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THEORETICAL PHYSICS

On the Localization Problem in Relativistic Quantum Mechanics

by

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Summary. A new axiomatics of the position operator in Relativistic Quantum Mechanics is formulated. The axioms are obtained by using the symmetry properties of the position observable in Classical Statistical Mechanics. The position operators for the Klein—Gordon and Dirac particles correspond to the results of Newton and Wigner.

0. Introduction. Since the classical papers by Newton and Wigner [6] and Wightman [8] appeared a lot has been written on the localization problem. However, up to now there is no solution of this problem everybody would agree to.

A full classification of the different possible approaches can be found in Kalnay's paper [3].

In view of the obscurities connected with the subject it is — in our opinion — sensible to look for the fundamental physical ideas a notion of localization should contain. The present paper is a step in this direction. It is based on an axiomatic treatment by Kijowski [4], which the author has used to construct the time operator in Quantum Mechanics.

The starting point is classical statistical mechanics. Here position can be described by giving the probability density of finding the particle on a hyperplane t=const of the Minkowski space. It will be obvious that such a probability density has some symmetry properties, which must be satisfied in Quantum Mechanics, too.

It is shown that the set of axioms obtained in this way gives us a unique notion of localization for the Klein—Gordon and Dirac particles. The corresponding position operators are Newton—Wigner-like.

Taking into consideration this result, it seems to us that from the point of view of classical correspondence the Newton—Wigner localization — in spite of its well-known failings — is the most natural one.

1. Position of a free particle with mass m in Relativistic Classical Mechanics. Consider an ensemble of classical particles with mass m. The motion of such a system is described by the probability density $f(x^i, p_i, t)$ of finding a particle at the moment of time t at the point (x^i, p_i) of the phase space. The function f satisfies the Liouville equation. For free particles we have:

$$f(x^i, p_i, t)=f\left(x^i-\frac{p_i}{p_0}t, p_i, 0\right).$$

It is obvious that $\int f(x, p, t)\, d^3p$ is the probability density of finding a particle at the point (x^i, t) and in particular

$$P(x^1=0)=\int f(0, x^2, x^3, p, t)\, d^3p\, dx^2\, dx^3$$

is the probability density of finding a particle on the hyperplane $x^1=0$ at the moment of time t. From now on let us consider particles at $t=0$. $P(x^1=0)$ can be written as

$$P(x^1=0)=\int f(x, p)\, \delta(x^1)\, d^3x\, d^3p\,. \tag{1.1}$$

The probability density of finding a particle at the hyperplane $x^1=\lambda$ is given by

$$P(x^1=\lambda):=A(\lambda)=\int f(x, p)\, \delta(x^1-\lambda)\, d^3x\, d^3p\,. \tag{1.2}$$

Then the average value of the first component of position is equal to

$$x^1_{av}=\int x^1 f(x, p)\, d^3x\, d^3p \tag{1.3}$$

and using (1.2)

$$x^1_{av}=\int \lambda A(\lambda)\, d\lambda\,. \tag{1.4}$$

It follows from (1.2) that $A(\lambda)$ can be treated as a value of the distribution

$$F(x^1, x^2, x^3, p_1, p_2, p_3)=\delta(x^1-\lambda)$$

on the test function $f \in \mathcal{D}(\mathcal{P})$, where $\mathcal{P}$ is the phase space. Thus $F \in \mathcal{D}'(\mathcal{P})$. Changing variables in $A(\lambda)$ we get

$$A(\lambda)=\int d^3x\, d^3p\, \delta(x^1)\, f(x^1+\lambda, x^2, x^3, p),$$

which shows that $A(\lambda)=F(\tau_{-\lambda}f)$, where τ_λ denotes the translation in the direction of the x^1-axis:

$$(\tau_\lambda f)(x, p):=f(x^1-\lambda, x^2, x^3, p)\,. \tag{1.5}$$

In particular, we have $F(\tau_0 f)=F(f)$. Now the average value (1.4) becomes a functional

$$x^1_{av}=x^1_{av}(F, f)=\int \lambda F(\tau_{-\lambda}f)\, d\lambda\,. \tag{1.6}$$

