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DENSITY OF PROBABILITY OF PRESENCE OF ELEMENTARY PARTICLES

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1. Introduction: nonrelativistic case

In the initial, nonrelativistic theory of quantum mechanics it is assumed that the only information we have about the state of a particle, at a given time, is its wave function Ψ , a complex function on R^3 or a complex function of three coordinates x, y, z . This function is assumed to be square integrable, $\Psi \in L^2$, and moreover one assumes

$$(1.1) \quad \iiint_{R^3} |\Psi(x, y, z)|^2 dx dy dz = 1.$$

Consider an observable physical quantity, taking its values in a set X . For example, the position of the particle is a quantity with values in $X = R^3$ and so is the velocity. The energy has values in $X = R$, and so on. In classical mechanics, a measurement of such a quantity is supposed to be obtainable with arbitrary accuracy, and, for a given state, the quantity has a definite value x in X . In quantum mechanics, this unlimited precision disappears. If we make a measurement of the quantity, for a particle having the wave function Ψ , we have only a probability law P_Ψ , depending on Ψ , that is, a positive measure on X , of total mass 1. Thus, if A is a subset of X , assumed to be measurable (P_Ψ), the probability that the measurement will give a result in $A \subset X$ is $P_\Psi(A)$. It is usually assumed that this probability law P_Ψ on X must be given by a spectral decomposition of the Hilbert space L^2 , with respect to X . Such a spectral decomposition is defined as follows. It is a map $P:A \rightarrow P(A) = L_A^2$, where A runs over a Borel field of subsets of X , and L_A^2 is a closed subspace of L^2 , with the following properties.

(a) $L_\phi^2 = \{0\}$, where $\phi =$ empty set of X , $0 =$ origin of the vector space L^2 ; $L_X^2 = L^2$.

(b) If A and B are disjoint subsets of X , L_A^2 and L_B^2 are orthogonal in L^2 .

(c) If A is the union of a finite or denumerable family of disjoint subsets A_n , then L_A^2 is the closure of the subspace of L^2 spanned by the $L_{A_n}^2$.

Thus the probability law P_Ψ of the physical quantity under consideration must be given by

$$(1.2) \quad P_{\Psi}(A) = \|\Psi_A\|^2 = \iiint_{R^3} |\Psi_A(x, y, z)|^2 dx dy dz,$$

where Ψ_A is the orthogonal projection of $\Psi \in L^2$ on the subspace $P(A) = L_A^2$ of L^2 . Axiom (a) ensures that $P_{\Psi}(\phi) = 0$, $P_{\Psi}(X) = 1$, and (b) and (c) ensure, according to Pythagoras' theorem, that P_{Ψ} is a completely additive set function; it is therefore, as desired, a probability law on X .

In this model the state of the particle is given by the wave function Ψ , the observable physical quantity by the spectral decomposition P , and thus a measurement of the quantity for the state of the particle is governed by the probability law P_{Ψ} on X , given by (1.2). There is in $L^2(R^3)$ a trivial spectral decomposition, that for which L_A^2 is the subspace of those Ψ which are zero outside A . It is regarded as the spectral decomposition associated with the observable: "position of the particle in R^3 ." Therefore, we have, in a measurement, the following probability for the particle to be found in the subset A of R^3

$$(1.3) \quad P_{\Psi}(A) = \iiint_A |\Psi(x, y, z)|^2 dx dy dz.$$

For this reason, $|\Psi|^2$ is the density of probability of presence. If now we look for the spectral decomposition corresponding to the first coordinate x of the particle, taking its values in R , it must be that for which, when $B \subset R$, the probability for a measurement of x to give a result in B is

$$(1.4) \quad \iiint_{x \in B} |\Psi(x, y, z)|^2 dx dy dz.$$

This spectral decomposition is also the spectral decomposition associated with the self-adjoint operator on L^2 "multiplication by x ." Multiplication by x is also said to be the operator associated with the measurement of x .

If now we consider the evolution in time of the given particle, we shall have, at every instant t , a wave function Ψ_t , and thus a function of time having values in L^2 . It will also be a function Ψ of the four variables x, y, z, t , defining for every t a function Ψ_t of the three variables x, y, z . The usual rules of quantum mechanics say that Ψ must satisfy some Schrödinger equation such as

$$(1.5) \quad i \hbar \frac{\partial \Psi}{\partial t} = H_t \Psi_t,$$

where, for every t , the H_t is a self-adjoint operator on L^2 . This self-adjointness ensures, according to known properties of Hilbert spaces, that any solution of (1.5) keeps the same norm in L^2 for every t ; if, for $t = 0$, it has the norm 1, which is required by (1.1), this equality remains valid for every t , and the solution defines a valid wave function for every t , and finally a valid motion of the particle. The Hamiltonian H , or the function $t \rightarrow H_t$, depends on the mechanical conditions under consideration.

