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Ket vectors in three-dimensional space and their cross product

Amelia Carolina Sparavigna[1] and Roberto Marazzato[2]
1 Department of Applied Science and Technology, Politecnico di Torino, Italy
2 Visiting Staff at Department of Mathematical Sciences, Politecnico di Torino, Torino, Italy

Abstract: In quantum mechanics, the ket notation for vectors was introduced in 1939 by Paul Dirac for describing the quantum states. In this framework, the dot product was easily rendered as a bra-ket operation. Here, we show that it is also possible to represent the cross product of vectors within this notation. We will consider the case of Euclidean vectors in a three-dimensional space with orthonormal basis vectors.

Keywords: Physics education research.

Introduction. In quantum mechanics, the ket notation for vectors is used for describing the quantum states. In this framework, the dot or inner product of two vectors is easily rendered as a bra-ket, such as $\langle a|b\rangle$ for vectors $|a\rangle$ and $|b\rangle$. The notation was introduced in 1939 by Paul Dirac [1]. It is known as Dirac notation and largely used in quantum physics.
The bra-ket notation and the related calculus, which is also represented by calculations with matrices, is not used in classical mechanics, probably because, for this mechanics, we need just Euclidean vectors in the three-dimensional space, with orthonormal unit vectors $|e_i\rangle$, with index i being 1,2 and 3. Being not used in classic mechanics, no expression of the cross product with ket and bra vectors is given. Here, we propose a simple expression for this product, involving permutation and projection operators.

Linear subspace. The ket-vectors belong to a linear subspace. To characterize the subspace as linear, we require that the subspace is closed under linear combinations [2,3]. Let call the linear subspace *S*. Let *K* be a field (in the cases we are here discussing, the field of real numbers), and *V* be a vector space over *K*. Suppose *S* a subspace of *V*, closed under operations of addition and multiplication by a scalar (the operation of addition is commutative and associative, the multiplication by a scalar is distributive and associative). We have the following theorem: *S* is a subspace if and only if *S* satisfies the following three conditions: 1) zero vector, $|0\rangle$, is in *S*; 2) if $|a\rangle$ and $|b\rangle$ are elements of *S*, then the sum $|a\rangle+|b\rangle$ is an element of *S*; 3) if $|a\rangle$ is an element of *S* and *c* is a scalar from *K*, then the product $c|a\rangle$ is an element of *S*. A relevant property is that, $\forall|a\rangle\in S$, we have the opposite element $-|a\rangle\equiv(-1)|a\rangle$, so that $|a\rangle-|a\rangle=|0\rangle$.

***K* real for dot product.** Since we aim discussing the use of ket vectors in the classical mechanics, let us confine ourselves to the case of *K* real. Let us write the dot product with ket vectors. Being $|a\rangle$ and $|b\rangle$, it is simply given by bra-ket $\langle a|b\rangle$, which is a *K* element. If we use the common vector notation, the dot product is $\vec{a}\cdot\vec{b}=\langle a|b\rangle$. It has the following properties:

$$\begin{aligned}&\langle a|b\rangle=\langle b|a\rangle\\ &\langle a|a\rangle\geq 0\\ &\langle a|c\rangle=\langle a|(\alpha|d\rangle+\beta|e\rangle)\rangle=\alpha\langle a|d\rangle+\beta\langle a|e\rangle\end{aligned}\qquad(1)$$

Two vectors are orthogonal when: $\langle a|b\rangle=\langle b|a\rangle=0$. The norm of a vector is: $N_a=\sqrt{\langle a|a\rangle}$.

Let us consider a subspace having three dimensions, such as the three-dimensional space. Let us consider, for this subspace, an orthonormal basis consisting of three vectors, $|e_1\rangle$, $|e_2\rangle$ and $|e_3\rangle$. Each vector of S is given by a linear combination of them. The dot product of two vectors becomes:

$$
\begin{aligned}
&|a\rangle = a_1|e_1\rangle + a_2|e_2\rangle + a_3|e_3\rangle \\
&|b\rangle = b_1|e_1\rangle + b_2|e_2\rangle + b_3|e_3\rangle \\
&\langle a|b\rangle = \langle b|a\rangle = a_1b_1 + a_2b_2 + a_3b_3
\end{aligned} \tag{2}
$$

However, ket and bra vectors can also be represented by columns and rows, so we can represent the dot product in the following manner:

$$
|a\rangle = \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}; \langle b| = \begin{pmatrix} b_1 & b_2 & b_3 \end{pmatrix} \Rightarrow \langle b|a\rangle = \begin{pmatrix} b_1 & b_2 & b_3 \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = a_1b_1 + a_2b_2 + a_3b_3 \tag{3}
$$

.

