mathcal{M}_2$.

Chapter 3

Daigonalizing Operators

Diagonal matrices are relatively easy to compute, and similar matrices share many properties, so diagonalizable matrices are well-suited for computation.

3.1 Eigenvalues and Eigenvectors

Let B be a linear operator. If ψ is a nonzero vector and b is a scalar such that $B\psi = b\psi$, then we say that ψ is an eigenvector of B and b is an eigenvalue of B.

Theorem 3.1.1. *If T is a linear operator which has an inverse T^{-1}, then operators B and TBT^{-1} have the same eigenvalues.*

3.1.1 Spectral Decomposition

Definition 3.1.2. *A family of projection operators E_x depending on a real parameter x is a spectral family if it has the following properties:*

1. *If $x \leq y$, then $E_x \leq E_y$ or $E_x E_y = E_x = E_y E_x$;*
2. *If ϵ is positive, then $E_{x+\epsilon}\psi \to E_x\psi$ as $\epsilon \to 0$ for any vector ψ and any x;*
3. *$E_x\psi \to 0$ as $x \to -\infty$ and $E_x\psi \to \psi$ as $x \to +\infty$*

Definition 3.1.3. *The set of points on x in which e_x increases is known as **spectrum***

Definition 3.1.4. *The set of points x at which E_x jumps is called the **point spectrum**.*

Definition 3.1.5. *The set of points x such that E_x increases continuously in the neighborhood of $x$nis called **continuous spectrum**.*

Theorem 3.1.6. *For each unitary operator U there is a unique spectral family of projection operators E_x such that $E_x = 0$ for $x \leq 0$ and $E_x = 1$ for $x \geq 2\pi$ and*

$$(\varphi, U\psi) = \int_0^{2\pi} e^{\imath x} d(\varphi, E_x\psi) \tag{3.1}$$

[1, Theorem 3.1.6]

Theorem 3.1.7. *A self-adjoint operator is bounded if and only if its spectrum is bounded.*

Proof. Let A be a self-adjoint operator with the spectral decomposition,

$$A = \int_{-\infty}^{\infty} x dE_x \tag{3.2}$$

for any vectors ψ and φ, letting $\varphi = \psi$, we get

$$(\varphi, E_x\psi) = (\psi, E_x^2\psi) = \|E_x\psi\|^2$$

and

$$\|\varphi\|, A^2\psi = \int_{-\infty}^{\infty} x^2 d\|E_x\psi\|^2$$

Suppose there is a positive number b such that the spectrum of A is in the interval $-b \leq x \leq b$. Then, $\|E_x\psi\|^2 = 0$ for $x < -b$ and $\|E_x\psi\|^2 = |\psi\|^2$ for $x \geq b$

$$\|A\psi\|^2 \leq b^2 \int_{-\infty}^{\infty} d\|E_x\psi\|^2 = b^2 \left\|\psi^2\right\|$$

Thus A is bounded. Suppose the spectrum is not bounded; suppose it has no upper bound. Then for each positive integer n, there is an integer $m > n$ such that the projection operator E_m–E_n is not zero.

Let ψ be a nonzero vector such that $(E_m–E_n)\psi = \psi$.

$$(E_xE_m - E_xE_n)\psi = (E_x - E_n)\psi = 0$$

$$\|A\psi\|^2 \geq n^2 \int_{-\infty}^{\infty} d\|E_x\psi\|^2 = n^2\|\psi\|$$

Thus, A is not bounded. □

[1, Theorem 3.1.7]

3.2 Functions of Commuting Operators

In Quantum Mechanics one often works with functions of two or more real variables and the corresponding functions of two or more Hermitian operators who commute with each other. Let A be a *Hermitian operator* with a pure point spectrum so that

$$A = \sum_k a_k I_k \tag{3.3}$$

where a_k is a different eigenvalue of A and I_k is the projection operator onto the eigenvector subspace for a_k. Let B be a bounded Hermitian operator which commutes with A. For each k and any vector x,

$$ABI_k x = BAI_k x = a_k BI_k x$$

so, $BI_k x$ is in the eigenvector subspace for a_k, for any vector x

$$BI_k x = I_k BI_k x$$

Taking adjoints on both sides,

$$I_k B = BI_k$$

Thus each I_k commutes with every bounded Hermitian operator which commutes with A.