Let us define the corresponding average deviation by

$$(\Delta x^1)^2=(\Delta x^1)^2(F, f)=\int d\lambda\, (\lambda-x^1_{av})^2\, F(\tau_{-\lambda}f)\,. \tag{1.7}$$

We will consider only distributions satisfying the condition

$$\int F(\tau_\lambda f)\, \lambda^2\, d\lambda<\infty \quad \text{for every } f \in \mathcal{D}(\mathcal{P})\,. \tag{1.8}$$

It means that $(\Delta x^1)^2(F, f)<\infty$. We note that F has the following properties:

1° $(\mathcal{D}(\mathcal{P}) \ni f \geq 0) \Rightarrow (F(f) \geq 0)$.

2° $\left(\int f(x, p)\, d^3x\, d^3p=1 \text{ for every } f \in \mathcal{D}(\mathcal{P})\right) \Rightarrow \left(\int F(\tau_\lambda f)\, d\lambda=1\right)$.

3° $F(\Lambda f)=F(f)$ for every $f \in \mathcal{D}(\mathcal{P})$

and all Lorentz transformations Λ preserving the hyperplane $x^1=0$.

4° $F(f)=F(f_1)$ where $f_1(x, p)=f(-\bar{x}, \bar{p})$.

The transformation $f \to f_1$ represents a space-time inversion.

1° is due to the demand that a probability density should not be negative. 2° says that for a normalized distribution of probability density the probability of finding a particle "somewhere" should be equal to one.

The Lorentz transformations preserving the hyperplanes $x^1=\lambda$ and $t=0$ are given by translations of the coordinates (x^2, x^3) and rotations in the 2-dimensional plane $x^1=\lambda$, $t=0$. Axiom 4° distinguishes $F(f)$ from all other $F(\tau_\lambda f)$, $\lambda \neq 0$.

The following theorem is true:

THEOREM 1. *If the distribution F satisfies the above axioms, then*

1) *for any* $f \in \mathcal{D}(\mathcal{P})$

$$x^1_{av}(F, f)=x^1_{av}(F_0, f),$$

where F_0 *gives the true probability density, i.e.* $F_0(x, p)=\delta(x^1)$.

2) *for any* $f \in \mathcal{D}(\mathcal{P})$

$$(\Delta x^1)^2(F, f) \geq (\Delta x^1)^2(F_0, f)\,.$$

3) *if for every* $f \in \mathcal{D}(\mathcal{P})$

$$(\Delta x^1)^2(F, f)=(\Delta x^1)^2(F_0, f) \text{ for a certain } F, \text{ then } F=F_0\,.$$

Every F satisfying our axioms defines a certain observable. It follows from the theorem that all such observables have the same average value. The position coordinate x is the unique element among them which has the smallest deviation.

Because the proof of this theorem is almost identical with that of theorem 1 in the paper of Kijowski [4], we can omit it here.

2. Position of the Klein-Gordon particle in Relativistic Quantum Mechanics. We describe the state of the system by a scalar field $\Psi \in L^2(\Gamma^+, d\Gamma^-)$, where Γ^+ is the positive part of the mass shell and $d\Gamma^+$ is the Haar measure on it. For a given inertial reference frame we are looking for the probability density of finding a particle on the hyperplane $x^1=\lambda$ at a given moment of time. The choice of this reference frame enables us to represent four-momentum as (p, p_0), where $p_0=(p^2+m^2)^{1/2}$, $p \in \boldsymbol{R}^3$.

Let us consider the unitary transformation

$$U: L^2(\Gamma^+, d\Gamma^+) \to L^2(\boldsymbol{R}^3, d\boldsymbol{R}^3)$$

given by

$$(U\Psi)(p)=\varphi(p):=\left(p_0(p)\right)^{-1/2}\, \Psi\left(p, p_0(p)\right)\,. \tag{2.1}$$

According to the general principles of Quantum Mechanics, our probability density should be given by a hermitian form on the space of the state vectors φ. Taking the test function space $\mathscr{D}(\boldsymbol{R}^3)$, where $\boldsymbol{R}^3$ is the momentum space, we can treat our probability density as

(2.2) $$\mathscr{D}(\boldsymbol{R}^3) \ni \varphi \to F(\varphi) = T_F(\varphi^*, \varphi),$$

where $T_F \in \mathscr{D}'(\boldsymbol{R}^3 \times \boldsymbol{R}^3)$.

