# Phys 221A – Quantum Mechanics – Lec02

UCLA, Fall 2014

Wednesday $8^{\text{th}}$ October, 2014

# 1 Introduction

Preliminary notes

- TA (Shahriar) office hours changed: Wednesday 3-4 PM in Knudsen 3-111.

## 1.1 More on Hilbert spaces

From now on we will be living in Hilbert space $G$ with vectors, for example $\psi$ or $\phi$. Recall that in the bra-ket notation we have $\psi = |\psi\rangle$ in the Hilbert space, a "ket". The inner product is given by

$$\begin{array}{rcl} G \times G & \to & \mathbb{C} \\ |\phi\rangle, |\psi\rangle & \mapsto & \langle\phi|\,\psi\rangle\,. \end{array} \tag{1}$$

We write elements in the dual space as $\langle\psi|$, a "bra". This is a linear map taking $G \to \mathbb{C}$ and mapping $|\phi\rangle \mapsto \langle\psi|\,\phi\rangle$.

Consider an operator $O : G \to G$ mapping $|\psi\rangle \mapsto O\,|\psi\rangle$. For example, $O = |\phi\rangle\langle\psi|$ for some $\phi, \psi \in G$. Then

$$O\,|\xi\rangle = (|\phi\rangle\langle\psi|)\,|\xi\rangle = |\phi\rangle\langle\psi|\,\xi\rangle\,. \tag{2}$$

Given operators $A, B, C$ we have

$$(AB)\,|\psi\rangle = A(B\,|\psi\rangle), \qquad ABC = A(BC) = (AB)C. \tag{3}$$

Recall the closure relation

$$1 = \sum_i |\alpha_i\rangle\langle\alpha_i| \tag{4}$$

where $\{|\alpha_i\rangle\}$ forms an orthonormal basis (so $\langle\alpha_i|\,\alpha_j\rangle = \delta_{ij}$).

Given an operator $O$, we have that $O$ is linear iff

$$O(c_1\,|\psi_1\rangle + c_2\,|\psi_2\rangle) = c_1 O\,|\psi_1\rangle + c_2 O\,|\psi_2\rangle \tag{5}$$

for all $c_i \in \mathbb{C}$, $|\psi_i\rangle \in G$. The operator $O^\dagger$ is the Hermitian conjugate or adjoint of $O$ iff

$$\langle\psi|\,O\phi\rangle = \left\langle O^\dagger\psi\right|\,\phi\rangle \tag{6}$$

for all $\psi, \phi \in G$. If $O^\dagger$ is the adjoint then $(O^\dagger)^\dagger = O$ and furthermore $\langle O\phi|\,\psi\rangle = \left\langle\phi\right|\,O^\dagger\psi\rangle$.

If $O^\dagger = O$ then $O$ is Hermitian or self-adjoint. If $UU^\dagger = 1$ (i.e. $U^\dagger = U^{-1}$) then $U$ is called unitary. Note that we have

$$\langle O\psi| = \langle\psi| O^\dagger, \tag{7}$$

or in other words

$$\langle O\psi| \phi\rangle = \langle\psi| O^\dagger |\phi\rangle = \left\langle\psi\middle| O^\dagger\phi\right\rangle. \tag{8}$$

A physical observable, i.e. a dynamical variable, must be represented by a linear operator $O$. Given a physical state $\psi$, where $\langle\psi| \psi\rangle = 1$, the "expectation value" of $O$ in the state $|\psi\rangle$ is given by

$$\langle O\rangle = \langle\psi| O\psi\rangle. \tag{9}$$

Note that if $O$ is Hermitian, i.e. $O = O^\dagger$, then $\langle O\rangle \in \mathbb{R}$ for any $\psi$.

## 1.2 Representation in a basis

In an orthonormal basis $|\alpha_i\rangle$ we have

$$|\psi\rangle = \sum_i |\alpha_i\rangle \langle\alpha_i| \psi\rangle = \sum_i c_i |\alpha_i\rangle \tag{10}$$

so we can write

$$\begin{aligned} O|\psi\rangle &= O\sum_i c_i |\alpha_i\rangle = \sum_i c_i O|\alpha_i\rangle & (11)\\ &= \sum_{ij} c_i |\alpha_j\rangle \langle\alpha_j| O |\alpha_i\rangle. & (12)\end{aligned}$$

Thus we can write $O|\psi\rangle$ in the basis as $\sum_j b_j |\alpha_j\rangle$ where $b_j = \sum_i O_{ji}c_i$ and

$$O_{ij} = \langle\alpha_i| O |\alpha_j\rangle \tag{13}$$

is called the matrix element.