Theorem 3.2.1. *Let A be a self-adjoint operator with the spectral decomposition*

$$A = \int_{-\infty}^{\infty} x dE_x \tag{3.4}$$

If B is a bounded self-adjoint operator such that $AB = BA$ then $E_x B = BE_x$ for every x. [1, theorem 3.2.1]

3.3 Complete Sets of Commuting Operators

Let $A1, A2, ..., A_N$ mutually commute Hermitian operators with pure point spectra. Then for each $r = 1, 2, ..., N$

$$A_r = \sum_k a_k^{(r)} I_k^{(r)}$$

where each $a_k^{(r)}$ is a different eigenvalue of A_r and $I_k^{(r)}$ is the projection operator. The projection operators $I_k^{(r)}$ commute with each other $\forall$ different r and k,

$$I_j^{(r)} I_k^{(s)} = I_k^{(s)} I_j^{(r)}$$

It projects onto the subspace of all vectors x such that $A_1 x = a_j^{(1)} x$ and $A_N x = a_l^{(N)} x$. These *projection operators* are mutually orthogonal and they have the completeness property that,

$$\sum_j \sum_k ... \sum_l I_j^{(1)} I_k^{(2)} ... I_l^{(N)} = 1$$

Suppose none of them projects onto a subspace of dimension larger than one. Then we say that the set of operators $A_1, A_2, ...A_N$ is a *Complete set of commuting operators.*

Definition 3.3.1. *When all operators are represented by diagonal matrices then it is called Spectral Representation.*

3.4 Operator Algebras

We use operator algebras to describe general properties of functions of non-commuting operators, for example, to say which operators are functions of a given set of non-commuting operators.

Definition 3.4.1. *(Schur's Lemma) An asymmetric set of bounded or Hermitian operators are irreducible if and only if multiples of the identity operator are the only bounded operators that commute with all operators in the set.*

[1, Definition 3.4.1]

3.4.1 Von Neumann Algebras, Functions of non-commuting opeators

Definition 3.4.2. *A set of bounded operators is a symmetric ring or symmetric algebra or *algebra if for any operators A and B in the set and any complex number c the operators $cA, A+B, AB$, and $A^\dagger$ also are in the set.*

[1, Definition 3.4.2]

Chapter 4

States

4.1 Measurable Quantities

In classical mechanics, the measurable quantities characteristic of a physical system are real or complex variables. Hermitian operators are analogs of real variables and Non-Hermitian operators are analogs of complex variables. A bounded non-Hermitian operator B can be written

$$B = ReB + ImB$$

4.1.1 Density matrix and traces

Definition 4.1.1. *A density matrix is a positive self-adjoint operator W such that if the set of vectors x is an orthonormal basis, then*

$$\sum_k (x_k, wx_k) = 1 \tag{4.1}$$

Theorem 4.1.2. *Let W be a density matrix and B a bounded operator. If the set of vectors x_k is an orthonormal basis and the set of vectors y_j is any other orthonormal basis, then*

$$\sum_k (x_k, WBx_k), \sum_k (y_j, WBy_j), \sum_k (x_k, BWx_k) and \sum_k (y_j, BWy_J)$$

are finite.

[1, Theorem 4.1.2] From the above theorem, we have

$$\mathrm{Tr}(BW) = \sum_j (x_j, BWx_j)$$

and call these the **trace** of BW. Furthermore, Tr(WB) = Tr(BW)

- Tr(WcB) = c Tr(BW)
- TrW(A + B) = Tr(WA) + Tr(WB)

4.2 Reprsentation of States

A state describes values of measurable quantities. In Quantum Mechanics, this description consists of probabilities. We assume that a state specifies a finite expectation value B for each bounded operator B. We assume that expectation values have the following properties-

1. If B is self-adjoint, then is real.
2. If B is self-adjoint and positive, then is non-negative.

4.3 Probabilities

Consider a state represented by a vector ψ, with $\|\psi\| = 1$, and consider a real measurable quantity represented by a self-adjoint operator A with spectral decomposition

$$A = \int_{-\infty}^{\infty} x dE_x \tag{4.2}$$

We assume that a function f of this quantity is represented by the operator $f(A)$. If $f(A)$ is bounded, it has a finite expectation value

$$\langle f(A)\rangle \ = (\psi, f(A)\psi) = \int_{-\infty}^{\infty} f(x) d(\psi, E_x\psi) = \int_{-\infty}^{\infty} f(x) d\,\|\psi\|^2$$

Indeed $\|E_x\psi\|^2$ is a monotonically increasing function of x, which converges to zero as $x \to \infty$ and to one as $x \to -\infty$, and $f(A)$ is the mean of $f(x)$ with respect to this probability distribution. If A is bounded, then A_n is bounded, and we have finite expectation values

$$\langle A^n\rangle \ = \int_{-\infty}^{\infty} x^n d\,\|E_x\psi\|^2$$

for $n = 0, 1, 2, ...$ These are the moments of the probability distribution. We can always use the unitary operators e^{itA}. As a function of all real t, their expectation values

$$\langle e^{itA}\rangle \ = \int_{-\infty}^{\infty} e^{itx} d\,\|E_x\psi\|^2$$

are the characteristic functions of the probability distribution.

