# QUANTUM MECHANICS
# Lecture 21

## Dirac notation
## Schrödinger equation in 3D

Enrico Iacopini

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D. J. Griffiths: paragraph 3.6, 4.1

# Dirac notation

In $QM$, very often, we have to evaluate **scalar products** $<\mathbf{u}|\mathbf{v}>$ between vectors of the Hilbert space, representing the physical states.

1. Dirac proposed to chop the bracket notation for the scalar product into two pieces:
   - the ***bra*** $<u|$;
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1. **But what represents the *bra* $< u|$ ?**
2. To answer, let us see what it does . . .
   It associates, in a linear way, a complex number to any vector of $\mathcal{H}$:

$$< u| \left(\alpha|v > + \beta|w >\right) = \alpha < u|v > + \beta < u|w >$$

3. It describes, therefore, a ***linear function* defined from** $\mathcal{H}$ to the complex field $C$.
4. The set of these linear functions forms a vector space.

$$\left(\alpha < u| + \beta < v|\right)|w > = \alpha < u|w > + \beta < v|w >$$

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1. So, the bra $< u|$ is an element of the dual space of $\mathcal{H}$ (space that the mathematicians have shown to be isomorphic to $\mathcal{H}$ itself).

2. According to this notation, for instance, the scalar product $< \mathbf{u}|\hat{Q}\mathbf{v} >$ becomes equal to the bra $< u|$ applied to the vector $\hat{Q}\mathbf{v}$.
   In other words, we have

$$< \mathbf{u}|\hat{Q}\mathbf{v} > \equiv < u|\hat{Q}|v >$$

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# Dirac notation

1. Let $|u>$ be a normalized vector and let us define the following operator
$$\hat{P} = |u><u|$$
(be careful: this has nothing to do with $<u|u>$ which is a non-negative number !).

2. When we apply the operator $\hat{P}$ to any vector $|v>$ of the Hilbert space, we obtain
$$\hat{P}|v> \equiv |u><u|v> = <u|v> \ |u>$$
which is the component of the vector $|v>$ *aligned* with the vector $|u>$.

3. The operator $\hat{P}$ is, in fact, the **projection operator** onto the one dimensional subspace of $\mathcal{H}$, generated by the vector $|u>$.

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Let $\{|e_n >\}$ be a numerable, orthonormal basis of $\mathcal{H}$, made, for instance, by the eigenvectors of some observable $\hat{Q}$, although this it is not essential: by hypothesis

$$< e_n|e_m >= \delta_{nm}$$

It turns out that the operator

$$\sum_n |e_n >< e_n|$$

is a ***representation of the identity***: we call it a **decomposition of the operator I**.

# Dirac notation



In fact, if $|u>$ is a generic vector, then we already know that

$$|u>=\sum_n c_n\,|e_n> \quad where \quad c_n=<e_n|u>$$

In other words

$$|u>=\sum_n <e_n|u>\;|e_n>\equiv$$

$$\equiv\sum_n |e_n><e_n|u>$$

$$\Leftrightarrow \quad \sum_n |e_n><e_n| = I$$

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1. Similarly, if $\{|e(s)>\}$ is a Dirac orthonormalized "continuous" basis, such that
$$< e(s)|e(t) >= \delta(s-t)$$
then
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1. Clearly, every orthonormal basis $\{|e(s)>\}$ defines its characteristic decomposition of the identity

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For instance, if we use the basis made by the normalized generalized eigenvectors
$|x>\equiv|e(x)>$
of the position operator $\hat{x}$, then the generic vector of the Hilbert space $|\psi>$ will be represented as

$$|\psi>=\int dx\,|x><x|\psi>=\int dx\,\psi(x)\,|x>$$

where $\psi(x)\equiv<x|\psi>$ is the usual "old" wave function which, according to the generalized statistical interpretation, is such that $|\psi(x)|^2$ gives the p.d.f. to measure, on the state $|\psi>$, the particle position between $x$ and $x+dx$.

