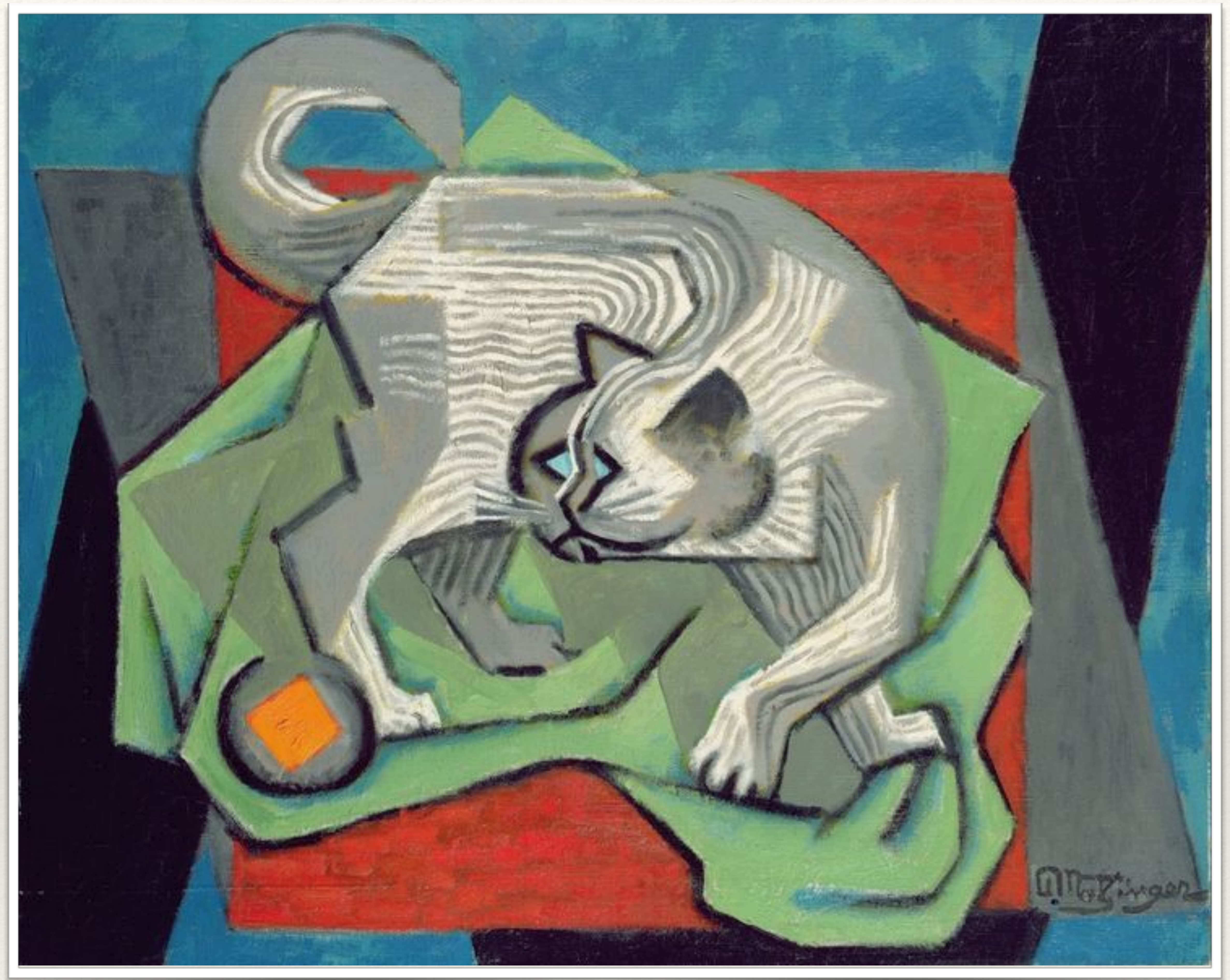
Prof. Steven Flammia

Quantum Mechanics

Lecture 1

Course administration;
Review of Dirac notation and state space;
Operators in quantum mechanics;
Observables, expected values, unitary dynamics.



Administration

- PHYS 3x34, advanced stream 3rd year Quantum Physics.
- Teaching assistant: Alistair Milne, amil1264@uni.sydney.edu.au
- Course website: www.physics.usyd.edu.au/~sflammia/Courses/QM2019/
- 4 Quizzes to be held during Lectures 5, 8, 11, 14.
- 2 Assignments, 1 Exam.
- Marks apportioned: 0.2 Q + 0.2 A + 0.6 E.

Why quantum physics?

