A very simple proof of the Bloch's Theorem

Marcello Colozzo

Abstract

We prove the famous Bloch's Theorem using the symmetry for discrete translations in Dirac notation.

1 Unitary transformations. The Translations group

Let S_q be a quantum system consisting of a nonrelativistic particle of mass m. In the presence of a conservative force field of potential energy $V(x)$, the Hamiltonian operator of the system is

$$\hat{H} = \frac{\hat{\mathbf{p}}^2}{2m} + V(\hat{\mathbf{x}}) \tag{1}$$

where $\hat{\mathbf{x}} = (\hat{x}, \hat{y}, \hat{z})$ and $\hat{\mathbf{p}} = (\hat{p}_x, \hat{p}_y, \hat{p}_z)$ are the hermitian operators representing the observable position $\mathbf{x}$ and the observable momentum $\mathbf{p}$ respectively. In Dirac notation [1]-[2], the eigenvalue equation for $\hat{\mathbf{x}}$ is written:

$$\hat{\mathbf{x}} |\mathbf{x}\rangle = \mathbf{x} |\mathbf{x}\rangle \tag{2}$$

The eigenket system $\{|\mathbf{x}\rangle\}$ is a complete orthonormal system in the Hilbert space $\mathcal{H}$ associated with the system:

$$\langle \mathbf{x}|\mathbf{x}'\rangle = \delta^{(3)}(\mathbf{x} - \mathbf{x}'), \qquad \int_{\mathbb{R}^3} d^3x \, |\mathbf{x}\rangle \langle \mathbf{x}| = \hat{1} \tag{3}$$

where $\delta^{(3)}(\mathbf{x} - \mathbf{x}') = \delta(x - x')\,\delta(y - y')\,\delta(z - z')$ us theDirac 3-delta function, while $\hat{1}$ is the identity operator in $\mathcal{H}$.

Assuming $\{|\mathbf{x}\rangle\}$ as the orthonormal basis of $\mathcal{H}$, we have that the representation of the impulse operator in this basis is [2]

$$\langle \mathbf{x}|\hat{\mathbf{p}}|\psi\rangle = -i\hbar \boldsymbol{\nabla} \psi(\mathbf{x}), \quad \forall |\psi\rangle \in \mathcal{H} \tag{4}$$

where $\psi(\mathbf{x}) = \langle \mathbf{x}|\psi\rangle$ i.e. the representation in the base of the ket coordinates $|\psi\rangle$. If $|\psi\rangle$ is the state ket of the particle at a given instant, $\psi(\mathbf{x})$ is the wave function at that instant.

Definition 1 *The* **translation operator** *according to an arbitrary direction* $\mathbf{l}$*, is defined by:*

$$\hat{T}(\mathbf{l}) |\mathbf{x}\rangle = |\mathbf{x} + \mathbf{l}\rangle \tag{5}$$

for any eigenket $|\mathbf{x}\rangle$ *of the position.*

In other words, the operator $\hat{T}(\mathbf{l})$ translates any $|\mathbf{x}\rangle$ into $|\mathbf{x} + \mathbf{l}\rangle$. From the completeness of the system $\{|\mathbf{x}\rangle\}$ it follows that the (5) uniquely defines the aforementioned operator, in the sense that the result of the application of $\hat{T}(\mathbf{l})$ to any ket is well defined $|\psi\rangle$ (expanded into position autoket):

$$|\psi\rangle = \int_{\mathbb{R}^3} d^3x \, |\mathbf{x}\rangle \langle \mathbf{x}|\psi\rangle$$

The square of the ket norm $|\psi\rangle$ is

$$||\psi||^2 = \langle \psi|\psi\rangle = \langle \psi|\hat{1}|\psi\rangle = \left\langle \psi | \int_{\mathbb{R}^3} d^3x \, |\mathbf{x}\rangle \langle \mathbf{x}| \, | \psi \right\rangle = \int_{\mathbb{R}^3} |\psi(\mathbf{x})|^2 \, d^3x$$

Interpreting $|\psi(\mathbf{x})|^2$ as the probability density of finding the particle in the volume element d^3x centered at $\mathbf{x}$, it must be $||\psi||^2 = 1$ or in any case $< +\infty$ and then normalized to 1. It follows that the Hilbert space $\mathcal{H}$ is identified with the functional space $\mathcal{L}^2(\mathbb{R}^3)$ whose elements are the summable square modulus functions in $\mathbb{R}^3$.

