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Lecture notes for FYS610 Many particle Quantum Mechanics

Note 2, 10.1 2018

Additions and comments to *Quantum Field Theory and the Standard Model* by Matthew D. Schwartz (2014)

The Hilbert space

Based upon the enormous success of standard non-relativistic Quantum Mechanics and of Quantum Electrodynamics, a clear consistent picture of the formal structure of quantum theories has evolved. This has not at all been influenced by the wide variety of *interpretations* of quantum mechanics that has been introduced. This general description is conveniently formulated in terms of Dirac's *bra-ket* notation.

Any *pure*, *i.e.* completely characterized, physical state is characterized by some vector, called a **state vector**, which shall be written $|\,\psi\,\rangle$, in an infinite-dimensional complex vector space, more precisely a **Hilbert space**, $\mathcal{H}$. Such a vector is also called a "ket" in the Dirac formalism. Since $\mathcal{H}$ is a vector space, the kets can be added and be multiplied by complex constants, so that if $|\,\phi\,\rangle, |\,\psi\,\rangle \in \mathcal{H}$, and a and b are complex numbers, we have:

$$|\,\chi\,\rangle = a|\,\phi\,\rangle + b|\,\psi\,\rangle \in \mathcal{H}\,.$$

An important point is that $|\,\psi\,\rangle$ and $c|\,\psi\,\rangle$ represents the *same* physical state, for any non-zero constant c. But if $|\,\phi\,\rangle \neq c|\,\phi\,\rangle$ for any non-zero c, the states $|\,\phi\,\rangle$ and $|\,\psi\,\rangle$ represent different physical states. Thus if we define a **ray** parallel to $|\,\psi\,\rangle$ as the set $\{c|\,\psi\,\rangle |\, c \in \mathbb{C}\}$ ($\mathbb{C}$ is the set of all complex numbers), we have a one-to-one relation between the *rays* of $\mathcal{H}$ and the states of a physical system.

Like any vector space, one can equip $\mathcal{H}$ with sets of basis vectors, $\{|\,e_i\,\rangle\}$. For a system of a fixed finite number of particles, we can even find countable sets of such basis vectors, which we can assume to be numbered by the natural numbers, $|\,e_1\,\rangle, |\,e_2\,\rangle\ \ldots\ |\,e_i\,\rangle\ \ldots$. A Hilbert space where this is possible, is called *separable*. But, as we shall see, this is not possible in the extension of the theory to an arbitrary number of particles, *i.e.* in quantum field theory.

The basis vectors are *linearly independent*, which for separable spaces means that all equations of the form:

$$\sum_{i=1}^{\infty} \psi_i |\,e_i\,\rangle = 0\,,$$

only have the solution $\psi_i = 0$ for all i. This and the following results can be extended to non-separable spaces, but for notational convenience we shall restrict ourselves to the separable case. From this, one can show that any ket can be expanded in terms of basis vectors in a *unique* manner, just like a vector in a finite-dimensional vector space:

$$|\,\psi\,\rangle = \sum_{i=1}^{\infty} \psi_i |\,e_i\,\rangle\,. \tag{2.1a}$$

For any Hilbert space, $\mathcal{H}$, one can define a **dual vector space**, $\mathcal{H}^*$, which is isomorphous to $\mathcal{H}$, *i.e.* there is a one-to-one, and hence invertible, correspondence between the vectors of $\mathcal{H}$ and $\mathcal{H}^*$. The construction of this dual space is not hard, but we shall not need it. It essentially amounts to a generalization of the observation that in finite dimensional vector spaces we can map the set of column vectors by transposition on the set of row vectors in a one-to-one fashion. A vector in $\mathcal{H}^*$ is called a "bra". The isomorphy between the spaces means that all ket's $|\,\psi\,\rangle$ of $\mathcal{H}$ are mapped on a bra in $\mathcal{H}^*$. The image of $|\,\psi\,\rangle$ we shall write $\langle\psi|$. In particular the basis vectors in $\mathcal{H}$ are mapped on basis vectors in $\mathcal{H}^*$, and *vice versa*: $|\,e_i\,\rangle \leftrightarrow \langle e_i|$. It turns out to be possible, and very convenient, to arrange things so that the mapping $\mathcal{H} \leftrightarrow \mathcal{H}^*$ is **anti-linear**, meaning that it is linear, except that numbers are mapped on their complex conjugates. We call this mapping **Hermitean conjugation**, and denote it by a dagger, †. Thus $|\,\psi\,\rangle$ in eq.(2.1a) is mapped as:

$$|\,\psi\,\rangle \leftrightarrow |\,\psi\,\rangle^\dagger = \langle\psi| = \sum_{i=1}^{\infty} \psi_i^* \langle e_i|\,. \tag{2.1b}$$

This operation corresponds to a simultaneously transposition and complex conjugation of a vector in a finite dimensional vector spaces.