- One of the most stunning intellectual achievements in human history.
- It raises deep philosophical and conceptual questions:
  - Determinism, causality, information, locality, *even reality itself*.
- Huge range of scientific and practical applicability:
  - Neutron stars, elementary particles, fission and fusion, magnetism, lasers, transistors, superconductors, chemistry, fiber optics, quantum computers...
- Despite a fearsome reputation, the principles of quantum physics are *simple*.

1927 Solvay conference

29 attendees, 17 Nobel laureates, 18 Nobel prizes.

Dirac notation

Recall that quantum mechanical systems are described by **states**.

Kets = column vectors

$$|\psi\rangle, |\phi\rangle, |\uparrow\rangle, |+\rangle, \text{ etc.}$$

Bras = row vectors

$$\langle\psi|, \langle\phi|, \langle\uparrow|, \langle+|, \text{ etc.}$$

Inner product

$$\langle\psi|\phi\rangle, \langle\uparrow|+\rangle, \text{ etc.}$$

Can express any vector in an **orthonormal basis.**

$$|\psi\rangle = \sum_j c_j |e_j\rangle \qquad \langle e_j | e_k \rangle = \delta_{jk}$$

(c_j complex)

$$\langle\psi| = \sum_j c_j^* \langle e_j|$$

States must be **normalized.**

$$\sum_j |c_j|^2 = \langle\psi|\psi\rangle = 1$$

Dirac notation

Example: spin-1/2 system

Basis:

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

Orthonormal:

$$\langle\uparrow|\uparrow\rangle = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 1 \qquad \langle\uparrow|\downarrow\rangle = \begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = 0$$

$$\langle\downarrow|\uparrow\rangle = \begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0 \qquad \langle\downarrow|\downarrow\rangle = \begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = 1$$

Other states can be expanded in the basis:

$$|+\rangle = \frac{1}{\sqrt{2}}(|\uparrow\rangle + |\downarrow\rangle) = \frac{1}{\sqrt{2}}\begin{pmatrix}1\\1\end{pmatrix}$$

$$\langle\uparrow|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 0\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}$$

$$\langle\downarrow|+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix}0 & 1\end{pmatrix}\begin{pmatrix}1\\1\end{pmatrix} = \frac{1}{\sqrt{2}}$$

We conclude:

$$|+\rangle = \langle\uparrow|+\rangle|\uparrow\rangle + \langle\downarrow|+\rangle|\downarrow\rangle$$

Finite-dimensional quantum systems

More generally, consider a system with a finite number of orthogonal states.

$$|\psi\rangle = \sum_n c_n |a_n\rangle \qquad \langle\psi| = \sum_n c_n^* \langle a_n| \qquad \langle a_n | a_m\rangle = \delta_{nm}$$ orthonormal basis

normalization:

$$\langle\psi|\psi\rangle = \sum_m c_m^* \langle a_m| \sum_n c_n |a_n\rangle = \sum_{n,m} c_m^* c_n \langle a_m | a_n\rangle = \sum_{n,m} c_m^* c_n \delta_{m,n} = \sum_n |c_n|^2 = 1$$

expansion coefficients:

$$\langle a_m|\psi\rangle = \langle a_m| \sum_n c_n |a_n\rangle = \sum_n c_n \langle a_m | a_n\rangle = \sum_n c_n \delta_{m,n} = c_n$$

$$\Rightarrow \quad |\psi\rangle = \sum_n \langle a_n|\psi\rangle |a_n\rangle$$

Finite-dimensional quantum systems

More generally, consider a system with a finite number of orthogonal states.

$$|\psi\rangle = \sum_n \langle a_n|\psi\rangle\,|a_n\rangle = \sum_n |a_n\rangle\langle a_n|\psi\rangle = \left(\sum_n |a_n\rangle\langle a_n|\right)|\psi\rangle$$

This holds for all $|\psi\rangle$, so therefore we must have:

$$\sum_n |a_n\rangle\langle a_n| = 1$$

We say that the basis forms a **resolution of the identity**. The equation itself is called a **completeness relation**.

Any expression of the form $|\psi\rangle\langle\phi|$ is called an **outer product**. Outer products (and sums of them) are linear operators: they act linearly and map vectors to vectors.

Operators

Any complete orthonormal basis forms a **resolution of the identity**.

