Intermediate Quantum Mechanics
Lecture 2 Notes (1/26/15)

Vector Spaces

Vector Spaces

- Mathematicians have developed many mathematical concepts that later have found use in physics. One of the more important of these is the concept of a **vector space**. Describing arrows in physical space (velocity, momentum, force, etc.) is one use of vector spaces.

- In addition, there are other more abstract uses of vectors in physics. The concept of complex vector spaces is at the heart of quantum mechanics. You can't really know quantum mechanics without a basic understanding of vector spaces.

- We'll spend two lectures on the linear algebra of vector spaces and their associated linear operators. For most of you, this will be a review, but you'll see vectors spaces from a physics rather than a mathematics perspective. I'll present a brief summary going over only the essential points needed for use in quantum mechanics without going into the full mathematical details.

Definition of a Vector Space

- A vector space is a collection of elements (vectors).

- We'll use the notation $|a\rangle$ to indicate a vector with label a. This is called a **ket**. You'll see why shortly. This is a notation that was invented by Dirac and has been used by physicists ever since. It is a very powerful notation (as you'll see) for quantum mechanics. Don't ask a mathematician about it, though. They use their own notation.

- There are two defined operations under which the vector space is closed.
  - Addition of vectors: $|a\rangle + |b\rangle$
  - Multiplication of a vector by a number: $\alpha\,|a\rangle$

- Closed means that the operation yields a vector in the space

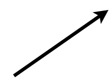
$$|a\rangle + |b\rangle = |c\rangle \qquad\qquad \alpha\,|a\rangle = |d\rangle$$

- This closure under addition of vectors and multiplication of a vector by a number are the important properties. Mathematicians also worry about:
  - commutativity of the addition
  - distribution of the addition over the multiplication
  - distribution of the multiplication over the addition
  - existence of the null vector
  - existence of an inverse for every vector

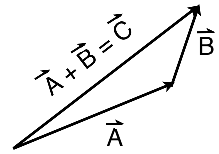
We won't be concerned with these. Any sensible vector space, including all of those that we will discuss, satisfies these. If you are interested you can check these properties for yourself.

Example of arrows in physical space

- You know about vectors (velocity, momentum, acceleration, etc.). These are all **arrows** in **physical space**. They have a **length** and a **direction**. Here is an arrow in the plane of the computer monitor.



- The addition of arrows is defined in the usual manner by the parallelogram rule.



Note that for arrows I'm using the familiar notation of a vector as a label with a half arrow on top rather than the more general ket notation.

- Multiplying an arrow by a number α changes the length of the arrow by a factor of α. If α is negative, the direction of the arrow is reversed.

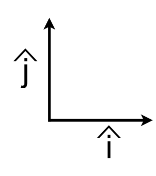
- Arrows in the plane of the monitor are elements of a 2-dimensional vector space. That is, any vector in the space can be expressed as the linear sum of two **linearly independent** vectors. We say that these vectors **span** the space. Three linearly independent vectors would be needed to express arrows in three dimensional space.

- The minimum number of linearly independent vectors needed to express any vector in the space is the **dimension** of the space.

Basis vectors

- It is almost always most useful to choose the linearly independent vectors that span the space to be perpendicular and of unit length. They are then called **basis vectors**.

- For arrows in 2 dimensions, we can choose the basis vectors: $\hat{i}$, $\hat{j}$



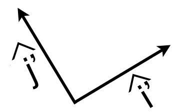
Then any vector $\vec{A}$ can be expressed as: $\quad \vec{A} \,=\, A_x\,\hat{i} \,+\, A_y\,\hat{j}$

- In this basis, $\vec{A}$ is determined by the two parameters, A_x and A_y. We can write this as a column matrix.

$$\begin{pmatrix} A_x \\ A_y \end{pmatrix}$$

- A_x and A_y are called the **components**.

- There are an infinite number of possible choices for basis vectors. We could, for example, choose: $\hat{i}'$, $\hat{j}'$.