It is physically reasonable to require probability conservation with respect to translations (definition 1), so if $|\psi'\rangle$ is the translated ket i.e. $\hat{T}(\mathbf{l})|\psi\rangle = |\psi'\rangle$, it must be

$$\langle\psi'|\psi'\rangle = \langle\psi|\psi\rangle \Longleftrightarrow \left\langle\psi|\hat{T}^\dagger(\mathbf{l})\hat{T}(\mathbf{l})|\psi\right\rangle = \langle\psi|\psi\rangle, \quad \forall|\psi\rangle \in \mathcal{H}$$

i.e. $\hat{T}^\dagger(\mathbf{l})\hat{T}(\mathbf{l}) = \hat{1} \Longleftrightarrow \hat{T}(\mathbf{l})\hat{T}^\dagger(\mathbf{l}) = \hat{1}$ or what is the same, the adjoint $\hat{T}^\dagger(\mathbf{l})$ of $\hat{T}(\mathbf{l})$ coincides with the inverse: $\hat{T}^\dagger(\mathbf{l}) = \hat{T}^{-1}(\mathbf{l})$. It follows that the operator $\hat{T}(\mathbf{l})$ is unitary.

Conclusion 2 *For a nonrelativistic quantum system, a translation is a unit transformation in the appropriate Hilbert space.*

We compose two successive translations:

$$\left(\hat{T}(\mathbf{l})\hat{T}(\mathbf{l}')\right)|\mathbf{x}\rangle = \hat{T}(\mathbf{l})\left(\hat{T}(\mathbf{l}')|\mathbf{x}\rangle\right) = \hat{T}(\mathbf{l})(|\mathbf{x}+\mathbf{l}'\rangle) = |\mathbf{x}+\mathbf{l}'+\mathbf{l}\rangle = \hat{T}(\mathbf{l}'+\mathbf{l}) \tag{6}$$

From the completeness of $\{|\mathbf{x}\rangle\}$ it follows

$$\hat{T}(\mathbf{l}+\mathbf{l}') = \hat{T}(\mathbf{l})\hat{T}(\mathbf{l}'), \quad \forall\mathbf{l},\mathbf{l}' \in \mathbb{R}^3$$

In the set $\mathcal{T} = \left\{\hat{T}(\mathbf{l}) \mid \mathbf{l} \in \mathbb{R}^3\right\}$ we can therefore define a law of internal composition χ:

$$\begin{aligned} &\chi : \mathcal{T} \times \mathcal{T} \longrightarrow \mathcal{T} \\ &\chi : \left(\hat{T}(\mathbf{l}), \hat{T}(\mathbf{l}')\right) \longrightarrow \hat{T}(\mathbf{l})\hat{T}(\mathbf{l}') \end{aligned} \tag{7}$$

which checks the following properties:

1. *Associative property*:
$$\hat{T}(\mathbf{l})\left(\hat{T}(\mathbf{l}')\hat{T}(\mathbf{l}'')\right) = \left(\hat{T}(\mathbf{l})\hat{T}(\mathbf{l}')\right)\hat{T}(\mathbf{l}'')$$

2. *Existence of the neutral element* $\hat{T}(\mathbf{0}) = \hat{1}$:
$$\hat{T}(\mathbf{0})|\psi\rangle = |\psi\rangle, \ \forall|\psi\rangle \in \mathcal{H}$$

3. *Existence of the inverse*:
$$\forall\hat{T}(\mathbf{l}) \in \mathcal{T}, \ \exists\hat{T}^\dagger(\mathbf{l}) \in \mathcal{T} \mid \hat{T}^\dagger(\mathbf{l})\hat{T}(\mathbf{l}) = \hat{T}(\mathbf{0})$$

From these properties it follows that the ordered pair $(\mathcal{T}, \chi)$ or the set $\mathcal{T}$ with the composition law (7), takes on the group structure.

Definition 3 *The group $(\mathcal{T}, \chi)$ is called* **translation group**.

The composition law (7) manifestly verifies the commutative property, so the translation group is abelian.

For an infinitesimal translation $d\mathbf{x}$ the operator (5) ddiffers from the identity operator 1 by a first order term on $d\mathbf{x}$ right:

$$T(d\mathbf{x}) = \hat{1} - i\hat{\mathbf{G}} \cdot d\mathbf{x} \tag{8}$$

where $\hat{\mathbf{G}} = \left(\hat{G}_x, \hat{G}_y, \hat{G}_z\right)$ with $\hat{G}_k$ Hermitian operators.

Definition 4 $\hat{\mathbf{G}}$ *is* **translation generator**.