Example: spin-1/2

$$|\uparrow\rangle\langle\uparrow| + |\downarrow\rangle\langle\downarrow| = \begin{vmatrix}1\\0\end{vmatrix}\begin{pmatrix}1 & 0\end{pmatrix} + \begin{vmatrix}0\\1\end{vmatrix}\begin{pmatrix}0 & 1\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 0\end{pmatrix} + \begin{pmatrix}0 & 0\\0 & 1\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} = 1$$

$$|+\rangle\langle+| + |-\rangle\langle-| = \frac{1}{2}\begin{vmatrix}1\\1\end{vmatrix}\begin{pmatrix}1 & 1\end{pmatrix} + \frac{1}{2}\begin{vmatrix}1\\1\end{vmatrix}\begin{pmatrix}1 & 1\end{pmatrix} = \frac{1}{2}\begin{pmatrix}1 & 1\\1 & 1\end{pmatrix} + \frac{1}{2}\begin{pmatrix}1 & -1\\-1 & 1\end{pmatrix} = \begin{pmatrix}1 & 0\\0 & 1\end{pmatrix} = 1$$

Different basis choices allow us to expand states in different bases:

$$|\psi\rangle = \langle+|\psi\rangle|+\rangle + \langle-|\psi\rangle|-\rangle \quad \text{(x-basis)}$$

$$|\psi\rangle = \langle\uparrow|\psi\rangle|\uparrow\rangle + \langle\downarrow|\psi\rangle|\downarrow\rangle \quad \text{(z-basis)}$$

It also follows that: $\langle a|b\rangle^* = \langle b|a\rangle$

Operators

In general, any linear operator of commensurate dimension can act on a state. Operators can be thought of as acting from the **left** or from the **right**.

$$A\,|\psi\rangle = |\phi\rangle \;\; \text{(from the left)} \quad \Leftrightarrow \quad \langle\psi|A^\dagger = \langle\phi| \;\; \text{(from the right)}$$

The Hermitian conjugate (complex conjugate + transpose) relates the two actions. Operator ordering follows the conventions of matrix multiplication.

$$(AB)^\dagger = B^\dagger A^\dagger \qquad BA\,|\psi\rangle = B\left(A\,|\psi\rangle\right) \qquad \langle\psi|A^\dagger B^\dagger = \left(\langle\psi|A^\dagger\right)B^\dagger$$

Operators do not commute!

$$\mathrm{AB} \neq \mathrm{BA} \;\; \text{(in general)}$$

Eigenstates and eigenvalues

Eigenvalues and eigenstates (or eigenvectors, same thing) are solutions to:

$$A\,|\,a_n\rangle = a_n\,|\,a_n\rangle$$

associated eigenvalue

eigenvector

The length of the eigenvector is not specified by this equation, but if it is nonzero, then the length can be chosen to be 1.

A huge fraction of practical quantum calculations involves finding eigenstates and eigenvalues.

Observables and expected values

Observables are operators that are also self-adjoint (or just Hermitian):

$$A = A^\dagger$$

They have a complete set of orthonormal eigenvectors and real eigenvalues.

$$A = \sum_n a_n |a_n\rangle\langle a_n| \qquad \Rightarrow A|a_n\rangle = a_n|a_n\rangle = A^\dagger|a_n\rangle = \left(\langle a_n|A\right)^\dagger = \left(\langle a_n|a_n\right)^\dagger = a_n^*|a_n\rangle\,.$$

$$\Rightarrow a_n = a_n^*$$

We are often interested in computing **expected values** of operators (usually for observables, but it can be done more generally).

$$\langle\psi|A|\psi\rangle = \sum_{m,n}\langle a_m|c_m^* c_n A|a_n\rangle = \sum_{m,n}\langle a_m|c_m^* c_n a_n|a_n\rangle$$

$$= \sum_{m,n} c_m^* c_n a_n \langle a_m|a_n\rangle = \sum_{m,n} c_m^* c_n a_n \delta_{mn} = \sum_n |c_n|^2 a_n$$

The Born rule and unitary dynamics

The probability of an outcome of a measurement is given by the Born rule.

Example: spin-1/2 $p_\uparrow = |\langle \uparrow | \psi \rangle|^2$

$p_\downarrow = |\langle \downarrow | \psi \rangle|^2$

More generally: $p_n = |\langle a_n | \psi \rangle|^2$

for a measurement in the basis $\{a_n\}$.

Unitary matrices are the inverse of their adjoint: $U^\dagger = U^{-1}$ by definition,

$$\Rightarrow U^\dagger U = U U^\dagger = 1.$$

Unitary dynamics therefore preserves total probability:

$$\sum_n p_n(U) = \sum_n |\langle a_n | U | \psi \rangle|^2 = \sum_n \langle a_n | U | \psi \rangle^* \langle a_n | U | \psi \rangle = \sum_n \langle \psi | U^\dagger | a_n \rangle \langle a_n | U | \psi \rangle$$

$$= \langle \psi | U^\dagger \left(\sum_n | a_n \rangle \langle a_n | \right) U | \psi \rangle = \langle \psi | U^\dagger 1 U | \psi \rangle = \langle \psi | U^\dagger U | \psi \rangle = \langle \psi | \psi \rangle = 1.$$