4.4 Probabilities for Complete Sets of Commuting Operators

Consider a set of quantities represented by a complete set of commuting Hermitian operators $A_1, A_2, ..., A_N$ with pure point spectra. Suppose that for a particular state, the probability is one that the set of values of these quantities is a particular set of eigenvalues Then the state is represented by an eigenvector of $A_1 A_2, ..., A_N$ for these eigenvalues.

$$\langle |a_j^1, a_k^2, ...a_i^N, \rangle \ \langle a_i^1, a_k^2, ...a_i^N\rangle| \ = \langle a_j^1, ...a_j^N \psi\rangle\|,$$

The space L^2 of functions $\psi(x) = \psi(x_1, x_2, x_3)$ can be used to describe a particle. The position is represented by the complete set of commuting operators $Q = (Q_1, Q_2, Q_3)$ defined by $(Q\psi)(x) = x\psi(x)$. For a state represented by a vector ψ of length one the probability that the components of the position are $\leq x, y, z$ is

$$\langle E_x^1 E_y^2 E_z^3 \rangle = \int \psi(u,v,w)^* (E_x^1 E_y^2 E_z^3 \psi)(u,v,w)\,\mathrm{du}\,\mathrm{dv}\,\mathrm{dw}$$

$$= \int_{-\infty}^{x} \mathrm{du} \int_{-\infty}^{y} \mathrm{dv} \int_{-\infty}^{z} \mathrm{dw}\,|\psi(u,v,w)|^2$$

Therefore the probability that the position is in an infinitesimal volume $\mathrm{du}\,\mathrm{dv}\,\mathrm{dw}$ at the point (x, y, z) is

$$|\psi(x,y,z)|^2\,\mathrm{dx}\,\mathrm{dy}\,\mathrm{dz}$$

The momentum divided by $\hbar$ is represented by the complete set of commuting operators $P = (P1, P2, P3)$ defined by

$$(P\psi)(x) = -i \bigtriangledown_{\psi}(x)$$

4.5 Uncertainty Principle

Consider a quantity represented by *Hermitian operator* A, for each state its *uncertainty* ΔA is defined by-

$$(\Delta A)^2 = \langle A^2 \rangle - \langle A^2 \rangle$$

Theorem 4.5.1. *Let A and B be Hermitian operators. For any state-*

$$(\Delta A)(\Delta B) \geq \frac{1}{2}|\langle AB - BA \rangle| \tag{4.3}$$

[1, Theorem 4.5.1]

4.5.1 Simultaneous Measurability

We interpret this as implying that position and momentum are not simultaneously measurable with unlimited precision. Commuting Hermitian Operator represents real quantities that are simultaneously measurable with unlimited precision. Let A_1 and A_2 be Hermitian operators with spectral decompositions

$$A_r = \int_{-\infty}^{\infty} x dE_x^{(r)} \tag{4.4}$$

for $r = 1, 2$.

4.5.2 Super-selection Rules

Every bounded Hermitian operator represents a measurable quantity. Consider the operator $e^{i2\pi J_3}$, which represents a rotation through an angle 2π about the z axis Let B be a bounded operator which represents a measurable quantity

$$e^{i2\pi J_3} B e^{-i2\pi J_3} = B \tag{4.5}$$

Definition 4.5.2. *A restriction of the operators that represent measurable quantities is called a super-selection rule.*

Definition 4.5.3. *If a bounded operator, such as $e^{-i2\pi J_3}$, commutes with every Hermitian operator which represents a measurable quantity, but is not a multiple of the identity operator, then we call it a super-selection operator.*

[2, Definitions]

Chapter 5

Equations of Motions

States describe values or probabilities for measurable quantities at given times. Equations of motion determine how these values or probabilities change in time. There are at least two ways to make expectation values depend on time.

- To work with states represented by vectors $x(t)$ which depend on the time t;
- Let each measurable quantity be represented by an operator A which is independent of time.

Then an expectation value has a time dependence,

$$\langle A \rangle \ (t) = (x(t)), Ax(t) \tag{5.1}$$

This is called the *Schrödinger picture*(5.1)

$$\langle A(t) \rangle \ = (x, A(t)x) \tag{5.2}$$

This is called *Heisenberg Picture*(5.2) [1]

5.1 Antiunitary Operators

For each vector x let Tx be a vector specified by T such that-

1. $T(x+y) = T(x) + T(y)$
2. $Tcx = c^* Tx$

Then T is an *antilinear operator*. Antilinear operator T has an inverse T^{-1} if T^{-1} is an antiliner operator such that

$$T^{-1}T = 1 = TT^{-1} \tag{5.3}$$

Antilinear operator T is **antiunitary** if it has an inverse T^{-1} and $\|Tx\| = \|x\| \, \forall x$

If T is an antiunitary antilinear operator then:

$$(Tx, Ty) = (x, y)^* \forall x, y \tag{5.4}$$

Due to Wigner's theorem, these transformations can either be unitary or antiunitary.