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1. But if we use, instead, the generalized momentum eigenvectors $|p>\equiv|e(p)>$, then we can represent the same vector as

$$|\psi>=\int dp\,|p><p|\psi>=\int dp\,\phi(p)\,|p>$$

where $\phi(p)\equiv<p|\psi>$ is now the momentum wave-function and $|\phi(p)|^2$ gives the p.d.f. to measure, on the state $|\psi>$, a momentum between $p$ and $p+dp$.

2. With the two different decompositions of the identity we have obtained **two different wave functions describing the same vector**, one in the coordinate space and the other in the momentum space, respectively.

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# QM in 3D

1. The generalization of the Schrödinger equation in three dimensions is quite straightforward.
2. The time-dependent Schrödinger equation says

$$i\hbar \frac{\partial \Psi}{\partial t} = \hat{H}\,\Psi$$

where, as alredy well known, the hamiltonian operator is obtained from the classical total energy

$$H = \frac{p^2}{2m} + V(\vec{r})$$

which, in three dimensions, becomes

$$\frac{1}{2m}(p_x^2 + p_y^2 + p_z^2) + V(\vec{r})$$

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# QM in 3D



Using the usual prescription

$$p_x \to -i\hbar\frac{\partial}{\partial x}; \quad p_y \to -i\hbar\frac{\partial}{\partial y}; \quad p_z \to -i\hbar\frac{\partial}{\partial z}$$

we obtain

$$i\hbar\frac{\partial\Psi}{\partial t} = -\frac{\hbar^2}{2m}\nabla^2\Psi + V(\vec{r})\,\Psi$$

where $\nabla^2$ is the **laplacian operator**

$$\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

and the meaning of the w.f. is now that the probability of finding the particle in the volume $dv = dx\,dy\,dz$ is $|\Psi(\vec{r}, t)|^2$, once the wave function $\Psi$ has been normalized to the unity in the whole space.

# QM in 3D



1. In order to give the wave-function definition that we have done previously, we have implicitly assumed that the three position coordinates can be measured simultaneously, or, in other words, that the operators $\hat{x}$, $\hat{y}$, $\hat{z}$ are compatible.

2. This is clearly true, because they are represented by the multiplication for $x$, $y$ and $z$, respectively, and the multiplication of real numbers **do** commute. So

$$[\hat{x}, \hat{y}] = [\hat{x}, \hat{z}] = [\hat{y}, \hat{z}] = 0$$

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1. Also the three momentum components represented by the operators $-i\hbar\partial_x$, $-i\hbar\partial_y$, $-i\hbar\partial_z$ **do commute** and, therefore, they describe compatible observables.

2. In fact, a particle can be in a simultaneous eigenvector (although of generalized type ...) of all the three momentum components.

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# QM in 3D



Concerning the compatiblity of position and momentum components, from the definition of the respective operators, it turns out, instead, that **homologous components are incompatible** and we have

$$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$$

whereas non-homologous components are indeed compatible

$$[x, p_y] = [x, p_z] = 0$$
$$[y, p_x] = [y, p_z] = 0$$
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# QM in 3D



1. But let us come back to the **Schrödinger equation in** $3D$.

2. If the energy potential $V = V(\vec{r})$ is time independent, similarly to the one-dimensional case, there will be a **complete set of stationary states**

$$\mathbf{\Psi}(\vec{r},t) = \psi(\vec{r})\, e^{-iEt/\hbar}$$

where the functions $\psi(\vec{r})$ satisfy the time independent Schrödinger equation, that now reads

$$-\frac{\hbar^2}{2m}\nabla^2\psi(\vec{r}) + V(\vec{r})\,\psi(\vec{r}) = E\,\psi(\vec{r})$$

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and the general solution of the time-dependent Schrödinger equation will be

$$\boldsymbol{\Psi}(\vec{r},t) = \sum_n c_n \, \Psi_n(\vec{r},t) = \sum_n c_n \, \psi_n(\vec{r}) \, e^{-iE_n t/\hbar}$$

where the coefficients $c_n$ are determined in the usual way, from the $\Psi(\vec{r},0)$

$$c_n = \int d^3r \;\; \psi_n^*(\vec{r}) \;\; \boldsymbol{\Psi}(\vec{r},0)$$

where the $\psi_n(\vec{r})$ are the solutions of the time independent Schrödinger equation, or, in other words, the **eigenfunctions of the Hamiltonian operator.**