On a Question of W. Pauli

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Abstract. We discuss the following problem posed by W. Pauli: to what extent is the state vector of a quantum system determined by the distribution functions of its physical observables?

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by

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It is a natural question to ask whether one can reconstruct the state vector of a quantum system from the distribution functions of its observables. Let us consider, for instance, a spinless particle in non-relativistic quantum mechanics. The possible states of such a particle are described by the rays of the complex Hilbert space $X = L^2(\mathbf{R}^3)$. Kinematically, one can measure the distribution of the position operator $\vec{x}$, of the momentum operator $\vec{p}$, of the angular momentum $\vec{L} = \vec{x} \times \vec{p}$, and of its projections L_ν. Denoting by $\{e_i^{(\nu)}\}$ the basis of common eigen-functions of L^2 and L_ν, we write, for $\psi_j \in L^2(\mathbf{R}^3)$,

$$\psi_j = \sum_{i=1}^{\infty} \alpha_{ij}^{(\nu)} e_i^{(\nu)}, j = 1, 2,$$

and ask whether the relations

$$\left|\alpha_{i1}^{(\nu)}\right| = \left|\alpha_{i2}^{(\nu)}\right|, |\psi_1(\vec{x})| = |\psi_2(\vec{x})|, \left|\hat{\psi}_1(\vec{p})\right| = \left|\hat{\psi}_2(\vec{p})\right| \tag{1}$$

for all $i, \vec{x}$, and $\vec{p}$ imply that $\psi_1 = \beta\psi_2$ with $\beta \in \mathbf{C}$; here

$$\hat{\psi}(\vec{p}) = \frac{1}{(2\pi)^{\frac{3}{2}}} \int_{\mathbf{R}^3} \psi(\vec{x}) \exp(ip\vec{x}) d\vec{x}$$

is the Fourier transform of ψ (cf. [6], [5], [7]). If one lets ν vary, the question can be naturally split up into two. First of all, we ask with W. Pauli [9, p. 17] how to describe the set of solutions

$$\left\{\psi | \psi \in L^2\left(\mathbf{R}^l\right), |\psi(\vec{x})| = W_1(\vec{x}), \left|\hat{\psi}(\vec{p})\right| = W_2(\vec{p})\right\} \tag{2}$$

for the given functions W_1, W_2. Secondly, one may consider a finite-dimensional vector space $Y \simeq \mathbf{C}^n$ and self-adjoint operators $A_\nu, 1 \le \nu \le m$, in Y; let

$$A_\nu e_{i\nu} = \lambda_{i\nu} e_{i\nu}, 1 \le i \le n.$$

On writing $x = \sum_{i=1}^{n} a_{i\nu}(x) e_{i\nu}$ for $x \in Y$, one may wish to describe the set of solutions

$$\mathcal{A}(b) = \{x \| a_{i\nu}(x)| = b_{i\nu}, 1 \le i \le n, 1 \le \nu \le m\}$$

for given $b_{i\nu}$. In particular, we ask under what conditions on A_ν the solution is unique (up to a scalar), so that

$$x, y \in \mathcal{A}(b) \Rightarrow y = \alpha x$$

with $\alpha \in \mathbf{C}$. Being unable to treat these difficult problems in full generality, we propose to collect here some of our observations (an interested reader may consult the references for physical motivation and some further results relating to this problem).

Let us start with the finite-dimensional problem. In this case we have the following proposition, [8].

Proposition 1. *If $m = 3$ and $n \geq 12$, the set $\mathcal{A}(b)$ contains at least two different solutions.*
Proof. Suppose, on the contrary, that the solution is unique. Then the map

$$x \mapsto |a_{i\nu}(x)|, 1 \leq i \leq n, 1 \leq \nu \leq 3$$

is a topological embedding of $\mathbf{CP}^{n-1}$ in $\mathbf{R}^{3n}$; since $3n > \frac{3(2(n-1)+1)}{2}$, it can be approximated by a differentiable embedding, [3]. Therefore, a non-immersion theorem, [10], shows that

$$3n \geq 4(n-1) - 2\log_2(n-1) - 1,$$

that is $n \leq 11$.

This proposition shows, in particular, that the distributions of the three projections of the spin do not determine the spin state of a system for high enough spins.