Now we demand that — similarly as in the classical case — the following axioms be satisfied:

1° $F(\varphi) \geq 0$ for every $\varphi \in \mathscr{D}(\boldsymbol{R}^3)$.

2° $(\|\varphi\|^2 = 1) \Rightarrow \left(\int d\lambda\, F(\tau_\lambda \varphi) = 1\right)$,

where τ_λ denotes the translation in the direction of the x^1-axis. In the momentum representation it is given by

$$(\tau_\lambda \varphi)(\boldsymbol{p}) = e^{i\lambda p_1} \varphi(\boldsymbol{p}).$$

3° For every $\varphi \in \mathscr{D}(\boldsymbol{R}^3)$

$$F(\Lambda\varphi) = F(\varphi)$$

if Λ is a Lorentz transformation preserving the hyperplanes $x^1 = \lambda$ and $t = 0$.

In the momentum representation translations of the position coordinates x^2 and x^3 are given by

(2.3) $$(\Lambda_a \varphi)(\boldsymbol{p}) = e^{ia^K p_K} \varphi(\boldsymbol{p}); \quad K = 2, 3.$$

4° We demand invariance under space-time inversion

(2.4) $$F(\varphi) = F(\varphi^*).$$

The value $F(\varphi)$ can be written as

(2.5) $$F(\varphi) = \int d^3p\, d^3q\, T(\boldsymbol{p}, \boldsymbol{q})\, \varphi^*(\boldsymbol{p})\, \varphi(\boldsymbol{q}).$$

We will use the notation $F(\varphi) = (\varphi | T\varphi)$, where

(2.6) $$(T\varphi)(\boldsymbol{p}) = \int d^3q\, T(\boldsymbol{p}, \boldsymbol{q})\, \varphi(\boldsymbol{q}).$$

Again we define the average value of x^1:

(2.7) $$x^1_{\text{av}} = \int \lambda F(\tau_{-\lambda} \varphi)\, d\lambda = \int d\lambda \left((\tau_{-\lambda} \varphi) | \lambda T(\tau_{-\lambda} \varphi)\right),$$

and its deviation:

(2.8) $$(\Delta x^1)^2 (F, \varphi) = \int d\lambda\, (\lambda - x^1_{\text{av}})^2 F(\tau_{-\lambda} \varphi) = \int d\lambda \left((\tau_{-\lambda} \varphi) | (\lambda - x^1_{\text{av}})^2 T(\tau_{-\lambda} \varphi)\right).$$

THEOREM 2. *If the distribution F satisfies the axioms, then*

1) *for any* $\varphi \in \mathscr{D}(\boldsymbol{R}^3)$

$$x^1_{\text{av}}(F, \varphi) = x^1_{\text{av}}(F_0, \varphi), \quad \textit{where } F_0(\varphi) = (\varphi | T_0 \varphi)$$

and

$$(T_0 \varphi)(p_1, p_2, p_3) = \int dq\, \varphi(q, p_2, p_3).$$

2) *for any* $\varphi \in \mathscr{D}(\boldsymbol{R}^3)$

$$(\Delta x^1)^2 (F, \varphi) \geq (\Delta x^1)^2 (F_0, \varphi)$$

3) *if for every* $\varphi \in \mathscr{D}(\boldsymbol{R}^3)$

$$(\Delta x^1)^2 (F, \varphi) = (\Delta x^1)^2 (F_0, \varphi), \quad \textit{then } F = F_0.$$

Idea of the proof (for further details see [4]). From axioms 1° and 4° we immediately have

$$F(\varphi) = F^*(\varphi) = F(\varphi^*),$$

which gives us

$$(\varphi | T^* \varphi) = (\varphi | T\varphi).$$

Using the polarization method for hermitian forms we obtain

$$(\varphi_1 | T^* \varphi_2) = (\varphi_1 | T\varphi_2).$$

Because $\overset{*}{\varphi}_1 \otimes \varphi_2$ are dense in $\mathscr{D}(\boldsymbol{R}^3 \times \boldsymbol{R}^3)$, we get