We are now in the position to define a **scalar product** in $\mathcal{H}$. Because of the linearity of the spaces, it suffices to define the product for the basis vectors:

$$\langle e_i| \cdot |\,e_j\,\rangle = \langle e_i|e_j\rangle = \delta_{ij}\,. \tag{2.2}$$

From this, we find the scalar product between to vectors $|\,\psi\,\rangle = \sum_k \psi_k |\,e_k\,\rangle$ and $|\,\phi\,\rangle = \sum_k \phi_k |\,e_k\,\rangle$ as;

$$\langle\phi|\psi\rangle = \sum_k \phi_k^* \psi_k = \langle\psi|\phi\rangle^*\,. \tag{2.3}$$

This formula explains the names "bra" and "ket", their scalar product is a "bracket". We see that this is nothing but a generalization to infinite-dimensional vectors of the usual complex scalar product. In particular, we can define the length of a vector as:

$$\||\,\psi\,\rangle\|^2 = \|\langle\psi|\|^2 = \langle\psi|\psi\rangle = \sum_k |\psi_k|^2\,. \tag{2.4}$$

We see that $\||\,\psi\,\rangle\|^2 > 0$ unless $\psi_k = 0$ for all k, in which case $|\,\psi\,\rangle = 0$, so the scalar product is positive definite. It can furthermore be shown that $\||\,\psi\,\rangle\|^2 < \infty$ for all vectors in $\mathcal{H}$. Since physical states are represented by rays, the length of $|\,\psi\,\rangle$ has no physical significance. Hence we are free to normalize our states so that $\||\,\psi\,\rangle\| = 1$, and this is often convenient.

By multiplying $|\,\psi\,\rangle$ in eq. (2.1a) with $\langle e_i|$, we find, not unexpectedly, from eq. (2.3) (cf. *BJ* [2.88]).

$$\psi_k = \langle e_k|\psi\rangle\,. \tag{2.5}$$

Inserting this back in eq. (2.1a), we then have:

$$|\,\psi\,\rangle = \sum_k |\,e_k\,\rangle\langle e_k|\psi\rangle = \left(\sum_k |\,e_k\,\rangle\langle e_k|\right)|\,\psi\,\rangle\,.$$

Since this is true for *any* $|\,\psi\,\rangle$, it means that we must have the operator identity:

$$\sum_k |\, e_k\,\rangle\langle e_k| = \mathbb{1}\,, \tag{2.6}$$

where $\mathbb{1}$ is the *unit operator* in $\mathcal{H}$. This equation, called the *resolution of the unit operator*, expresses the *completeness* of the basis.

Operators

An **operator** in a Hilbert space $\mathcal{H}$ is simply a function mapping a vector (ket) of $\mathcal{H}$ onto another vector in the same space. With very few exceptions, the most important one being the *time reversal operator*, we only need *linear operators* in Quantum Mechanics. A linear operator, $\mathcal{O}$, is one that satisfies:

$$\mathcal{O}\left(a|\,\psi\,\rangle + b|\,\phi\,\rangle\right) = a\,\mathcal{O}|\,\psi\,\rangle + b\,\mathcal{O}|\,\phi\,\rangle\,, \tag{2.7}$$

for arbitrary $|\,\psi\,\rangle$ and $|\,\phi\,\rangle$ in $\mathcal{H}$ and complex numbers a, b. Since $\mathcal{O}|\,\psi\,\rangle$ is also a vector in $\mathcal{H}$, it can be expanded in any basis, using eq. (2.5).

$$\mathcal{O}|\,\psi\,\rangle = \mathcal{O}\,\mathbb{1}|\,\psi\,\rangle = \sum_k \mathcal{O}|\,e_k\,\rangle\langle e_k|\psi\rangle = \sum_k \psi_k \mathcal{O}|\,e_k\,\rangle\,. \tag{2.8}$$

