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QUANTUM BOCHNER THEOREMS AND INCOMPATIBLE OBSERVABLES

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A quantum version of Bochner's theorem characterising Fourier transforms of probability measures on locally compact Abelian groups gives a characterisation of the Fourier transforms of Wigner quasi-joint distributions of position and momentum. An analogous quantum Bochner theorem characterises quasi-joint distributions of components of spin. In both cases quantum states in which a true distribution exists are characterised by the intersection of two convex sets. This may be described explicitly in the spin case as the intersection of the Bloch sphere with a regular tetrahedron whose edges touch the sphere.

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1. BOCHNER'S THEOREM ON LOCALLY COMPACT ABELIAN GROUPS

The Fourier transforms

$$f(x) = \int_{\mathbb{R}} e^{ixy}\, \mathrm{d}\mu(y) \tag{1}$$

of probability measures μ on the real line $\mathbb{R}$ have three easily established properties:

- *normalisation:* $f(0) = 1$
- *continuity*: f is continuous
- *nonnegative-definiteness*: for arbitrary $N \in \mathbb{N}$, $z_1, z_2, \ldots, z_N \in \mathbb{C}$ and $x_1, x_2, \ldots, x_N \in \mathbb{R}$,

$$\sum_{j,k=1}^{N} \bar{z}_j z_k f(-x_j + x_k) \geq 0.$$

Conversely, Bochner's theorem [1] is that every complex-valued function f satisfying these properties is the Fourier transform of a unique probability measure on $\mathbb{R}$. A generalisation [8] replaces ($\mathbb{R}$,+) by an arbitrary locally compact Abelian topological group (lcAg), characterising the Fourier transforms of probability measures as complex-valued functions on the dual group of continuous homomorphisms to the group $\mathbb{T}$ of unimodular complex numbers with the same three properties of normalisation, continuity and nonnegative-definiteness.

2. OBSERVABLES AND STOCHASTIC PROCESSES

Bochner's theorem on the real line allows us to *define* a real valued observable in quantum mechanics as a continuous unitary representation $\mathbb{R} \ni x \mapsto U_x \in \mathcal{U}(\mathcal{H})$ of $(\mathbb{R}, +)$ in the underlying Hilbert space $\mathcal{H}$, in that, given such a representation and a state represented by a density operator ρ on $\mathcal{H}$ it is not difficult to show that the function

$$f(x) = \operatorname{tr} \rho U_x$$

is normalised, continuous and nonnegative-definite. The corresponding probability measure μ for which (1) holds gives us directly the probability distribution of the observable in the state ρ. This definition of observable, while somewhat indirect, has the pedagogical advantage of combining rigour with avoidance of involvement of either the spectral theorem for an unbounded self-adjoint operator or Stone's theorem. Of course Bochner's theorem also provides a relatively easy route to proofs of both these theorems.

Given two observables $(U_x)_{x\in\mathbb{R}}$ and $(V_x)_{x\in\mathbb{R}}$ in this sense which are *compatible*, in the sense that U_x commutes with V_y for arbitrary $x, y \in \mathbb{R}$, it may be verified easily that the function on $\mathbb{R}^2$

$$f(x, y) = \operatorname{tr} \rho U_x V_y \tag{2}$$

is normalised, continuous and nonnegative-definite. Bochner's theorem for the lcAg $\mathbb{R}^2$ allows us to define the *joint probability distribution* of these observables as the probability measure M on $\mathbb{R}^2$, identified as its own dual group, for which

$$f(x, y) = \int_{\mathbb{R}^2} e^{i(xx'+yy')} \,\mathrm{d}M(x', y').$$

Note that M gives the correct marginal distributions for the two observables $(U_x)_{x\in\mathbb{R}}$ and $(V_x)_{x\in\mathbb{R}}$, for which the corresponding Fourier transforms are given in terms of (2) by the functions $x \mapsto f(x, 0)$ and $x \mapsto f(0, x)$ respectively.