There is a one-to-one map from vectors $\psi$ to column vectors $\mathbf{c} = (c_1, \ldots, c_n)^\top$ (where $n = \dim G$) such that $\psi = \sum_i c_i |\alpha_i\rangle$, as well as a map from operators $O$ to $n \times n$ matrices $\hat{O} = (O_{ij})$. Thus we can write $G \cong \mathbb{C}^n$ (note that $n$ is not necessarily finite). Note that given a vector $\phi$ represented by $\mathbf{b}$, we can write $\langle\phi| \psi\rangle = \mathbf{b}^\dagger \cdot \mathbf{c}$. Furthermore if $|\phi\rangle = O|\psi\rangle$ then $\mathbf{b} = \hat{O}\mathbf{c}$.

A Hermitian operator $O$ corresponds to a Hermitian matrix $\hat{O}$, and similarly a unitary operator $U$ corresponds to a unitary matrix $\hat{U}$. Thus given Hermitian $O$ and unitary $U$ we have $O_{ij} = O^*_{ji}$ and $\hat{U}\hat{U}^\dagger = \hat{1}$. Given two orthonormal bases $\{|\alpha_i\rangle\}$ and $\{|\alpha'_i\rangle\}$ we can always write $\hat{O}' = \hat{U}^\dagger\hat{O}\hat{U}$ where $U_{ij} = \left\langle\alpha_i\middle| \alpha'_j\right\rangle$ and happens to be unitary. We can show this last statement:

$$(\hat{U}\hat{U}^\dagger)_{ij} = \sum_k U_{ik}U^*_{jk} = \sum_k \langle\alpha_i| \alpha'_k\rangle \langle\alpha'_k| \alpha_j\rangle = \langle\alpha_i| \alpha_j\rangle = \delta_{ij}. \tag{14}$$

A little more on operators. We define

$$\begin{aligned} [A, B] &= AB - BA, &&\text{the commutator, and} & (15)\\ \{A, B\} &= AB + BA, &&\text{the anti-commutator.} & (16)\end{aligned}$$

Then we have

$$AB = \frac{1}{2}[A, B] + \frac{1}{2}\{A, B\} \tag{17}$$

$$= BA = -\frac{1}{2}[A, B] + \frac{1}{2}\{A, B\} \tag{18}$$

Notice that $\{A, B\}$ is Hermitian and $[A, B]$ is anti-Hermitian ($O^\dagger = -O$). Furthermore, if $A$ and $B$ are Hermitian then

$$(AB)^\dagger = B^\dagger A^\dagger = BA \neq AB. \tag{19}$$

Finally we can split any operator $O$ into a Hermitian part $\zeta_+$ and an anti-Hermitian part $\zeta_-$:

$$O = \frac{1}{2}(\zeta_+ + \zeta_i), \quad \zeta_+ = O + O^\dagger, \quad \zeta_- = O - O^\dagger. \tag{20}$$

## 1.3 Onward to physics

The eigenvectors of a Hermitian operator yield a complete orthonormal basis. If $A$ and $B$ are Hermitian operators and $[A, B] = 0$ then the operators yield a complete set of simultaneous eigenvectors (which form an orthonormal basis). When this happens we call $A, B$ compatible observables.

In the hydrogen atom we have quantum numbers:

- principle quantum number $n = 1, 2, \ldots$ where $E \sim -1/n^2$, eigenvalues of the Hamiltonian $H$,
- angular momentum quantum number $\ell = 0, 1, \ldots, n-1$, eigenvalues of $L^2$,
- magnetic quantum number $m = -\ell, \ldots, \ell$, eigenvalues of $L_z$,
- spin quantum number $s = \pm 1/2$, eigenvalues of $S_z$.

We can show that

$$[H, L^2] = [L^2, L_z] = [H, L_z] = 0 \tag{21}$$

so that $H, L^2, L_z$, and $S_z$ are compatible observables uniquely identified by their quantum numbers $(n, \ell, m, s)$.

Generally, a complete set of compatible observables whose eigenvalues, or quantum numbers, uniquely label their common eigenvectors (resolving all degeneracies). Thus each $|\alpha_i\rangle$ in the corresponding orthonormal basis is labelled by the set of quantum numbers. Typically this complete set is provided by $H$ and corresponding symmetry generators.