2. Relativistic case

In special relativity no distinction is made between the three space variables x, y, z and the time variable t . The universe is a space E_4 , a four-dimensional affine space, having an associated vector space \vec{E}_4 . We note that E_4 is not a vector space, it has no origin, and there is no sum of any two points; \vec{E}_4 is the space of vectors of E_4 . If a and b are two points of E_4 , then $\overrightarrow{b-a}$ is a vector, belonging to \vec{E}_4 . On E_4 is given a quadratic form, with signature (3.1) measuring the "universe lengths." A physical coordinate system is an orthonormal basis of E_4 , given by an origin of E_4 and four vectors of \vec{E}_4 . If $x_1, x_2, x_3, x_4 = ct$ are called the corresponding coordinates of an event (an event is a point of E_4), the observer sees x_1, x_2, x_3 as its space coordinates and t as its time. A sense of time and an orientation of \vec{E}_4 are also given.

The complete motion of a particle will be a wave function Ψ , a complex function on E_4 . For a physical coordinate system Ψ becomes a function of four variables x_1, x_2, x_3, t , and we are led back to the situation of section 1.

We shall consider that a given particle in given mechanical conditions is characterized by all its possible motions. We may assume that all these possible motions will be all the elements of norm 1 in a Hilbert space \mathcal{H} of functions on E_4 . For instance, in the nonrelativistic case, for a particle characterized by the Hamiltonian H , the Hilbert space \mathcal{H} was formed by all the functions Ψ of four variables x, y, z, t satisfying (1.5) and belonging to $L^2_{x,y,z}$ for every t . The norm in \mathcal{H} was given by

$$(2.1) \quad \|\Psi\|_{\mathcal{H}}^2 = \iiint_{E^3} |\Psi(x, y, z, t)|^2 dx dy dz,$$

the result being independent of t because of the self-adjointness of H_t . We can certainly not have the same kind of results in the relativistic case, because it is not Lorentz invariant.

It is an uninteresting restriction to force Ψ to be a function; we shall only assume Ψ to be a distribution on E_4 , a wave distribution. Remember that a distribution Ψ is a continuous linear form on the space $\mathcal{D}(E_4)$ of the infinitely differentiable functions on E_4 , with compact support. The value of Ψ on $\varphi \in \mathcal{D}$ will be denoted by $\Psi(\varphi)$ or $\langle \Psi, \varphi \rangle$. \mathcal{H} will be a subspace of the space $\mathcal{D}'(E_4)$ of the distributions on E_4 . \mathcal{H} will also have a given structure as a Hilbert space, and we shall assume that the norm in \mathcal{H} is such that convergence in \mathcal{H} implies convergence in the sense of distributions. There are infinitely many choices of \mathcal{H} , each of which gives a possible particle in some well-defined physical situation, and all the $\Psi \in \mathcal{H}$, with norm 1 in \mathcal{H} , give all the possible motions of such a particle in the situation considered. We are only interested in spaces $\mathcal{H} \neq \{0\}$ since we have to deal with elements of \mathcal{H} of norm 1.

3. Free scalar elementary particle

For a detailed proof of the formulas given here, such as (3.3) and (4.5), see Schwartz [1].

If the particle is free (no external fields), it has to be Lorentz universal, or Lorentz invariant, in the sense that a Lorentz transformation on a possible motion Ψ must give a new possible motion.

Thus we shall assume that, for any element σ of the Lorentz group and any Ψ of \mathcal{H} , the transformed distribution $\sigma\Psi$ also belongs to \mathcal{H} , and has the same norm in \mathcal{H} , that is,

$$(3.1) \quad \|\sigma\Psi\|_{\mathcal{H}} = \|\Psi\|_{\mathcal{H}}.$$

Note that the transformed distribution $\sigma\Psi$ is defined, for any function $\varphi \in \mathcal{D}$ which is infinitely differentiable with compact support, by

$$(3.2) \quad \sigma\Psi(\varphi) = \Psi(\sigma^{-1}\varphi) = \Psi[\varphi(\sigma x)].$$

Therefore, σ is a unitary operator on the Hilbert space \mathcal{H} , and the Lorentz group G has here a unitary representation in \mathcal{H} . We shall define as a *free elementary particle* a free particle (thus Lorentz invariant) for which \mathcal{H} is *minimal*, in the sense that no Lorentz invariant Hilbert space $\mathcal{H}' \neq \{0\}$ contained in \mathcal{H} exists except $\mathcal{H}' = \mathcal{H}$ with a proportional norm. Therefore the unitary representation of the Lorentz group G is simply an irreducible unitary representation.