Theorem 5.1.1. *Wigner's Theorem- Any symmetry transformation can be represented on Hilbert space of physical states by an operator that is either linear and unitary or antilinear and antiunitary.*

[4, Theorem 5.1.1]

5.2 Schrödinger picture

Suppose the state at time $t = 0$ is represented by a vector $x(0)$ and the state at another time t is represented by a vector $x(t)$. We assume that every vector $x(0)$ such that $\|x(0)\| = 1$ represents a possible state at time zero and similarly for $x(t)$ such that $\|x(t)\| = 1$ Let there be two possible states at time zero such that $x(0)$, $y(0)$ and time t such that $x(t)$, $y(t)$. Then $|x(0), y(0)|^2$ is the probability of finding the state represented by $x(0)$ and $|x(t), y(t)|^2$is the probability of finding the state represented by $y(t)$. These probabilities should be the same-

$$|(x(0), y(0))|^2 = |(x(t), y(t))|^2$$

From Wigner's theorem, it follows that there is an operator $T(t)$ which is either linear and unitary or antilinear and anti-unitary. $U(t)$ is another unitary or antiunitary operator such that if $x(0)$ represents the state at time zero, then $U(t)x(0)$ represents the state at time t, then

$$|U(t)x(0)\rangle \langle U(t)x(0)| = |T(t)x(0)\rangle \langle T(t)x(0)|$$

Theorem 5.2.1. *Stone's Theorem states that there is a unique self-adjoint operator H such that*

$$U(t) = e^{-itH} \tag{5.5}$$

[1, Theorem 5.2.1]
If $\psi(0)$ represents the state at time zero, then

$$\psi(t) = U(t)\psi(0) = e^{-itH}\psi(0)$$

represents the state at time t. If $\psi(t)$ is in the domain of H, then

$$i\frac{d}{dt}\psi(t) = H\psi(t) \tag{5.6}$$

This is the *Schrödinger equation* and H is the *Hamiltonian.*

5.3 Heisenberg Picture

Directly we cannot deduce *Hamiltonian* from the Schrödinger equation, so we transfer to the Heisenberg picture. In the Schrödinger picture, the expectation value of a quantity is represented by

$$\langle A\rangle\ (t) = (e^{-itH}\psi, Ae^{-itH}\psi) = (\psi, e^{itH}Ae^{-itH}\psi) \tag{5.7}$$

We assume that it has the same time dependence in the Heisenberg picture. Therefore the quantity represented by the operator $A = A(0)$ at time zero must be represented by the operator

$$A(t) = e^{itH} A e^{-itH} = e^{itH} A(0) e^{-itH} \tag{5.8}$$

Because this is a unitary transformation, it preserves the general properties of operators.

1. If $A(0)$ is bounded, then $A(t)$ is bounded;
2. $A(0)$ is Hermitian. Then $A(t)$ is Hermitian;
3. If $A(0)$ is positive, then $A(t)$ is positive.
4. $A(0)$ and $A(t)$ have the same spectrum

If the projection operators in the spectral decomposition of $A(0)$ are $E_x(0)$, similarly for $A(t)$

$$E_x(t) = e^{itH} E_x(0) e^{-itH}$$

Algebraic relations between noncommuting operators are also preserved in time. If $A(0)$, $B(0)$, and $C(0)$ are operators such that

$$A(0) = B(0) + C(0)$$

then,

$$A(t) = B(t) + C(t)$$

similarly, we have

$$A(0) = B(0)C(0)$$

then,

$$A(t) = B(t)C(t)$$

The quantity represented by the Hamiltonian operator H is a constant of the motion, because

$$e^{itH} H e^{-itH} = H$$

in classical mechanics suggests that $\hbar H$ represents the energy. Here $\hbar = 1$ and $H = energy$ For example, consider a single particle. Let the position and momentum at time zero be represented by the operators Q and P defined by

$$(Q\psi)(x) = x\psi(x)$$

and

$$(P\psi)(x) = -i \bigtriangledown \psi(x)$$

on the space L^2 of functions $\psi(x)$. Then the position and momentum at the time t are represented by

$$Q(t) = e^{itH} Q e^{-itH}$$

and

$$P(t) = e^{itH} P e^{-itH}$$

The nonrelativistic energy for a particle of mass m in a static potential $V(x)$ is represented by the operator

$$H = \frac{1}{2m} p^2 + V(Q) \tag{5.9}$$

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