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

$$(1.1) \qquad \int\!\!\!\int\!\!\!\int_{R^3} |\Psi(x, y, z)|^2 \, dx \, dy \, dz = 1.$$

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 $P:A \to P(A) = L^2_A$, where A runs over a Borel field of subsets of X, and L^2_A is a closed subspace of L^2, with the following properties.

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

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

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

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

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

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

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

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

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

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

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

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 $\vec{E}_4$, 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 $\mathcal{3C}$ of functions on E_4. For instance, in the nonrelativistic case, for a particle characterized by the Hamiltonian H, the Hilbert space $\mathcal{3C}$ 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 $\mathcal{3C}$ was given by

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

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 $\langle \Psi, \varphi \rangle$. $\mathcal{3C}$ will be a subspace of the space $\mathcal{D}'(E_4)$ of the distributions on E_4. $\mathcal{3C}$ will also have a given structure as a Hilbert space, and we shall assume that the norm in $\mathcal{3C}$ is such that convergence in $\mathcal{3C}$ implies convergence in the sense of distributions. There are infinitely many choices of $\mathcal{3C}$, each of which gives a possible particle in some well-defined physical situation, and all the $\Psi \in \mathcal{3C}$, with norm 1 in $\mathcal{3C}$, give all the possible motions of such a particle in the situation considered. We are only interested in spaces $\mathcal{3C} \neq \{0\}$ since we have to deal with elements of $\mathcal{3C}$ 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 $\mathcal{3C}$, the transformed distribution $\sigma\Psi$ also belongs to $\mathcal{3C}$, and has the same norm in $\mathcal{3C}$, that is,

$$(3.1) \qquad \qquad ||\sigma\Psi||_{\mathcal{3C}} = ||\Psi||_{\mathcal{3C}}.$$

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

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

Therefore, σ is a unitary operator on the Hilbert space $\mathcal{3C}$, and the Lorentz group G has here a unitary representation in $\mathcal{3C}$. We shall define as a *free elementary particle* a free particle (thus Lorentz invariant) for which $\mathcal{3C}$ is *minimal*, in the sense that no Lorentz invariant Hilbert space $\mathcal{3C}' \neq \{0\}$ contained in $\mathcal{3C}$ exists except $\mathcal{3C}' = \mathcal{3C}$ 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 $\mathcal{3C} \subset \mathfrak{D}'(E_4)$, Lorentz invariant and minimal, may be obtained by different techniques, all using Fourier transforms. The result is the following. Of course, for every $\mathcal{3C}$, one can also take the same with a proportional norm, but we shall not distinguish them.

(a) There is one special $\mathcal{3C}$, 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 $\mathcal{3C}_1$, depending on one real parameter. These cannot be physically interpreted.

(c) There is a normal series, physically interpretable. It depends on a parameter $m_0 \geqq 0$, 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 $\mathcal{K}_{m_0, +}$ may be described in the following way. Consider the distribution on $\vec{E}_4$

$$(3.3) \qquad 2\pi\Delta^-_{\frac{2\pi cm_0}{h}}(\vec{X})$$

$$= \text{p.v.} \left[\frac{\frac{\pi cm_0}{2h} N_1\left(\frac{2\pi cm_0}{h}\sqrt{-\vec{X}^2}\right)}{\sqrt{-\vec{X}^2}} Y(-\vec{X}^2) + \frac{\frac{cm_0}{h} K_1\left(\frac{2\pi cm_0}{h}\sqrt{\vec{X}^2}\right)}{\sqrt{\vec{X}^2}} Y(X^2) \right]$$

$$+ i\left[\frac{\frac{\pi cm_0}{h}\epsilon(X_0)J_1\left(\frac{2\pi cm_0}{h}\sqrt{-\vec{X}^2}\right)}{\sqrt{-\vec{X}^2}} Y(-\vec{X}^2) - \frac{1}{2}\epsilon(X_0)\delta(\vec{X}^2) \right].$$

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 $\tau \geqq 0$, and $= 0$ for $\tau < 0$; ϵ is defined as the function $\epsilon(\tau) = \text{sign of } \tau = +1$ for $\tau \geqq 0$, 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 $\mathcal{K}_{m_0, +}$ if and only if the expression

$$(3.4) \qquad \frac{|\langle \Psi, \varphi\rangle|}{\langle 2\pi\Delta^-_{\frac{2\pi cm_0}{h}}*\bar{\varphi}, \varphi\rangle^{1/2}}$$

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 $\mathcal{K}_{m_0, +}$.

