Lecture 3

2. Quantum Spin Systems

2.3 States

A <u>state</u> of a quantum system with algebra of observables $\mathcal{A}$ is a <u>normalized</u>, <u>positive</u> linear functional on $\mathcal{A}$.

For example, when $\mathcal{A} = B(\mathcal{H})$ for some Hilbert space of states $\mathcal{H}$, this means that:

i) $\omega : \mathcal{A} \to \mathbb{C}$ is <u>linear</u>

i.e. $\omega(\lambda A + \mu B) = \lambda \omega(A) + \mu \omega(B)$

for all $A, B \in \mathcal{A}$ and $\lambda, \mu \in \mathbb{C}$.

ii) ω is <u>positive</u>, i.e.

$\omega(A^* A) \geq 0$ for all $A \in \mathcal{A}$.

<u>and</u>

iii) ω is <u>normalized</u>, i.e.

$\omega(\mathbb{1}) = 1$.

$\boxed{\text{Note: positive here = non-negative}}$:(

As we discussed last class

- $\omega(A)$ – the <u>expected value</u> of A in the state ω
- $\mathrm{var}(A) = \omega\big((A - \omega(A)\mathbb{1})^*(A - \omega(A)\mathbb{1})\big) = \omega(A^*A) - |\omega(A)|^2$

  is the <u>variance</u> of A

In general, there are many states on $\mathcal{A}$.

For any unit vector $\psi \in \mathcal{H}$ (i.e. $\|\psi\| = 1$),

$\omega_\psi : \mathcal{A} \to \mathbb{C}$ given by

$$\omega_\psi(A) = \langle \psi, A\psi \rangle \quad \text{for all } A \in \mathcal{B}(\mathcal{H})$$

is a state. Such states are called <u>vector states</u>.

In fact, defining $P_\psi : \mathcal{H} \to \mathcal{H}$ by setting

$$P_\psi(\phi) = \langle \psi, \phi \rangle \psi$$

one sees that $P_\psi^2 = P_\psi = P_\psi^*$, i.e. P_ψ is an orthogonal projection,

P_ψ is the orthogonal projection onto the one-dimensional subspace of $\mathcal{H}$ spanned by ψ, and moreover,

$$\omega_\psi(A) = \mathrm{Tr}[P_\psi A] \quad \text{for all } A \in \mathcal{B}(\mathcal{H})$$

Convexity

It is clear that the set of states on an observable algebra $\mathfrak{A}$ is convex.

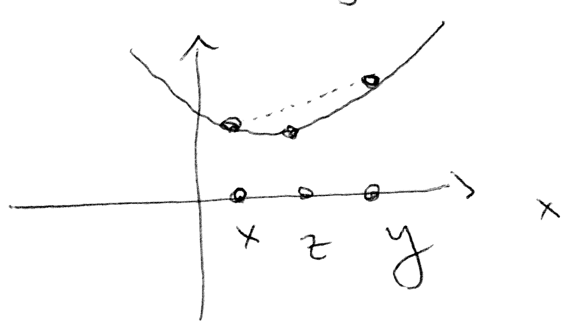
Recall: let X be a real or complex vector space. A set $C \subset X$ is said to be convex if:

For all $x, y \in C$ and $\theta \in [0,1]$, $\theta x + (1-\theta) y \in C$.

In words, the line segment connecting any two elements of C is contained in C.

- Of course, this is different from the notion of convexity for functions...
  Let $I \subset \mathbb{R}$ be an interval. $f : I \to \mathbb{R}$ is said to be convex if for all $x, y \in I$

$$f(\theta x + (1-\theta) y) \leq \theta f(x) + (1-\theta) f(y)$$



For any $x \leq z \leq y$, $\exists\ \theta_z$ with $0 \leq \theta_z \leq 1$ and

$$z = \theta_z x + (1-\theta_z) y$$

i.e. z is a convex combination of x and y

$$f(\theta_z x + (1-\theta_z) y) = f(z) \leq \theta_z f(x) + (1-\theta_z) f(y)$$

line between $f(x)$ and $f(y)$

Here the set of states is a subset of the dual of $\mathfrak{A}$, denoted by $\mathfrak{A}^*$, which is the vector space of all bounded linear functionals over $\mathfrak{A}$.

<u>Moreover</u> If ω_1 and ω_2 are states on $\mathfrak{A}$ and $0 \le \theta \le 1$, then $\omega_\theta : \mathfrak{A} \to \mathbb{C}$ defined by

$$\omega_\theta(A) = \theta\omega_1(A) + (1-\theta)\omega_2(A)$$

<u>Satisfies:</u> i) ω_θ is linear
ii) ω_θ is positive
iii) ω_θ is normalized

~~and~~ Hence ω_θ is a state, and so the set of states is convex.

- The <u>extreme points</u> of the convex set of states on $\mathfrak{A}$ are called <u>pure states</u>.
- If ω is a state on $\mathfrak{A}$ and ω is not pure, then ω is called a <u>mixed state</u>.

<u>Recall:</u>
<u>Def.</u> An extreme point of a convex set C is a point $x \in C$ for which: if $x = \theta y + (1-\theta) z$ for some $y, z \in C$ and $0 \le \theta \le 1$, <u>then</u> $y = x$ and/or $z = x$ (i.e. $\theta \in \{0, 1\}$).

In words, the extreme points of a convex set are points for which there is no non-trivial convex decomposition. Said differently, extreme points are not interior points of any line segment lying entirely in C.

We now look closer at states on M_d.

First, some more linear algebra.