In (3), the vectors of the basis are rendered as:

$$
|e_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} \qquad |e_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad |e_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} \tag{4}
$$

Cross products of basis vectors. Usually, the Cartesian frame of reference is characterized by the unit vectors $\hat{\mathrm{i}}, \hat{\mathrm{j}}, \hat{\mathrm{k}}$ that fulfil the right-hand rule for the spatial orientation of them. How can we represent a cross products, such as $\hat{i} \times \hat{j} = \hat{k}$, of basis vectors with bra and ket? If we solve this problem, since any vector can be represented as a linear combination of the basis vectors, we are able of writing the cross product of any two vectors.

Let us try to write $\hat{k} = \hat{i} \times \hat{j}$. If we use the Dirac notation, it could be: $|e_3\rangle = |e_1\rangle \times |e_2\rangle$.

Let us consider operator T, given by the following permutation matrix:

$$
T = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \tag{5}
$$

We can easily see that we have the following relations:

$$
\begin{aligned}
&|e_2\rangle = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \mathrm{T}|e_1\rangle \quad ; \quad |e_3\rangle = \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \mathrm{T}|e_2\rangle \\
&|e_1\rangle = \begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \mathrm{T}|e_3\rangle
\end{aligned} \tag{6}
$$

Therefore:

(7) $\quad |e_3\rangle = |e_1\rangle \times |e_2\rangle = \mathrm{T\,T}\,|e_1\rangle \;;\quad |e_1\rangle = |e_2\rangle \times |e_3\rangle = \mathrm{T\,T}\,|e_2\rangle \;;\quad |e_2\rangle = |e_3\rangle \times |e_1\rangle = \mathrm{T\,T}\,|e_3\rangle$

However, we need also products such as $-|e_3\rangle = |e_2\rangle \times |e_1\rangle$. A solution to have them is simply to give:

(8) $\quad -|e_3\rangle = |e_2\rangle \times |e_1\rangle = -\mathrm{I\,T\,T}\,|e_2\rangle$

In (8), I is the identity operation.
To calculate a cross product of two vectors, we have also to add conditions $|e_i\rangle \times |e_i\rangle = 0$. And then, the cross product of two vectors, which is usually defined as:

(9) $\quad \left(|a\rangle \times |b\rangle\right)_i = \varepsilon_{ijk}\left(\sum_{j,k} a_j b_k\right)$ (ε_{ijk} is the Levi-Civita symbol),

can be rendered with T operator in the following expression:

$$
\begin{aligned}
&|a\rangle \times |b\rangle = (a_1|e_1\rangle + a_2|e_2\rangle + a_3|e_3\rangle) \times (b_1|e_1\rangle + b_2|e_2\rangle + b_3|e_3\rangle) \\
&= a_2 b_1 |e_2\rangle \times |e_1\rangle + a_3 b_1 |e_3\rangle \times |e_1\rangle + a_1 b_2 |e_1\rangle \times |e_2\rangle + a_3 b_2 |e_3\rangle \times |e_2\rangle \\
&+ a_1 b_3 |e_1\rangle \times |e_3\rangle + a_2 b_3 |e_2\rangle \times |e_3\rangle \\
&= -a_2 b_1 |e_1\rangle \times |e_2\rangle + a_3 b_1 |e_3\rangle \times |e_1\rangle + a_1 b_2 |e_1\rangle \times |e_2\rangle - a_3 b_2 |e_2\rangle \times |e_3\rangle \\
&- a_1 b_3 |e_3\rangle \times |e_1\rangle + a_2 b_3 |e_2\rangle \times |e_3\rangle \\
&= (a_1 b_2 - a_2 b_1)\,\mathrm{T\,T}|e_1\rangle + (-a_1 b_3 + a_3 b_1)\,\mathrm{T\,T}|e_3\rangle + (a_2 b_3 - a_3 b_2)\,\mathrm{T\,T}|e_2\rangle
\end{aligned}
\tag{10}
$$

In (10), it could be questionable the fact that we consider, for instance, $a_i|e_i\rangle \times b_j|e_j\rangle = a_i b_j |e_i\rangle \times |e_j\rangle$, and that we imposed conditions $|e_i\rangle \times |e_i\rangle = 0$.