In this basis, the components would be: $A_{x'}$, $A_{y'}$.

Representation of a vector

- The symbol $\vec{A}$ indicates the actual vector independent of what set of basis vectors are used. If we choose the $\hat{i}$, $\hat{j}$ basis we can represent the vector in this basis as

$$\begin{pmatrix} A_x \\ A_y \end{pmatrix}$$

- We indicate this as:

$$\vec{A} \implies \begin{pmatrix} A_x \\ A_y \end{pmatrix}$$

We should not use an equal sign since $\begin{pmatrix} A_x \\ A_y \end{pmatrix}$ is not the vector. It is just a representation of the vector. If we choose a different basis, for example, $\hat{i}'$ and $\hat{j}'$, the vector $\vec{A}$ would be represented as:

$$\vec{A} \implies \begin{pmatrix} A_{x'} \\ A_{y'} \end{pmatrix}$$

- This might seem rather pedantic but in quantum mechanics realizing that the same vector (a state of asystem) can be represented in various ways (for example, the position or the momentum representation) will be important.

Inner Product

- We will be interested only in vector spaces for which an **inner product** is defined. This is an operation on two vectors that yields a number.

- In the case of arrows, the inner product is the familiar dot product of two vectors. For 2-dimensional arrows:

$$\vec{A} \cdot \vec{B} = A_x B_x + A_y B_y$$

item It can easily be shown that:

$$\vec{A} \cdot \vec{B} = |\vec{A}||\vec{B}| \cos\theta$$

where $|\vec{A}|$ and $|\vec{B}|$ are the lengths of arrows $\vec{A}$ and $\vec{B}$, respectively, and θ is the angle between the two arrows. This shows that the dot (inner) product is independent of the choice of basis vectors. We also have that:

$$\vec{A} \cdot \vec{B} \;=\; \text{projection of } \vec{A} \text{ on } \vec{B} \;=\; \text{projection of } \vec{B} \text{ on } \vec{A}$$

- We require that the inner product operation be linear, that is:

$$\vec{A} \cdot (\alpha\,\vec{B} + \beta\,\vec{C}) \;=\; \alpha\,\vec{A} \cdot \vec{B} + \beta\,\vec{A} \cdot \vec{C}$$

- The inner product of basis vectors is:

$$\hat{i} \cdot \hat{j} \;=\; \delta_{ij} \;=\; \begin{cases} 1 & \text{if} \quad i = j \\ 0 & \text{if} \quad i \neq j \end{cases}$$

- The inner product of an arrow with itself is the square of the length of the arrow.

$$\vec{A} \cdot \vec{A} \;=\; A_x^2 + A_y^2 \;=\; |\vec{A}|^2$$

Other examples of vector spaces

- Besides 2-d and 3-d arrows, lets look at other examples of vector spaces.
- What about 1-d arrows. These are the numbers on the real number line. So, the real numbers form a 1-dimensional vector space.
- So far, we have only considered physical arrows. Now let's consider abstract vectors spaces where the space is not a physical space. An example is the collection of all 2×2 real matrices.

$$|a\rangle \;\Longrightarrow\; \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$$

  These form a vector space. You can easily show that they satisfy closure under matrix addition and multiplication of a matrix by a real number. What is the dimension of this space?

- Although we can only think about 1, 2 or 3-dimensional physical space, we can fairly easily abstract the idea of a vector space to higher dimensions. Warning: don't try to envision a 4, 5 or 6-dimensional arrow. You can't do it. Our brains are "hardwired" to only be able to think in 3 (or fewer dimensions) physical dimensions. [Most theorist I know have trouble even thinking in 3 dimensions.] Even though we can't envision vectors of more than three dimensions, we can easily abstract the mathematics of vector spaces to higher dimensions.
- A vector space in n dimensions would have n basis vectors and n components. A vector in this space could be represented by:

$$|a\rangle \;\Longrightarrow\; \begin{pmatrix} a_1 \\ a_2 \\ \cdot \\ \cdot \\ \cdot \\ a_n \end{pmatrix}$$

Infinite dimensional vector spaces

- As we consider higher and higher dimension spaces, we can go to the limit of an infinite dimensional space where:

$$|f\rangle \implies \begin{pmatrix} f_1 \\ f_2 \\ \cdot \\ \cdot \\ \cdot \end{pmatrix}$$

  This space has an infinite number of basis vectors and an infinite number of components.