- The matrix $A \in M_d$ is said to be <u>non-negative</u> (a.k.a. positive) if

$$\langle v, Av \rangle \geq 0 \quad \text{for all } v \in \mathbb{C}^d.$$

- The matrix $A \in M_d$ is said to be <u>strictly positive</u> if

$$\langle v, Av \rangle > 0 \quad \text{for all } v \in \mathbb{C}^d / \{0\}.$$

For homework we will prove the following

- $A \in M_d$ is non-negative $\iff$ $\exists B \in M_d$ and $A = B^* B$.

- $A \in M_d$ is strictly positive $\iff$ $A \in M_d$ is non-negative and A is invertible

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Some comments on this

1) From these facts, one concludes that

$A \in M_d$ is non-negative $\Rightarrow$ A is self-adjoint and the eigenvalues of A are non-negative.

2) We now better understand our definition of state.

Recall: A map $\omega: \mathcal{A} \to \mathbb{C}$ is said to be positive if

$$\omega(A^* A) \geq 0 \quad \text{for all } A \in \mathcal{A}.$$

When $\mathcal{A} = M_d$, $A^* A$ is non-negative for every $A \in \mathcal{A}$. Thus a map is "positive" if it takes non-negative operators to non-negative values.

Let us now return to the study of states on M_d.

In homework we will show that

- A state ω on M_d is a pure state if and only if ω is a vector state.

- For any state ω on M_d, $\exists \rho \in M_d$ for which ρ is non-negative, $Tr[\rho]=1$, and

$$\omega(A) = Tr[\rho A] \quad \text{for all } A \in M_d.$$

A number of comments are in order.

1) In general, any non-negative matrix ρ with $Tr[\rho]=1$ is called a <u>density matrix</u>. In words, these are the quantum mechanical analogues of probability densities. (More on this below.)

2) It is also clear that given a density matrix $\rho \in M_d$, $\omega_\rho : M_d \to \mathbb{C}$ defined by setting

$$\omega_\rho(A) = Tr[\rho A] \quad \text{for all } A \in M_d$$

is a state on M_d.

In this case, there is a 1-to-1 correspondence between states and density matrices on M_d.

$$\omega(A) = \mathrm{Tr}[\rho A] \qquad \text{for all } A \in M_d$$

1 to 1 correspondence.

3) Given a density matrix $\rho \in M_d$, the spectral theorem applies. In this case, there is an orthonormal basis of eigenvectors of ρ, which we label $\{v_1, v_2, \dots, v_d\} \subset \mathbb{C}^d$, and ρ may be written as:

$$(*) \quad \rho = \sum_{i=1}^{d} \lambda_i P_{v_i}$$

where:
- $\lambda_i \geq 0$ is an eigenvalue of ρ corresponding to the eigenvector v_i
- P_{v_i} is the orthogonal projection onto the one dimensional subspace of $\mathbb{C}^d$ spanned by v_i
- $1 = \mathrm{Tr}[\rho] = \sum_{i=1}^{d} \lambda_i$.

Using this representation of ρ (see (*) above), this homework problem shows that

$$\omega(A) = Tr[\rho A] = \sum_{i=1}^{d} \lambda_i Tr[P_{v_i} A]$$
$$= \sum_{i=1}^{d} \lambda_i \omega_{v_i}(A) \quad \text{for all } A \in M_d.$$

In words, any state ω on M_d is a finite convex combination of vector states.

<u>Note</u>: For a density matrix $\rho \in M_d$, writing

$$\rho = \sum_{i=1}^{d} \lambda_i P_{v_i}$$

where $\{v_1, v_2, \ldots, v_d\}$ form an orthonormal basis of $\mathbb{C}^d$, this is often called the <u>Schmidt decomposition</u> of ρ.

- If ρ corresponds to a pure state, then $\lambda_i = 1$ for some $1 \leq i \leq d$ and $\rho = P_{v_i}$ corresponds to a vector state. (This is part of the homework...)
- If ρ does not correspond to a pure state, then the corresponding state is mixed. The interpretation is: the system is in state ω_{v_i} with probability λ_i. Thus $\rho \longleftrightarrow$ probability density.

Let us finally consider the special case of $d=2$.

In the homework, we will show that:

1) $\rho \in M_2$ is a density matrix if and only if

$$\rho = \begin{pmatrix} r & \mu \\ \bar{\mu} & 1-r \end{pmatrix}$$ for some $r \in [0,1]$ and $\mu \in \mathbb{C}$ satisfying $|\mu|^2 \leq r(1-r)$.

2) $\rho \in M_2$ is a density matrix if and only if

$$\rho = \frac{1}{2}\mathbb{1} + \vec{x}\cdot\vec{\sigma} \quad \text{where } \vec{x}\cdot\vec{\sigma} = \sum_{i=1}^{3} x_i \sigma^i$$

with $\vec{x} = (x_1, x_2, x_3) \in \mathbb{R}^3$ satisfying $\sqrt{\sum_{i=1}^{3} x_i^2} = \|\vec{x}\| \leq 1$

and $\{\sigma^1, \sigma^2, \sigma^3\}$ are the Pauli matrices.

One can further check that the pure states in M_2 are in 1 to 1 correspondence with the unit vectors $\vec{x} \in \mathbb{R}^3$. The set of unit vectors in $\mathbb{R}^3$ is sometimes referred to as the Bloch sphere.

The key to 2) is to recall that we have proven that $\{\sigma^0, \sigma^1, \sigma^2, \sigma^3\}$ form an orthonormal basis of M_2!