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

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

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

The Hilbert space $\mathfrak{IC}_{m_0, -}$ 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 $\mathfrak{IC}$ instead of $\mathfrak{IC}_{m_0, \pm}$. Then every Ψ of $\mathfrak{IC}$ 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^1_{loc} 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 $\mathfrak{IC}_{t_0}$ of $\mathfrak{D}'(R^3)$, having a one-to-one correspondence $\Psi \rightarrow \Psi_{t_0}$ with $\mathfrak{IC}$. Carrying over the Hilbert structure of $\mathfrak{IC}$ onto $\mathfrak{IC}_{t_0}$, we define $\mathfrak{IC}_{t_0}$ as a Hilbert space contained in $\mathfrak{D}'(R^3)$, which may be called the cross section of the Hilbert space $\mathfrak{IC}$ 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 $\mathfrak{IC}_{t_0}$, relative to X. If $A \rightarrow P(A) = (\mathfrak{IC}_{t_0})_A$ is this spectral decomposition, the probability of finding the value of a measurement of the quantity in A, when the wave function is $\Psi \in \mathfrak{IC}$, with $\|\Psi\| = 1$, will be

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

where $(\Psi_{t_0})_A$ is the orthogonal projection of Ψ_{t_0} on $(\mathfrak{IC}_{t_0})_A$. Since $\|\Psi_{t_0}\| = \|\Psi\|$, where the Hilbert structure on $\mathfrak{IC}_{t_0}$ is defined by carrying over that of $\mathfrak{IC}$, 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 $(\mathfrak{IC}_{t_0})_A$ is formed by all the Ψ equal to zero outside A, because, as is seen by studying the scalar product in $\mathfrak{IC}_{t_0}$, in this case $(\mathfrak{IC}_{t_0})_A$ and $(\mathfrak{IC}_{t_0})_B$ would not be orthogonal subspaces in $\mathfrak{IC}_{t_0}$. 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 $\mathfrak{IC}_{t_0}$. 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 $\Psi_{t_0} \to \oplus$, from $\mathcal{K}_{t_0}$ 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) $$\Psi_{t_0} \to \oplus \text{ implies } \tau\Psi_{t_0} \to \tau\oplus$$

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 $\mathcal{K}_{t_0}$ and $(\mathcal{K}_{t_0})_A$ will be the set of $\mathcal{K}_{t_0}$ 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 $\Psi_{t_0} \to \oplus$ can be found. It is given as follows. If Δ is a Laplacian on R^3, by Fourier transform $\mathfrak{F}$ there is classically defined an operator

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

Thus, one has

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

or

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

where ρ is the distance from the origin.

Actually, it may be written as a convolution,

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

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 $\mathcal{K}_{t_0}$ 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 $\oplus' \to \oplus''$ is given, using the Fourier transform $\mathfrak{F}$, by the formula

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

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

Therefore, all the possible operations $\Psi_{t_0} \to \oplus$ are of the form

$$(4.8) \qquad \oplus = \mathfrak{L} * \Psi_{t_0},$$

where

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

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 $\mathfrak{L}$ is a distribution of positive type, having a positive measure as Fourier transform. But I do not see any physical reason for $\mathfrak{L}$ 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 $\mathfrak{L}$, 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].

REFERENCES

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[2] T. D. NEWTON and E. P. WIGNER, "Invariant theoretical determination of position operators," *Phys. Rev.*, Vol. 76 (1949), p. 191(A).