- Now let's go to the next level of abstraction. In the above the basis vectors and components while infinite in number are discreet. Let's go to the case where they are continuous. Then the components rather than being a function of the discreet index i will be a function of a continuous variable x.

$$|f\rangle \implies f(x)$$

- The set of real analytic function on a given interval form an infinite dimensional vector space. An infinite number of components, one for each value of the continuous variable x, are needed to specify a vector (real function). It is easy to show that the set of all analytic real function on a given interval satisfy the closure conditions. Analytic means that the function can be written in the form of a power series. That means that it is infinitely differentiable. A good synonym for analytic might be "well behaved".

- In the case of discreet basis vectors, the inner product of two vectors $|a\rangle$ and $|b\rangle$ is given by the sum of the product of components:

$$\sum_i a_i b_i = a_1 b_1 + a_2 b_2 \cdots$$

  For the case of the vector space of real functions, the sum over products of components becomes an integral over x so that the inner product of two functions $|f\rangle$ and $|g\rangle$ is:

$$\int f(x) g(x)\, dx$$

The Complex Number System

- Quantum mechanics is based on complex vector spaces. We'll discuss those but first an aside on complex numbers.

- The complex number system is the ultimate (perfect) number sense. If we start with the whole (counting) numbers, we find that there isn't always a solution to the problem of finding the inverse of addition, e.g., $a + 8 = 5$. This leads us to extend the number system to positive and negative integers but then there isn't always a solution to the problem of the inverse of multiplication, e.g., $a \times 5 = 3$. We then extend the number system to the rational numbers (ratios of integers) but then there isn't always a solution to the problem of the inverse of raising to a power, e.g., $a^2 = 2$. We're then led to the real numbers that in addition to the rational numbers includes such numbers as: $\sqrt{2}$, π, e, etc. But even with the real numbers, we can't solve even such a simple equation as: $x^2 + 1 = 0$. For that, we need the complex numbers.

- We introduce the imaginary number $i = \sqrt{-1}$. A general complex number is then: $z = a + ib$ where a and b are real numbers. We are now at the end of the line. There is no need to introduce any additional numbers. Any complex number raised to any complex power, $z_1^{z_2}$, is always a complex number. The Fundamental Theorem of Algebra that states that any equation of the form:

$$a_0 + a_1 z + a_2 z^2 + \cdots + a_n z^n = 0$$

  where the a's are any complex numbers, has all complex number solutions.

History of the The Complex Numbers

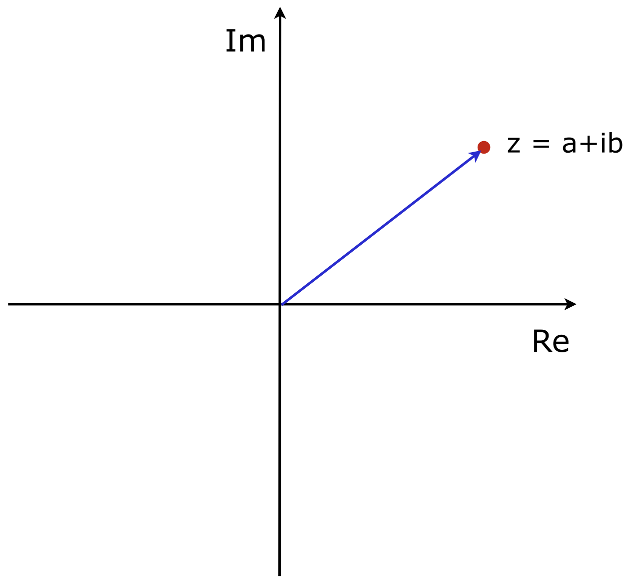
- The complex number were discovered in the 16th century primarily by a group of Italian mathematicians. They like mathematicians for centuries after them believed that they were a Platonic ideal having nothing to do with reality.