Our second observation is as follows. For an odd prime p, let $X = \{f | f : \mathbf{Z}/p\mathbf{Z} \to \mathbf{C}\}$. Clearly, $X \simeq \mathbf{C}^p$; we choose two bases of X:

$$\{\delta_n | 0 \leq n \leq p-1\},$$

and

$$\{\chi_a | 0 \leq a \leq p-1\}$$

with

$$\delta_n(m) = \begin{cases} 0, n \neq m \\ 1, n = m \end{cases}, \chi_a(m) = \exp\left(\frac{2\pi i a m}{p}\right),$$

and consider the elements ψ_a given by

$$\psi_a(m) = \exp\left(2\pi i \frac{am^2}{p}\right), 0 \leq a \leq p-1.$$

Write $\psi_a = \sum_{j=0}^{p-1} b_{aj}\delta_j$, $\psi_a = \sum_{j=0}^{p-1} c_{aj}\chi_j$.

Proposition 2. *If $1 \leq a \leq p-1$, then $|c_{aj}| = \frac{1}{p}$, and $|b_{aj}| = 1$.*

Proof. Clearly, $b_{aj} = \psi_a(j)$, and $c_{aj} = \frac{1}{p}\sum_{m=0}^{p-1} \psi_a(m)\overline{\chi_j(m)}$, so that

$$|c_{aj}|^2 p^2 = \sum_{0\le n,m\le p-1} \psi_a(m)\overline{\chi_j(m)\psi_a(n)}\chi_j(n)$$
$$= \sum_{0\le n,m\le p-1} \chi_j(n-m)\exp\left(2\pi i\frac{a(m^2-n^2)}{p}\right);$$

on replacing the variable of summation, one obtains

$$|c_{aj}|^2 p^2 = \sum_{0\le k,n\le p-1} \chi_j(k)\chi_j(-k(2n+k))$$
$$= \sum_{k=0}^{p-1}\overline{\chi_j(k^2)}\,\chi_j(k)\sum_{n=0}^{p-1}\overline{\chi_j(2kn)} = p.$$

Passing to the infinite-dimensional case, we note the following analogue of Proposition 2. Let $f_\alpha(x) = \exp(i\alpha x^2)$, then $\hat{f}_\alpha(p) = \frac{1}{\sqrt{2\alpha i}}\exp\left(-\frac{ip^2}{4\alpha}\right)$; so that for any **real** $\alpha \neq 0$ we get the same distribution functions $|f_\alpha(x)|$, $|\hat{f}_\alpha(p)|$ independent of α. However, $f_\alpha \notin L^2(\mathbf{R})$. We owe this observation to Y. Aharonov [1].

The following example is known for many years, [6] (cf. also [2]). Let $\psi \in L^2(\mathbf{R})$, write $\psi(x) = \rho(x)\exp(i\varphi(x))$ with $\rho(x) = |\psi(x)|$, and let $\psi_1(x) = \rho(x)\exp(-i\varphi(-x))$. Then

$$\psi_1(p) = \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \rho(-x)\exp(-i\varphi(-x) + ipx)dx$$
$$= \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty} \rho(-x)\exp(-i\varphi(x) - ipx)dx,$$

so that $\hat{\psi}_1(p) = \hat{\psi}(p)$ if $\rho(-x) = \rho(x)$, and in particular

$$\rho(x) = \rho(-x) \text{ for } x \in \mathbf{R} \Rightarrow |\psi(x)| = |\psi_1(x)|, \left|\hat{\psi}(p)\right| = \left|\hat{\psi}_1(p)\right|$$
$$\text{for } x, p \in \mathbf{R}.$$

Although one of us believes that the following conjecture holds true, we have no other results for $X = L^2(\mathbf{R})$.

Conjecture (A.M. Perelomov). Let $\psi, f \in L^2(\mathbf{R})$ and suppose that $|\psi(x)| = |f(x)|$, $|\hat{\psi}(p)| = |\hat{f}(p)|$ for $x, p \in \mathbf{R}$. Then either $f = \alpha\psi$, or $f = \alpha\psi_1$ with $\alpha \in \mathbf{C}$.

Let now $X = L^2(\mathbf{R}^l)$. The above example shows that if $\psi(x) = \psi_0(|x|)$, $\psi_1(x) = \overline{\psi(x)}$, then $|\psi(x)| = |\psi_1(x)|$, and $|\hat{\psi}(p)| = |\hat{\psi}_1(p)|$ for $x, p \in \mathbf{R}^l$, $|x| := \sqrt{x_1^2 + \ldots + x_l^2}$ (cf.

[4]). In particular, we see that relations (1) do not, in general, imply $\psi_1 = \beta\psi_2$ with $\beta \in \mathbf{C}$ since the angular momentum vanishes for a spherically symmetric state.