What we call here the Lorentz group is the *proper inhomogeneous Lorentz group*, that is, the group of all the affine operators of E_4 onto itself, preserving the given quadratic form, on \vec{E}_4 , the orientation, and the sense of time. The word *inhomogeneous* simply means that we consider affine operators of E_4 (for example, translations), and the word *proper* means that we restrict ourselves to operators preserving orientation (determinant +1) and sense of time.

The complete list of all these Hilbert spaces $\mathcal{H} \subset \mathcal{D}'(E_4)$, Lorentz invariant and minimal, may be obtained by different techniques, all using Fourier transforms. The result is the following. Of course, for every \mathcal{H} , one can also take the same with a proportional norm, but we shall not distinguish them.

(a) There is one special \mathcal{H} , one-dimensional, all the elements of which are constant functions Ψ . It may be interpreted as the vacuum.

(b) There is a series of spaces \mathcal{H}_1 , depending on one real parameter. These cannot be physically interpreted.

(c) There is a normal series, physically interpretable. It depends on a parameter $m_0 \geq 0$, which may be interpreted as the rest mass of the particle, and a parameter \pm , which may be interpreted as the electric charge.

In this way the only particles we have found are the π -mesons, with spin 0. We find, in this way, every possible mass m_0 , including 0, which is not true in nature! One can generalize and find all the known elementary particles by looking for finite-dimensional vector-valued elementary particles, for which Ψ is finite-dimensional vector-valued, that is, Ψ has a finite number of scalar components. We find here charged particles only, because we considered complex-valued

wave distributions Ψ . With real-valued distributions neutral particles are obtained.

The Hilbert space $\mathcal{H}_{m_0,+}$ may be described in the following way. Consider the distribution on \vec{E}_4

$$(3.3) \quad 2\pi\Delta_{\frac{2\pi cm_0}{h}}^-(\vec{X}) \\ = \text{p.v.} \left[\frac{\frac{\pi cm_0}{2h} N_1\left(\frac{2\pi cm_0}{h} \sqrt{-\vec{X}^2}\right)}{\sqrt{-\vec{X}^2}} Y(-\vec{X}^2) + \frac{cm_0}{h} K_1\left(\frac{2\pi cm_0}{h} \sqrt{\vec{X}^2}\right) Y(\vec{X}^2) \right] \\ + i \left[\frac{\frac{\pi cm_0}{h} \epsilon(X_0) J_1\left(\frac{2\pi cm_0}{h} \sqrt{-\vec{X}^2}\right)}{\sqrt{-\vec{X}^2}} Y(-\vec{X}^2) - \frac{1}{2} \epsilon(X_0) \delta(\vec{X}^2) \right].$$

In this rather complicated formula N_1 is a Neumann function; K_1 a Kelvin function; J_1 a Bessel function (one could use a shorter formula with Hankel functions); Δ^- is the name of the distribution, one of the "singular functions," that is, distribution of quantum mechanics; p.v. means Cauchy's principal value; \vec{X}^2 means the value on the vector $\vec{X} \in \vec{E}_4$ of the Lorentz quadratic form; Y means the Heaviside function where $Y(\tau) = 1$ for $\tau \geq 0$, and $= 0$ for $\tau < 0$; ϵ is defined as the function $\epsilon(\tau) = \text{sign of } \tau = +1$ for $\tau \geq 0$, and -1 for $\tau < 0$, so that if X_0 is the fourth component of \vec{X} in any coordinate system X_1, X_2, X_3, X_0 then $\epsilon(X_0)$, for elements \vec{X} of the interior or the surface of the light cone, is $+1$ for \vec{X} in the positive light cone, -1 for X in the negative light cone; $\delta(\vec{X}^2)$ is defined from the $\delta(u)$ of one variable u by the change of variables $u = \vec{X}^2$ (we denote here distributions in the physical way, as functions); c is the velocity of light; h is Planck's constant. The parameter is written cm_0/h so that m_0 may be interpreted as rest mass of the particle. Then a distribution Ψ on E_4 belongs to $\mathcal{H}_{m_0,+}$ if and only if the expression

$$(3.4) \quad \frac{|\langle \Psi, \varphi \rangle|}{\langle 2\pi\Delta_{\frac{2\pi cm_0}{h}}^* \varphi, \varphi \rangle^{1/2}}$$

is bounded when φ runs over $\mathfrak{D}(E_4)$. Here $*$ means convolution. In this case the upper bound is the norm of Ψ in $\mathcal{H}_{m_0,+}$.