- The complex numbers have many interesting properties and provide a valuable tools at solving mathematical problems. One of their first uses was in finding the real roots of general cubic equations (or determining that there weren't any real roots). They also have an important use in solving driven, damped oscillatory systems, for example, AC circuits. Without complex numbers the algebra would often be horrendous. Of course, in the end, if it is a physical system, only the real part of the solution has meaning.

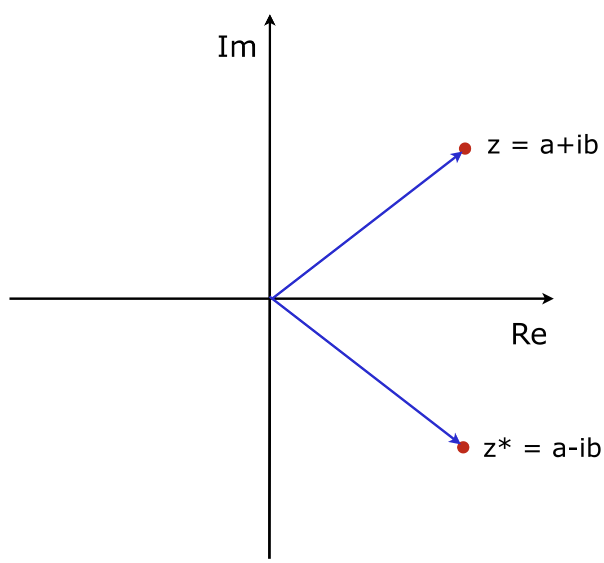
- It must have come as a shock to the physicists in the first half of the 20th century when they discovered that this ultimate number system was essential to the quantum mechanics, the most basic of all physical theories. It still seems really remarkable. In quantum mechanics, complex numbers are not just tools, they are essential. Without complex numbers there is no quantum mechanics. In a few lectures from now, we'll see why.

The complex number plane and complex conjugation

- We can represent the complex number, $z = a + ib$, in a plane defined by the real and imaginary axes.



- **Complex conjugation** is a very important operation on complex numbers. The complex conjugate of $z = a + ib$ is $z^* = a - ib$. It is a reflection about the real axis.



- The product of a complex number and its complex conjugate is always positive and real. It is the square of the magnitude (or modulus) of the complex number.

$$zz^* = (a + ib)(a - ib) = a^2 + b^2 = |z|^2$$

The Euler Relation

- One of the most remarkable and important equations in mathematics is the Euler relation.

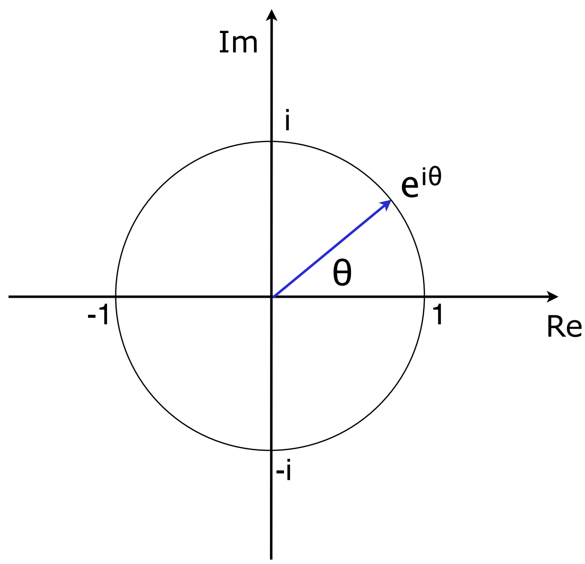
$$e^{i\theta} = \cos\theta + i\sin\theta$$

where e is the base of the natural logarithm with value 2.718...