Finally, we discuss the structure of the set (2) assuming that ψ (and therefore $\hat{\psi}$) is of Gaussian shape:

$$\psi(x) = a\ \exp\left(-\frac{1}{2}x^tAx\right), a \in \mathbf{C}, A = A^t, A \in GL(l,\mathbf{C}),$$

and ReA is positive definite. Let us start with the following simple observation.

Lemma. *Let $\psi \in L^2(\mathbf{R}^l)$. For any linear transformation $C : \mathbf{R}^l \to \mathbf{R}^l$ with* $\det C \neq 0$, *we have $\hat{\psi}_C(p) = |\det C|^{-1}\ \hat{\psi}\left(\left(C^{-1}\right)^tp\right)$, and $||\psi_C|| = |\det C|^{-1/2}||\psi||$; here $\psi_C(x) := \psi(Cx)$.*

Proof.

$$\hat{\psi}_C(p) = (2\pi)^{-\frac{l}{2}} \int_{\mathbf{R}^l} \psi(Cx)\exp\left(ip^tx\right)dx =$$

$$= |\det C|^{-1}(2\pi)^{-\frac{l}{2}} \int_{\mathbf{R}^l} \psi(y)\exp\left(ip^tC^{-1}y\right)dy;$$

and

$$||\psi_C||^2 = \int_{\mathbf{R}^l} |\psi(Cx)|^2dx = |\det C|^{-1}||\psi||^2.$$

On writing $A = A_1 + iA_2$ with real symmetric $A_j, j = 1,2$, one remarks that $C^tAC = I + \mathrm{diag}(\lambda_1,...,\lambda_l)$ for some linear transformation C since A_1 is positive definite. It follows then that

$$\left|\hat{\psi}(p)\right| = b\exp\left(-\frac{1}{2}p^tB_1p\right), B_1 = \mathrm{diag}(\mu_1^2,\ldots,\mu_l^2),$$

with $0 < \mu_j \leq 1,\ 1 \leq j \leq l$. Thus we let

$$W_1(x) = \pi^{-\frac{l}{4}}\exp\left(-\frac{1}{2}x^tx\right), W_2(p) = \pi^{-\frac{l}{4}}b\exp\left(-\frac{1}{2}p^tB_1p\right)$$

with $b = \prod_{j=1}^{l}\mu_j$, $B_1 = \mathrm{diag}(\mu_1^2,\ldots,\mu_l^2)$, and write

$$\psi(x) = W_1(x)\exp\left(-\frac{1}{2}ix^tA_2x\right),\ \hat{\psi}(p) = W_2(p)\exp\left(-\frac{1}{2}ip^tB_2p\right).$$

It follows then that $(I + iA_2)(B_1 + iB_2) = I$, or $B_1 - A_2B_2 = I$, $A_2B_1 + B_2 = C$. Thus it suffices to find all the (real symmetric) solutions A_2 of the equation $A_2^2 = C$ with $C = (I - B_1)B_1^{-1}$, so that $C = \mathrm{diag}(...,(1-\mu_j^2)\mu_j^{-2},...)$. We introduce the set

$$\mathcal{L} = \left\{\mathrm{diag}(\ldots,\lambda_j,\ldots)|\lambda_j^2 = \left(1-\mu_j^2\right)\mu_j^{-2}, 1 \leq j \leq l\right\}$$

containing precisely 2^l elements and remark that the general solution of our equation is of the shape $A_2 = \sigma^t D\sigma$ with $D \in \mathcal{L}$, $\sigma^t = \sigma^{-1}$, $\sigma B_1 = B_1\sigma$. Thus our set of solutions splits into 2^l orbits of the group $G = \{\sigma | \sigma \in O(l), \sigma B_1 = B_1\sigma\}$. As a simple example., one may choose $\psi_0(\vec{x}) = a\exp\left(-\alpha_1|\vec{x}|^2 - i\alpha_2(x_1^2 + x_2^2 - x_3^2)\right)$ with $\alpha_1 > 0, \alpha_2 \in \mathbf{R}\backslash\{0\}$ and remark that $|\psi_\sigma(\vec{x})| = |\psi_0(\vec{x})|$, $\left|\hat{\psi}_\sigma(\vec{p})\right| = \left|\hat{\psi}_0(\vec{p})\right|$ for any σ in 0(3), as soon as we let $\psi_\sigma(\vec{x}) = \psi_0(\sigma\vec{x})$. In particular, the set (2) may contain infinitely many different solutions (this example has been suggested by M. Kontsevich [4]).

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