More generally, given an arbitrary family $\big((U_x^\lambda)_{x\in\mathbb{R}}\big)_{\lambda\in\Lambda}$ of mutually compatible observables, using Bochner's theorem on the groups $\mathbb{R}^n$ we can construct a corresponding stochastic process, in the sense [5] of a family of mutually coherent joint probability distributions $M_{(\lambda_1,\lambda_2,\ldots,\lambda_n)}$, $n \in \mathbb{N}, \lambda_1, \lambda_2, \ldots, \lambda_n \in \Lambda$ on $\mathbb{R}^n$ for which

$$\operatorname{tr} \rho U_{x_1}^{\lambda_1} U_{x_2}^{\lambda_2} \cdots U_{x_n}^{\lambda_n} = \int_{\mathbb{R}^2} e^{i(x_1y_1+x_2y_2+\cdots+x_ny_n)} \,\mathrm{d}M_{(\lambda_1,\lambda_2,\ldots,\lambda_n)}(y_1, y_2, \ldots, y_n).$$

3. BOCHNER'S THEOREM FOR CANONICAL PAIRS

Of course quantum mechanics has to deal with incompatible observables such as momentum and position of a particle. If $(U_x)_{x\in\mathbb{R}}$ and $(V_x)_{x\in\mathbb{R}}$ denote the avatars of the momentum and position observables p and q as continuous unitary representations of $\mathbb{R}$ then we have the Weyl commutation rule

$$U_x V_y = e^{ixy} V_y U_x. \tag{3}$$

If, ignoring the noncommutativity, we use (2) to define the Fourier transform of a joint probability distribution, then, since

$$(U_x V_y\}^* = V_y^* U_x^* = V_{-y} U_{-x} = e^{-ixy} U_{-x} V_{-y}$$

we have

$$\bar{f}(x,y) = \mathrm{tr}\,(\rho U_x V_y)^* = \mathrm{tr}\,((U_x V_y)^* \rho) = \mathrm{tr}\,(\rho (U_x V_y)^*) = e^{-ixy} f(-x,-y).$$

Thus f fails to satisfy the necessary condition $\bar{f}(x,y) = f(-x,-y)$ for nonnegative-definiteness.

A more plausible candidate for joint Fourier transform which does satisfy this condition is got by replacing the operators $U_x V_y$ in (2) by the family of *Weyl operators* $W_{x,y}$, defined for $(x,y) \in \mathbb{R}^2$ by

$$W_{x,y} = e^{-\frac{1}{2}ixy} U_x V_y = e^{\frac{1}{2}ixy} V_y U_x.$$

Because of (3) these satisfy

$$W_{x,y} W_{x',y'} = e^{\frac{1}{2}i(xy'-yx')} W_{x+x',y+y'}, \tag{4}$$

thus they form a *multiplier representation* of the group $\mathbb{R}^2$ with *multiplier*

$$\omega((x,y),(x',y')) = e^{\frac{1}{2}i(xy'-yx')}.$$

Then the candidate joint Fourier transform

$$f(x,y) = \mathrm{tr}\,\rho W_{x,y} \tag{5}$$

is normalised and continuous, as in the commutative case. But instead of being nonnegative-definite, it is *ω-nonnegative-definite,* meaning that, for arbitrary $N \in \mathbb{N}$, $z_1, z_2, \ldots, z_N \in \mathbb{C}$ and $(x_1,y_1),(x_2,y_2),\ldots,(x_N,y_N) \in \mathbb{R}^2$,

$$\sum_{j,k=1}^{N} \bar{z}_j z_k \omega(-(x_j,y_j),(x_k,y_k)) f(-x_j+x_k,-y_j+y_k) \geq 0.$$