All the Ψ of $\mathcal{H}_{m_0,+}$ are solutions of the Klein-Gordon equation

$$(3.5) \quad \square \Psi - \frac{4\pi^2 c^2 m_0^2}{h^2} \Psi = 0.$$

This equation is here *not assumed*; we find it as a *consequence* of our hypothesis that \mathcal{H} is Lorentz invariant and minimal.

The Hilbert space $\mathcal{H}_{m,-}$ is obtained in the same way from Δ^+ , which is obtained from Δ^- by changing i into $-i$.

4. Density of probability of presence

From now on we shall write \mathcal{H} instead of $\mathcal{H}_{m,\pm}$. Then every Ψ of \mathcal{H} is a priori a distribution. Actually one can prove it is a function, that is, a locally integrable function defined almost everywhere on E_4 .

Consider a physical coordinate system. Thus Ψ becomes a function of (x, y, z, t) , locally integrable, defined almost everywhere. Therefore, if we fix the time $t = t_0$, then Ψ is *not defined* as a function of x, y, z , since a hyperplane $t = t_0$ is a set of measure zero in E_4 . But one can prove the following result: it is possible to choose Ψ (initially defined only almost everywhere) so that it is a *continuous function* of t , with values in the space L_{loc}^1 of the locally integrable functions of (x, y, z) . Because of the continuity in t , the function Ψ is then determined not merely almost everywhere in E_4 but, *for every t* , almost everywhere with respect to (x, y, z) .

Finally, Ψ defines for $t = t_0$, a well-defined Lebesgue class of functions Ψ_{t_0} , and also a well-defined distribution Ψ_{t_0} on R^3 . Moreover, it can be proved that a knowledge of Ψ_{t_0} , *the cross section of Ψ over the hyperplane $t = t_0$* , completely determines Ψ (quantum-mechanical determinism). The system of the function Ψ_{t_0} is a subspace \mathcal{H}_{t_0} of $\mathcal{D}'(R^3)$, having a one-to-one correspondence $\Psi \rightarrow \Psi_{t_0}$ with \mathcal{H} . Carrying over the Hilbert structure of \mathcal{H} onto \mathcal{H}_{t_0} , we define \mathcal{H}_{t_0} as a Hilbert space contained in $\mathcal{D}'(R^3)$, which may be called the cross section of the Hilbert space \mathcal{H} by $t = t_0$. Now any physical observable quantity at the time t_0 , with values in a set X , must be measured by a spectral decomposition of \mathcal{H}_{t_0} , relative to X . If $A \rightarrow P(A) = (\mathcal{H}_{t_0})_A$ is this spectral decomposition, the probability of finding the value of a measurement of the quantity in A , when the wave function is $\Psi \in \mathcal{H}$, with $\|\Psi\| = 1$, will be

$$(4.1) \quad P_\Psi(A) = \|(\Psi_{t_0})_A\|^2,$$

where $(\Psi_{t_0})_A$ is the orthogonal projection of Ψ_{t_0} on $(\mathcal{H}_{t_0})_A$. Since $\|\Psi_{t_0}\| = \|\Psi\|$, where the Hilbert structure on \mathcal{H}_{t_0} is defined by carrying over that of \mathcal{H} , we have that P_Ψ is, as desired, a probability law on X . We are interested in the measurement of the position of the particle at the time t_0 , whose physical quantity, the position, has values in R^3 . Here the result is essentially different from that of the nonrelativistic case. One cannot postulate that the manifold $(\mathcal{H}_{t_0})_A$ is formed by all the Ψ equal to zero outside A , because, as is seen by studying the scalar product in \mathcal{H}_{t_0} , in this case $(\mathcal{H}_{t_0})_A$ and $(\mathcal{H}_{t_0})_B$ would not be orthogonal subspaces in \mathcal{H}_{t_0} . In other words, $|\Psi_{t_0}|^2$ cannot be the density of probability of presence. In yet other words, the "position operator" in coordinate x_i for $i = 1, 2, 3$, cannot be multiplication by x_i , as it is in the nonrelativistic case, because such an operator is not self-adjoint in the Hilbert space \mathcal{H}_{t_0} . In the physical literature a density of probability of presence for the meson is often considered

which is not even positive! What should be the spectral decomposition relative to R^3 , corresponding to the measurement of position at the time t_0 ?