Then, let us refine our approach, involving, besides the permutation T, also the projection operator. This refined approach will give us an expression of the cross product with a more compact form, which is also self-consistent.

Projections and cross product. Let us write $|e_1\rangle\langle e_1|$ and use it to work on a vector:

(11) $\quad |e_1\rangle\langle e_1|a\rangle = a_1|e_1\rangle$

It means that $|e_1\rangle\langle e_1|$ is an operator which is projecting vector $|a\rangle$ on the 1-axis. The same happens for the other two vectors of the basis, and therefore:

(12) $\quad \left(\sum_i |e_i\rangle\langle e_i|\right)|a\rangle = \left(|e_1\rangle\langle e_1| + |e_2\rangle\langle e_2| + |e_3\rangle\langle e_3|\right)|a\rangle = a_1|e_1\rangle + a_2|e_2\rangle + a_3|e_3\rangle = \mathrm{I}|a\rangle$

This is the identity operator. This operator can be used in other operations such as the cross product. And in fact, let us use it with operator T.

Let us consider the following calculus:

$$\sum_{i,j} \mathrm{T}\left|e_j\right\rangle\left\langle b\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|a\right\rangle = a_1 b_2\left|e_3\right\rangle + a_2 b_3\left|e_1\right\rangle + a_3 b_1\left|e_2\right\rangle \tag{13}$$

And also:

$$-\sum_{i,j} \mathrm{T}\left|e_j\right\rangle\left\langle a\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|b\right\rangle = -b_1 a_2\left|e_3\right\rangle - b_2 a_3\left|e_1\right\rangle - b_3 a_1\left|e_2\right\rangle \tag{14}$$

Adding these two expressions, the cross product of two vectors is easily obtained from ket and bra vectors, in the following form:

$$\left|a\right\rangle\times\left|b\right\rangle = \sum_{i,j} \mathrm{T}\left|e_j\right\rangle\left\langle b\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|a\right\rangle - \sum_{i,j} \mathrm{T}\left|e_j\right\rangle\left\langle a\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|b\right\rangle \tag{15}$$

Using Einstein notation:

$$\left|a\right\rangle\times\left|b\right\rangle = \mathrm{T}\left|e_j\right\rangle\left\langle b\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|a\right\rangle - \mathrm{T}\left|e_j\right\rangle\left\langle a\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|b\right\rangle \tag{16}$$

It is also evident that:

$$\left|a\right\rangle\times\left|a\right\rangle = \mathrm{T}\left|e_j\right\rangle\left\langle a\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|a\right\rangle - \mathrm{T}\left|e_j\right\rangle\left\langle a\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|a\right\rangle = 0 \tag{17}$$

Therefore, this expression contains conditions $\left|e_i\right\rangle\times\left|e_i\right\rangle = 0$. Moreover, it is also given that:

$$\left|b\right\rangle\times\left|a\right\rangle = \mathrm{T}\left|e_j\right\rangle\left\langle a\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|b\right\rangle - \mathrm{T}\left|e_j\right\rangle\left\langle b\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|a\right\rangle = -\left|a\right\rangle\times\left|b\right\rangle \tag{18}$$

So we have, for instance:

$$\left|e_1\right\rangle\times\left|e_2\right\rangle = \mathrm{T}\left|e_j\right\rangle\left\langle e_2\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|e_1\right\rangle - \mathrm{T}\left|e_j\right\rangle\left\langle e_1\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|e_2\right\rangle = \left|e_3\right\rangle \tag{19}$$

$$\left|e_2\right\rangle\times\left|e_1\right\rangle = \mathrm{T}\left|e_j\right\rangle\left\langle e_1\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|e_2\right\rangle - \mathrm{T}\left|e_j\right\rangle\left\langle e_2\middle|e_j\right\rangle\left\langle e_j\middle|\mathrm{T}\middle|e_i\right\rangle\left\langle e_i\middle|e_1\right\rangle = -\left|e_3\right\rangle \tag{20}$$

In this manner, defining the cross product as in (15) or (16), we have easily the properties of the cross vector in ket-bra notation, given in a self-consistent manner.

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