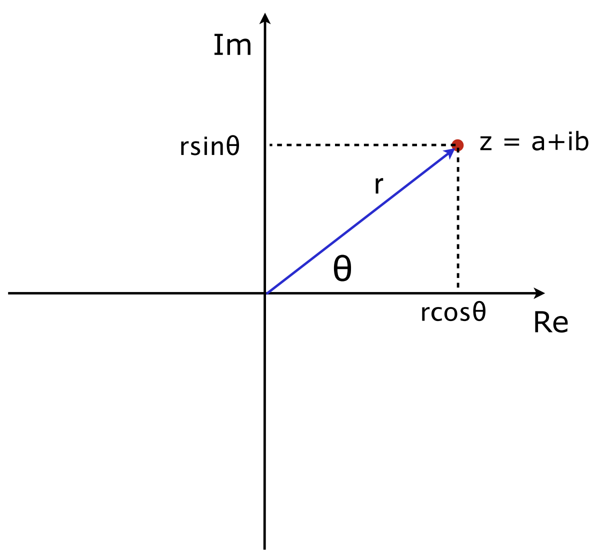
- The complex number $e^{i\theta}$ has unit modulus

$$e^{i\theta}(e^{i\theta})^* \;=\; e^{i\theta}e^{-i\theta} \;=\; 1$$

It represents complex numbers on the unit circle in the complex plane



Another expression for a complex number is then: $\quad z \;=\; r\cos\theta + ir\sin\theta \;=\; re^{i\theta}$



Complex vector space

- A complex vector space is the same as a real vector space except that in multiplication of a vector by a number we allow the number to be a complex number.

- The complex numbers themselves form a 1-dimensional complex vector space. From the figures of the complex plane above, you might think that they also form a 2-dimensional real vector space but, it's best not to think of them that way.

- For simplicity and clarity, I'll discuss a 2-dimensional complex vector space. It's easy to extend this discussion to a higher dimension space.

- We choose two basis vectors. I'll label them $|1\rangle$ and $|2\rangle$. Then just as for a real vector space, a general vector, $|a\rangle$, can be expressed as a linear combination of the the basis vectors:

$$|a\rangle \;=\; a_1\,|1\rangle \,+\, a_2\,|2\rangle$$

  where now the a's are complex numbers.

- Warning: do not try to think of complex arrows. You'll go crazy. Just think of complex vectors in terms of the mathematical properties they have, analogous to those of arrows.

Dual space

- For a complex vector space, we need the concept of the complex conjugate of a vector. We notate the complex conjugate of $|a\rangle$ by $\langle a|$ called a **bra**.

$$\text{If} \qquad |a\rangle \;\Longrightarrow\; \begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \qquad \text{then} \qquad \langle a| \;\Longrightarrow\; (a_1^*,\, a_2^*)$$

- The set of all bra's form a dual vector space. There is a one-to-one correspondence between ket vectors and the corresponding dual bra vectors.

Inner product

- We now define the inner product for a complex vector space as:

$$\langle a\,|\,b\,\rangle \;=\; (a_1^*,\, a_2^*)\begin{pmatrix} b_1 \\ b_2 \end{pmatrix} \;=\; a_1^*b_1 \,+\, a_2^*b_2$$

- The reason for defining the inner product this way is so that the inner product of a vector with itself is real and positive:

$$\langle a\,|\,a\,\rangle \;=\; (a_1^*,\, a_2^*)\begin{pmatrix} a_1 \\ a_2 \end{pmatrix} \;=\; a_1^*a_1 \,+\, a_2^*a_2 \;=\; |a_1|^2 \,+\, |a_2|^2$$

- $\langle a\,|\,a\,\rangle$ is the square of the "length" (norm) of $|a\rangle$.

- The reason for writing the bra as a row matrix is that the inner product is then given by the rules of matrix multiplication as above.