Indeed

$$\begin{aligned}
& \sum_{j,k=1}^{N} \bar{z}_j z_k \omega(-(x_j,y_j),(x_k,y_k)) f(-x_j+x_k,-y_j+y_k) \\
= & \sum_{j,k=1}^{N} \bar{z}_j z_k \omega(-(x_j,y_j),(x_k,y_k))\, \mathrm{tr}\,\rho W_{-x_j+x_k,-y_j+y_k} \\
= & \sum_{j,k=1}^{N} \bar{z}_j z_k\, \mathrm{tr}\,\rho W_{-x_j,-y_{jk}} W_{x_k,y_k} \\
= & \ \mathrm{tr}\,\rho \left(\sum_{j=1}^{N} \bar{z}_j W^*_{x_j,y_j}\right)\left(\sum_{k=1}^{N} z_k W_{(x_k,y_k)}\right) \\
= & \ \mathrm{tr}\,\rho \left(\sum_{j=1}^{N} z_j W_{x_j,y_j}\right)^* \sum_{k=1}^{N} z_k W_{(x_k,y_k)} \geq 0
\end{aligned}$$

using (4) together with the facts that $W^*_{x_j,y_j} = W_{-x_j,-y_j}$ and that $\operatorname{tr}\rho T^*T \geq 0$ for an arbitrary bounded operator T.

It is easily be verified using (3) that, for fixed $(x, y) \in \mathbb{R}^2$ the map $\mathbb{R} \ni t \mapsto W_{tx,ty} = e^{-\frac{1}{2}it^2xy}U_{tx}V_{ty}$ is a unitary representation of $\mathbb{R}$ whose infinitesimal generator $-i\frac{\mathrm{d}}{\mathrm{d}t}W_{tx,ty}\,|_{t=0}$ is given formally by

$$-i\frac{\mathrm{d}}{\mathrm{d}t}W_{tx,ty}\,|_{t=0} = xp + yq$$

where p and q are the infinitesimal generators $p = -i\frac{\mathrm{d}}{\mathrm{d}x}U_x\,|_{t=0}$ and $q = -i\frac{\mathrm{d}}{\mathrm{d}x}V_x\,|_{t=0}$. This suggests that the function (5) be written formally as

$$f(x, y) = \operatorname{tr}\rho e^{i(xp+yq)}, \tag{6}$$

and reinforces its claim to be the Fourier transform of a joint probability distribution of the momentum and position observables. It can be shown [7] that f is necessarily square-integrable and is thus indeed the Fourier–Plancherel transform of a square integrable function on $\mathbf{R}^2$. However the resulting *Wigner distribution* [9] may not be a true probability distribution in that it gives rise to negative probabilities.

Assume now that the representations $(U_x)_{x\in\mathbb{R}}$ and $(V_x)_{x\in\mathbb{R}}$satisfying (3) are irreducible, equivalently by the von Neumann uniqueness theorem [6] that they are unitarily equivalent to the Schrödinger representations in $L^2(\mathbb{R})$ given by

$$(U_xf)(t) = f(x + t),\ (V_yf)(t) = e^{iyt}f(y).$$

Then the following *quantum Bochner's theorem* can be proved [2, 3].

Theorem 3.1. There is a one-one correspondence, given by (5) between the sets of density operators ρ on $\mathcal{H}$ and of complex-valued functions f on $\mathbb{R}^2$ which are normalised, continuous and ω-positive definite.

4. WIGNER QUASIDENSITIES

While true joint probability distributions are characterised by their Fourier transforms, which are normalised continuous nonnegative-definite functions, Wigner distributions are characterised by Fourier transforms which are normalised, continuous and ω-nonnegative definite. The intersection of these two sets is by no means empty. For example in the pure state whose density operator in the Schrödinger representation is the projection $\rho = |\psi_0\rangle\langle\psi_0|$ onto the ground state

$$\psi_0(t) = \pi^{-\frac{1}{4}}e^{-\frac{1}{2}t^2}$$

of the oscillator $\frac{1}{2}(p^2 + q^2)$. it may be verified that the corresponding Wigner distribution is the joint Gaussian distribution with density