By analogy with classical mechanics: $\hat{\mathbf{G}} = \varkappa \hat{\mathbf{p}}$ being $\varkappa > 0$ a constant with the dimensions of the reciprocal of an action. Old Quantum Theory says $\varkappa = \hbar^{-1}$, so

$$T(d\mathbf{x}) = \hat{1} - i\frac{\hat{\mathbf{p}}}{\hbar} \cdot d\mathbf{x} \tag{9}$$

For (6) any translation $\hat{T}(\mathbf{l})$ is the result of the composition of N translations $\hat{T}\left(\frac{\mathbf{l}}{N}\right)$ and in the limit for $N \to +\infty$

$$\hat{T}(\mathbf{l}) = \lim_{N \to +\infty} \left(\hat{1} - i\frac{\hat{\mathbf{p}}}{\hbar} \cdot \frac{\mathbf{l}}{N}\right)^N = e^{-\frac{i}{\hbar}\hat{\mathbf{p}} \cdot \mathbf{l}} \tag{10}$$

2 Eigenfunctions of the momentum operator

Without loss of generality we consider the one-dimensional case:

$$\hat{H} = \frac{\hat{p}^2}{2m} + V(\hat{x}) \tag{11}$$

Since $\left[\hat{H}, \hat{p}\right] \neq \hat{0}$ i.e. $\hat{H}$ does not commute with the momentum, it follows that p is not a constant of motion. On the other hand

$$\left[\hat{p}, \hat{T}(l)\right] = \hat{0}, \quad \forall l \in \mathbb{R}$$

so that the operators $\hat{p}$ and $\hat{T}(l)$ have in common a complete orthonormal system of simultaneous eigenkets. Recall that the spectrum of $\hat{p}$ is purely continuous: $\sigma(\hat{p}) \equiv \sigma_c(\hat{p}) = (-\infty, +\infty)$ so the simultaneous eigenfunctions we are looking for are eigenfunctions in the improper sense ($\Longrightarrow \notin \mathcal{L}^2(\mathbb{R})$). We write the respective eigenvalue equations:

$$\begin{cases} \hat{p}\,|p\rangle = p\,|p\rangle \\ \hat{T}(l)\,|p\rangle = \tau(p)\,|p\rangle \end{cases} \tag{12}$$

But $\hat{T}(l) = e^{-\frac{i}{\hbar}\hat{p}l}$ so $\tau(p) = e^{-\frac{i}{\hbar}pl}$, $\forall l \in \mathbb{R}$. In the coordinate representation, the second of (12) is written:

$$\left\langle x|\hat{T}(l)\,|p\right\rangle = e^{-\frac{i}{\hbar}pl} \underbrace{\langle x|p\rangle}_{u_p(x)} \tag{13}$$

where $u_p(x)$ is the eigenfunction of the impulse corresponding to the eigenvalue p. For the above, $u_p(x)$ is also an eigenfunction of $\hat{T}(l)$ with eigenvalue $e^{-\frac{i}{\hbar}pl}$, $\forall l \in \mathbb{R}$. To evaluate the first member of (13) we observe that

$$\left\langle x|\hat{T}(l)\,|p\right\rangle = \left(\langle x|\,\hat{T}(l)\right) \cdot |p\rangle$$

$$\langle x|\,\hat{T}(l) \overset{\text{DC}}{\leftrightarrow} \hat{T}^\dagger(l)\,|x\rangle = |x - l\rangle$$

where DC=dual correspondence. It follows

$$\left\langle x|\hat{T}\left(l\right)|p\right\rangle = \left\langle x-l|p\right\rangle = u_p\left(x-l\right)$$

so (**??**) is written:

$$u_p\left(x-l\right) = e^{-\frac{i}{\hbar}pl}u_p\left(x\right), \quad \forall l \in \mathbb{R}$$

equivalent to

$$u_p\left(x\right) = e^{-\frac{i}{\hbar}pl}u_p\left(x+l\right), \quad \forall l \in \mathbb{R} \tag{14}$$

which is a functional equation in $u_p\left(x\right)$. Since $u_p\left(x\right)$ is an eigenfunction in the improper sense, we attempt the solution:

$$u_p\left(x\right) = \varphi_p\left(x\right)e^{\frac{i}{\hbar}px} \tag{15}$$

where $\varphi_p\left(x\right)$ it is a real function to be determined. By inserting the (15) into (14):

$$\varphi_p\left(x\right) \equiv \varphi_p\left(x+l\right), \quad \forall l \in \mathbb{R}$$

cioè $\varphi_p\left(x\right)$ is a periodic function of arbitrary period, i.e. a constant A. It follows that the eigenfunctions of the impulse are

$$u_p\left(x\right) = Ae^{\frac{i}{\hbar}px}$$

The real constant A is obtained from the normalization of the eigenfunctions $u_p\left(x\right)$. Precisely, reasoning in terms of autokets:

$$\begin{aligned} \left\langle p|p'\right\rangle = \delta\left(p-p'\right) &\Longleftrightarrow \left\langle p|\hat{1}|p'\right\rangle = \delta\left(p-p'\right) \\ \left\langle p\right|\int_{-\infty}^{+\infty}dx\left|x\right\rangle\left\langle x\right|\left|p'\right\rangle = \delta\left(p-p'\right) &\Longleftrightarrow \int_{-\infty}^{+\infty}u_p^*\left(x\right)u_{p'}\left(x\right)dx = \delta\left(p-p'\right) \\ A^2\int_{-\infty}^{+\infty}e^{-\frac{i}{\hbar}\left(p-p'\right)x}dx = \delta\left(p-p'\right) \end{aligned} \tag{16}$$

But

$$\delta\left(\alpha\right) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{-i\alpha x}dx$$

i.e. the Fourier transform of the function $f(x) = 1$, so from the last of the (16) we obtain= $\pm\left(2\pi\hbar\right)^{-1/2}$. Assuming $A > 0$ we finally obtain the eigenfunctions of the impulse:

$$u_p\left(x\right) = \frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px} \tag{17}$$

Ne concludiamo che le autofunzioni dell'impulso sono onde piane di numero d'onde $k = \frac{p}{\hbar}$. Nel caso speciale della particella libera le (17) sono anche autofunzioni dell'energia con autovalore $E = \frac{p^2}{2m}$, per cui lo spettro dell'hamiltoniano della particella libera è puramente continuo: $\sigma\left(\hat{H}\right) = [0, +\infty)$ ed è degenere con ordine di degenerazione 2 giacché agli autokets $\left|p\right\rangle$ e $\left|-p\right\rangle$ corrisponde lo stesso autovalore dell'energia.

3 Bloch Theorem

Let us consider the case of a period periodic potential a:

$$V(x+na) \equiv V(x), \quad \forall n \in \mathbb{Z} \tag{18}$$

It follows

$$\left[\hat{H}, \hat{T}(a)\right] = \hat{0}$$

so $\hat{H}$ and $\hat{T}(a)$ they have in common a complete orthonormal system of simultaneous eigenkets. We write the respective eigenvalue equations:

$$\begin{cases} \hat{H}|k\rangle = E(k)|k\rangle \\ \hat{T}(a)|k\rangle = \tau(k)|k\rangle \end{cases} \tag{19}$$

where $k \in \mathbb{R}$. The unitarity of $\hat{T}(a)$ suggests $\tau(k) = e^{-ika}$. In the coordinate representation, the second of (19) is written:

$$\left\langle x|\hat{T}(a)|k\right\rangle = e^{-ika}\underbrace{\langle x|k\rangle}_{u_k(x)} \tag{20}$$

being $u_k(x)$ the energy eigenfunction corresponding to the eigenvalue $E(k)$. Along the lines of the procedure in the previous section, we arrive at the functional equation

$$u_k(x) = e^{-ika}u_k(x+a) \tag{21}$$

Let's try the solution:

$$u_k(x) = \varphi_k(x)e^{ikx} \tag{22}$$

here $\varphi_k(x)$ is a real function to be determined. Inserting the (22) into (21):

$$\varphi_k(x) \equiv \varphi_k(x+a)$$

i.e. $\varphi_k(x)$ it is a periodic function of period a, i.e. with the same period as the potential $V(x)$. It follows that the energy eigenfunctions of a particle in a periodic potential are amplitude-modulated plane waves. The modulation envelope is a periodic function with the same period as the potential. This conclusion is the statement of *Bloch Theorem*. The real number k is the wave number of the aforementioned plane wave, and unlike the case of the free particle it is not identified with the impulse i.e. $k \neq p/\hbar$.

For k varying from $-\infty$ to $+\infty$, the eigenvalues $e^{-ika}$of the translation operator $\hat{T}(a)$ repeat with periodicity $2\pi/a$ since $e^{-ika} = \cos(ka) + i\sin(ka)$. It follows that for the values of k and therefore of the corresponding eigenfunctions u_k, is sufficient to refer to a single interval $\left[-\frac{\pi}{a} + \frac{2n\pi}{a}, \frac{\pi}{a} + \frac{2n\pi}{a}\right]$, $\forall n \in \mathbb{Z}$. For a question of symmetry it is preferable to take the interval $\left[-\frac{\pi}{a}, \frac{\pi}{a}\right]$ known as the *first Brillouin zone*.

References

[1] Dirac P.AM., I principi della meccanica quantistica.

[2] Sakurai J.J. Modern Quantum Mechanics.