(2.9) $$T^*(\boldsymbol{p}, \boldsymbol{q}) = T(\boldsymbol{p}, \boldsymbol{q}).$$

From axioms 3° we have

$$(\varphi | T\varphi) = (\Lambda_a \varphi | T\Lambda_a \varphi),$$

which gives for every $a^k \in \boldsymbol{R}^1$

$$T(\boldsymbol{p}, \boldsymbol{q}) \equiv T(\boldsymbol{p}, \boldsymbol{q})\, e^{ia^K (p_K - q_K)}; \quad K = 2, 3.$$

It means that $T(\boldsymbol{p}, \boldsymbol{q})$ should be of the form

(2.10) $$T(\boldsymbol{p}, \boldsymbol{q}) = K(\boldsymbol{p}, \boldsymbol{q})\, \delta(q_2 - p_2)\, \delta(q_3 - p_3)$$

and

$$(T\varphi)(\boldsymbol{p}) = \int dq_1\, K(\boldsymbol{p}, q_1, p_2, p_3)\, \varphi(q_1, p_2, p_3).$$

Now let us apply axiom 2°:

$$\int d\lambda\, F(\tau_{-\lambda} \varphi) = \int d\lambda\, (\tau_{-\lambda} \varphi | T\tau_{-\lambda} \varphi) =$$
$$= \int d\lambda \left(\varphi | (\tau_\lambda T) \varphi\right) = \left(\varphi | \left(\int d\lambda\, \tau_\lambda T\right) \varphi\right) = (\varphi | \varphi).$$

But

$$(\tau_\lambda T)(\boldsymbol{p}, \boldsymbol{q}) = T(\boldsymbol{p}, \boldsymbol{q})\, e^{i\lambda (q_1 - p_1)}.$$

This means that

$$\left(\int d\lambda\, \tau_\lambda T\right)(\boldsymbol{p}, \boldsymbol{q}) = T(\boldsymbol{p}, \boldsymbol{q})\, \delta_1(q_1 - p_1),$$
$$= K(\boldsymbol{p}, \boldsymbol{q}) \cdot \delta(q_1 - p_1)\, \delta(p_2 - q_2)\, \delta(p_3 - q_3) = K(\boldsymbol{p}, \boldsymbol{p})\, \delta^{(3)}(\boldsymbol{q} - \boldsymbol{p}).$$

Hence we see that

(2.11) $$K(\boldsymbol{p}, \boldsymbol{q}) \equiv 1.$$

Using axiom 1° it can be shown that

$$(2.12)\qquad \begin{aligned} &1.\quad \frac{\partial K}{\partial p}=0 \\ &2.\quad \frac{\partial^2 K}{\partial p^2}\leqslant 0 \end{aligned} \Bigg\} \text{ on the diagonal}$$

$$3.\quad \left(\frac{\partial^2 K}{\partial p^2}\equiv 0 \text{ on the diagonal}\right) \Rightarrow (K\equiv 1).$$

Now we can easily show (2.1)

$$(2.13)\qquad x^1_{\text{av}}(F,\varphi)=\int d\lambda\,(\tau_{-\lambda}\varphi\,|\,\lambda T\tau_{-\lambda}\varphi)=(\varphi\,|-i\delta_1' T\varphi)=(-i\varphi'\,|\,\delta_1\varphi)=x^1_{\text{av}}(F_0,\varphi),$$

where we have used

$$-i\delta_1'(q_1-p_1)=\int \lambda e^{i\lambda(q_1-p_1)}\,d\lambda$$

and (2.11), (2.12). 1. Furthermore it can be shown that

$$(2.14)\qquad (\Delta x^1)^2(F,\varphi)-(\Delta x^1)^2(F_0,\varphi)= \\ =\int \lambda^2\big(F(\tau_{-\lambda}\varphi)-F_0(\tau_{-\lambda}\varphi)\big)\,d\lambda=-(\varphi\,|\,\delta_1 T''\varphi).$$

Using (2.12).2 and (2.12).3 we have 2) and 3) of Theorem 2.

As in the classical case we propose to treat $F_0(\varphi)$ as the true probability density of finding the particle on the plane $x^1=0$ at time $t=0$.