Since any vector in $\mathcal{H}$ can be expanded in terms of basis vectors, a linear operator is completely specified by its actions on a complete set of these. Using eqs. (2.1a) and (2.6), the scalar product of $\mathcal{O}|\,\psi\,\rangle$ with an arbitrary bra $\langle\phi|$ can be written, using the notational convention that $\mathcal{O}|\,\psi\,\rangle = |\,\mathcal{O}\psi\,\rangle$:

$$\langle\phi|\mathcal{O}\psi\rangle = \langle\phi|\left(\mathbb{1}|\,\mathcal{O}\psi\,\rangle\right) = \sum_l \langle\phi|e_l\rangle\langle e_l|\mathcal{O}\psi\rangle = \sum_{k,l}\langle\phi|e_l\rangle\langle e_l|\mathcal{O}e_k\rangle\langle e_k|\psi\rangle = \sum_{k,l}\phi_l^*\,\mathcal{O}_{lk}\psi_k\,, \tag{2.9}$$

where the **matrix element** $\mathcal{O}_{ji}$ is defined by:

$$\mathcal{O}_{ji} = \langle e_j|\mathcal{O}e_i\rangle\,. \tag{2.10}$$

This is evidently the generalization of the usual rule for finding the matrix elements of a linear operator in a finite dimensional complex vector space. It follows that an operator is completely specified by all its matrix elements in some basis.

For any linear operator $\mathcal{O}$ we define the adjoint, or Hermitean conjugate, $\mathcal{O}^\dagger$ in analogy with eq. (2.1b):

$$|\,\mathcal{O}\psi\,\rangle^\dagger = \langle\mathcal{O}\psi| = \langle\psi|\mathcal{O}^\dagger\,. \tag{2.11}$$

Then from eq. (2.3) and (2.9):

$$\langle\mathcal{O}\psi|\phi\rangle = \left(\langle\psi|\mathcal{O}^\dagger\right)|\,\phi\,\rangle = \langle\phi|\mathcal{O}\psi\rangle^* = \sum_{k,l}\phi_l\,\mathcal{O}_{lk}^*\psi_k^* = \sum_{k,l}\psi_k^*\left(\mathcal{O}^{*\mathsf{T}}\right)_{kl}\phi_l\,.$$

Hence we can identify, just as for finite dimensional matrices:

$$\mathcal{O}^\dagger = \mathcal{O}^{*\mathsf{T}} \qquad \Longleftrightarrow \qquad \mathcal{O}_{ij}^\dagger = \mathcal{O}_{ji}^*\,, \tag{2.12}$$

so from eq. (2.9), with $\mathcal{O} \to \mathcal{O}^\dagger$:

$$\langle \mathcal{O}\psi|\phi\rangle = \sum_{k,l} \phi_l \, \mathcal{O}^\dagger_{kl} \psi^*_k = \langle \psi|\mathcal{O}^\dagger \phi\rangle \, .$$

Interchanging $\mathcal{O} \leftrightarrow \mathcal{O}^\dagger$, we thus can calculate matrix elements as:

$$\mathcal{O}_{ij} = \langle e_i|\mathcal{O}e_j\rangle = \langle \mathcal{O}^\dagger e_i|e_j\rangle = \langle e_i|\mathcal{O}|\, e_j\rangle \, . \tag{2.13}$$

Here the last equality is the definition of $\langle e_i|\mathcal{O}|\, e_j\rangle$. We say that we have to use the Hermitean conjugate of an operator when acting on a bra. An **Hermitean operator**, satisfying $\mathcal{O} = \mathcal{O}^\dagger$, acts in the same manner on ket's and bra's.

We note that by a double use of the resolution of the unit, we can write any operator in any basis as:

$$\mathcal{O} = \mathbb{1}\, \mathcal{O}\, \mathbb{1} = \sum_{i,j} |\, e_i \,\rangle\langle e_i|\mathcal{O}|\, e_j\rangle\langle e_j| = \sum_{i,j} |\, e_i \,\rangle \mathcal{O}_{ij} \langle e_j| \, . \tag{2.14}$$

In particular, if $\mathcal{O}$ is Hermitean, and the basis $\{|\, e_i \,\rangle\}$ consists of its normalized eigenvectors, $\mathcal{O}|\, e_i \,\rangle = O_i|\, e_i \,\rangle$ so $\mathcal{O}_{ij} = \langle e_i|\mathcal{O}|\, e_j\rangle = O_i \delta_{ij}$, this simplifies to:

$$\mathcal{O} = \sum_i |\, e_i \,\rangle O_i \langle e_i| \, . \tag{2.15}$$

References:

BJ) B. H. Bransden and C. J. Joachain: *Physics of Atoms and Molecules* (1983), ch. 2.1-3.