It is natural to ask whether there exists a one-to-one norm preserving, linear transformation $\Psi_{t_0} \rightarrow \oplus$, from \mathcal{H}_{t_0} onto $L^2(R^3)$, that is, covariant with the inhomogeneous proper orthogonal group Γ of R^3 . That is, Ψ_{t_0} must be such that

$$(4.2) \quad \Psi_{t_0} \rightarrow \oplus \text{ implies } \tau\Psi_{t_0} \rightarrow \tau\oplus$$

whenever τ belongs to Γ . Note that Γ is the group of affine operators of R^3 , preserving lengths and the orientation. Here inhomogeneous means that it contains the translations, proper that it preserves the orientation.

In this case the trivial spectral decomposition of $L^2(R^3)$ will define a spectral decomposition of \mathcal{H}_{t_0} and $(\mathcal{H}_{t_0})_A$ will be the set of \mathcal{H}_{t_0} corresponding to the set of L^2 formed by all the \oplus equal to zero outside A . Such a spectral decomposition will be acceptable as a spectral decomposition for the measurement of the position of the particle at the time t_0 , and $|\oplus|^2$ will be acceptable as a possible density of probability of presence at the time t_0 , for the particle having the wave function Ψ or the instantaneous t_0 -wave function Ψ_{t_0} .

In fact, such a map $\Psi_{t_0} \rightarrow \oplus$ can be found. It is given as follows. If Δ is a Laplacian on R^3 , by Fourier transform \mathcal{F} there is classically defined an operator

$$(4.3) \quad \sqrt{2} \left(-\frac{\Delta}{4\pi^2} + \frac{c^2 m_0^2}{h^2} \right)^{1/4}.$$

Thus, one has

$$(4.4) \quad \oplus = \sqrt{2} \left(-\frac{\Delta}{4\pi^2} + \frac{c^2 m_0^2}{h^2} \right)^{1/4} \Psi$$

or

$$(4.5) \quad \mathcal{F}\oplus = \sqrt{2} \left(\rho^2 + \frac{c^2 m_0^2}{h^2} \right)^{1/4} \mathcal{F}\Psi_{t_0},$$

where ρ is the distance from the origin.

Actually, it may be written as a convolution,

$$(4.6) \quad \oplus = \Psi_{t_0} * \frac{\left[2^6 \left(\frac{cm_0}{h} \right)^7 \pi^{-1} \right]^{1/4}}{\Gamma\left(-\frac{1}{4}\right)} \rho^{-7/4} K_{7/4} \left(2\pi \frac{cm_0}{h} \rho \right),$$

where K is a Kelvin function, decreasing, classically, exponentially at infinity. As we observe, \oplus is obtained from Ψ_{t_0} by a convolution, which is a *nonlocal* operation. Therefore, knowledge of Ψ_{t_0} in an open set Ω of R^3 does not allow us to know \oplus in Ω ; for this, a complete knowledge of Ψ_{t_0} is necessary.

There are infinitely many other isometries of \mathcal{H}_{t_0} onto $L^2(R^3)$ having the same property of covariance with the orthogonal group. Namely, one can take the previous one followed by any unitary transformation of L^2 onto itself, commuting with the inhomogeneous proper orthogonal group of R^3 . Such a unitary trans-

formation $\oplus' \rightarrow \oplus''$ is given, using the Fourier transform \mathfrak{F} , by the formula

$$(4.7) \quad \mathfrak{F}\oplus'' = (\mathfrak{F}\oplus')e^{if(\rho)},$$

where $f(\rho)$ is an arbitrary measurable function of the distance ρ from the origin of R^3 .

Therefore, all the possible operations $\Psi_{\iota_0} \rightarrow \oplus$ are of the form

$$(4.8) \quad \oplus = \mathcal{L} * \Psi_{\iota_0},$$

where

$$(4.9) \quad \mathfrak{F}\mathcal{L} = \sqrt{2} \left(\rho^2 + \frac{c^2 m_0^2}{h^2} \right)^{1/4} e^{if(\rho)}.$$

Since the coefficient of $e^{if(\rho)}$ is real and nonnegative, while $e^{if(\rho)}$ itself is never real and nonnegative unless $f(\rho) = 2k\pi$, it can be seen that there is one and only one transformation of the form (4.9), where \mathcal{L} is a distribution of positive type, having a positive measure as Fourier transform. But I do not see any physical reason for \mathcal{L} to be of positive type.

I should rather think that in the correspondence between the physical particle and the mathematical representation, there remains some arbitrariness. One example is the choice of \mathcal{L} , and the simplest choice is given in (4.6). The same can be done for vector-valued (spin) particles.

REMARK. Of course, the formulas and equations given here are well known in physics; only the point of view and the method of exposition are new (and, eventually, the mathematical rigor!).

Our density of probability of presence was already introduced by Newton and Wigner [2].

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