From Eq. (2.13) we can derive the expression for the position operator

$$(2.15)\qquad x^i=-i\frac{\partial}{\partial p_i},\quad \text{such that } x^i_{\text{av}}=(\varphi\,|\,x^i\varphi).$$

In the space $L^2(\Gamma^+, d\Gamma^+)$ it is given by

$$(2.16)\qquad x^i_\Gamma=p_0^{1/2}\left(-i\frac{\partial}{\partial p_i}\right)p_0^{-1/2}=-i\left(\frac{\partial}{\partial p_i}-\frac{1}{2}\frac{p_i}{p_0^2}\right),$$

which is the well-known Newton—Wigner position operator for a spinless particle of mass m.

Important remark. In our proof we have assumed that the first and second derivatives of the distribution T (·, ·) exist. That is a Newton—Wigner-like regularity condition.

3. Position of the Dirac particle. We will describe the state of a particle with mass $m\neq 0$ and spin $s=1/2$ in the Foldy—Wouthuysen picture [2]. In this picture the Dirac equation takes the form

$$(3.1)\qquad (H\Psi)(p)=\gamma^0 p_0\Psi(p),\quad \text{where } \gamma^0=\begin{pmatrix} I & 0\\ 0 & -I\end{pmatrix}.$$

Solutions of positive and negative energies are described by spinor fields Φ and X, where

$$(3.2)\qquad \begin{aligned} \Phi(p)&=\frac{1+\gamma^0}{2}\Psi(p)=\begin{pmatrix}\Psi_1\\ \Psi_2\\ 0\\ 0\end{pmatrix}(p),\\ X(p)&=\frac{1-\gamma^0}{2}\Psi(p)=\begin{pmatrix}0\\ 0\\ \Psi_3\\ \Psi_4\end{pmatrix}(p).\end{aligned}$$

Eq. (3.1) shows that states of positive and negative energies are not mixed under the action of the hamiltonian. We see that every spinor on the mass shell Γ^+ is a solution of (3.1) for $p_0>0$.

Let us consider states of positive energies. They are described by spinor fields Ψ:

$$\Psi_A\in L^2(\Gamma^+, d\Gamma^+):\quad A=1,2.$$

and after the unitary transformation (2.1) by spinor fields φ:

$$\varphi_A\in L^2(R^3, dR^3):\quad A=1,2.$$

The invariant scalar product on hyperplanes $t=$const. is given by

$$(3.3)\qquad (\varphi,\chi)=\int d^3p\,\varphi_A^*(p)\,\chi_A(p).$$

We look for the probability density of finding a particle on the hyperplane $x^1=\lambda$ at the moment of time $t=0$. We assume again that it should be a bilinear functional of φ. Now our test functions are fields φ, $\varphi_A\in\mathscr{D}(R^3)$, and the probability densities are hermitian forms:

$$\varphi\to F(\varphi)=T_F(\varphi^*,\varphi),$$

where

$$F(\varphi)=\int d^3p\,d^3q\,\varphi_A^*(p)\,T_F(p,q)_{AB}\,\varphi_B(q).$$

We define

$$(3.4)\qquad (T\varphi)_A(p)=\int d^3q\,T_F(p,q)_{AB}\,\varphi_B(q),\quad \text{then } F(\varphi)=(\varphi\,|\,T\varphi).$$

We assume that the same axioms as in the spinless case have to be satisfied. An analogous theorem can easily be shown.

THEOREM 3. *If the distribution F satisfies the axioms, then*

(3.5) 1) *for every* φ, $\varphi_A\in\mathscr{D}(R^3)$.

$$x^1_{\text{av}}(F,\varphi)=x^1_{\text{av}}(F_0,\varphi),\quad \text{where } F_0(\varphi)=(\varphi\,|\,T_0\varphi)$$

and

$$(T_0\varphi)_A(p)=\int dq\,\varphi_A(q,p_2,p_3).$$

(3.5) [continued] 2) *for every* φ, $\varphi_A \in \mathcal{D}(\mathbf{R}^3)$,

$$(\Delta x^1)^2 (F, \varphi) \geqslant (\Delta x^1)^2 (F_0, \varphi).$$

3) *if for every* φ, $\varphi_A \in \mathcal{D}(\mathbf{R}^3)$,

$$(\Delta x^1)^2 (F, \varphi) = (\Delta x^1)^2 (F_0, \varphi), \text{ then } F = F_0.$$

Again we propose to treat $F_0(\varphi)$ as the probability density we have been looking for. The average value of the position can be written in the form $x^i_{av} = (\varphi | x^i \varphi)$, which is the definition of the position operator. From (3.5) we obtain

$$x^i = -i \frac{\partial}{\partial p_i}. \tag{3.6}$$

In the state space $L^2(\Gamma^+, d\Gamma^+)$ we have

$$x^i_\Gamma = p_0^{1/2} \left(-i \frac{\partial}{\partial p_i}\right) p_0^{-1/2} \tag{3.7}$$

and after transforming (3.7) into the Dirac picture:

$$x^i_{\Gamma, D} = \frac{p_0 + m - \gamma \cdot p}{(2p_0(p_0+m))^{1/2}} p_0^{1/2} \left(-i \frac{\partial}{\partial p_i}\right) p_0^{-1/2} \frac{p_0 + m + \gamma \cdot p}{(2p_0(p_0+m))^{1/2}}. \tag{3.8}$$

(3.8) is the Newton—Wigner position operator for a particle with spin $s = 1/2$.

Remark. (3.7) differs from the Foldy—Wouthuysen operator of mean position. A discussion on the difference between the Foldy—Wouthuysen and the Newton—Wigner operator can be found in [1].

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Е, Киёвски, Г. Рудольф, **О проблеме положения в релятивистской квантовой механике**

Содержание. Сформулирована новая аксиоматика оператора положения в релятивисткой квантовой механике. Используя свойства симметрии величины положения в классической статистической механике получено аксиомы для квантового случая. Операторы положения для частиц Клейна—Гордона и Дирака соответствуют результатам Невтона и Вигнера.

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EXPERIMENTAL PHYSICS

Zeeman Coherences Relaxation in the Ground State of Alkali-Metal Atoms Induced by Spin-Exchange Collisions and Collisions with Buffer Gas Atoms

by

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Presented by A. JABŁOŃSKI on March 1, 1976

Summary. The evolution equation of the ground state density matrix elements (Zeeman ground state coherences) of alkali metal vapour due to spin-exchange collisions is given. Then the influence of spin-exchange collisions on transversal relaxation rates and Zeeman frequency shifts due to sudden collisions (collisions with buffer gas or coated walls of the cell) is considered. The evolution equation of Zeeman coherences in the case when both relaxation processes are active is solved for $F=1$.

In [1] the authors deal with off-diagonal density matrix elements relaxation of the given state of the hyperfine (*hf*) structure (Zeeman coherences) in the ensemble of polarized alkali metal atoms in the ground state induced by weak, sudden collisions in which the motion-narrowing condition is fulfilled. This condition is fulfilled in the case of collisions with light noble-gas atoms or with paraffin-(silicones)-coated walls of the cell [2, 3].

In this work the transversal relaxation (the relaxation of coherence) induced by spin-exchange collisions between alkali metal atoms is considered and the Zeeman coherences relaxation caused by both relaxation processes — spin-exachange and sudden collisions — in a large range of the static magnetic field H_0 is described. In the greater part of this range of H_0 there was no exact theoretical information about the relaxation of coherences.

In [2] transversal relaxation rates T_2^{-1}, due to sudden collisions, in the case of $\delta^{mm'}_{m+r\,m'+r} T_2 < 1$ were found.
There is:

$$\delta^{mm'}_{m+r\,m'+r} = \omega_{mm'} - \omega_{m+r\,m'+r}, \qquad r = \pm 1,$$

$$\omega_{mm'} = E_m - E_{m'}; \quad E_m, E_{m'} \text{ — Zeeman sublevels energy.}$$

For $\delta^{mm'}_{m+r\,m'+r} T_2 \gg 1$ transversal relaxation rates were given in that paper as well as in [4]. In [1] the relaxation rates and Zeeman frequency shifts, as a function of the quantity $\delta^{mm'}_{m+r\,m+r}$, were discussed and the Zeeman coherences evolution equation of alkali metal atoms in states with the quantum number of the total angular momen-