$$\gamma(u, v) = \pi^{-1}e^{-(u^2+v^2)} \tag{7}$$

whose Fourier transform is the function

$$f_0(x, y) = e^{-\frac{1}{4}(x^2+y^2)}$$

which is thus both nonnegative definite and ω-nonnegative definite. It follows from the fact that the entry-by entry product $[A_{j,k}B_{j,k}]$ of nonnegative-definite matrices is itself nonnegative-definite that the product of an ω_1-nonnegative-definite and an ω_2-nonnegative-definite function is $\omega_1\omega_2$-nonnegative-definite. Also, an ω-nonnegative definite function is also $\bar{\omega}$-nonnegative-definite. Thus the product ff_0 of an ω-nonnegative definite function f with the function f_0 is both ω-nonnegative definite (since f_0 is nonnegative-definite)and nonnegative-definite (since f_0 is $\bar{\omega}$-nonnegative-definite and $\omega\bar{\omega} \equiv 1$). However such functions ff_0 never correspond to pure states. It can be shown [4] that the only normalised continuous and simultaneously ω-nonnegative definite and nonnegative definite functions f which correspond as in to pure state density operators ρ are of form $\rho = |\psi\ \rangle\langle\psi\ |$ where the state vectors in Schrödinger representation is the exponential of a quadratic polynomial,

$$\psi(t) = \exp(at^2 + bt + c),\ \ a, b, c \in \mathbb{C},\ \ \mathrm{Re}\, a < 0.$$

The corresponding Wigner densities, generalising (7), are bivariate Gaussians

$$\gamma(u, v) = \pi^{-1} e^{-\frac{1}{2}(A(u-l)^2 + 2B(u-l)(v-m) + C(v-m)^2)},\ \ A, B, C, l, m \in \mathbb{R}$$

whose covariance matrices Γ achieve equality in the generalised Heisenberg uncertainty relation

$$\det\Gamma \geq \frac{1}{4}$$

so that $AC - B^2 = 4$.

5. SPIN COMPONENTS

The Pauli spin matrices

$$\sigma_x = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \sigma_y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \sigma_z = \begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$$

satisfy

$$\begin{aligned} \sigma_x^2 &= \sigma_y^2 = \sigma_z^2 = I, \\ \sigma_y\sigma_z &= -\sigma_z\sigma_y = i\sigma_x,\ \sigma_z\sigma_x = -\sigma_x\sigma_z = i\sigma_y,\ \sigma_x\sigma_y = -\sigma_y\sigma_x = i\sigma_x. \end{aligned}$$

Thus, together with the identity matrix I they form a multiplier unitary representation $e \mapsto I$, $x \mapsto \sigma_x$, $y \mapsto \sigma_y$, $z \mapsto \sigma_z$ of the *Klein 4-group* G which is the Abelian group whose four elements e, x, y, z satisfy

$$\begin{aligned} x^2 &= y^2 = z^2 = e, \\ yz &= zy = x,\ zx = xz = y,\ xy = yx = z. \end{aligned}$$

The multiplier ω for this representation is nontrivial, that is, it cannot be expressed in the form

$$\omega(g, h) = \frac{\phi(g + h)}{\phi(g)\phi(h)} \tag{8}$$

for some $\mathbb{T}$-valued function ϕ on G and the multiplier representation cannot thereby be reduced to a true representation, since for example $\omega(x,y) \neq \omega(y,x)$ which is incompatible with (8).

Regarding G as a lcAg with the discrete topology, and noticing that G is isomorphic to the direct sum $\mathbb{Z}_2 \oplus \mathbb{Z}_2$ of two copies of the two element group and is therefore isomorphic to its dual, let us determine the convex set of all normalised ω-nonnegative-definite functions f on the dual group $\hat{G}$. We require that the matrix

$$\begin{bmatrix} 1 & f(x) & f(y) & f(z) \\ f(x) & 1 & if(z) & -if(y) \\ f(y) & -if(z) & 1 & if(x) \\ f(z) & if(y) & -if(x) & 1 \end{bmatrix}$$

be nonnegative. Applying the Schur criterion we find from the nonnegativity in turn, of the principal 2×2 minors

$$1 - f(x)^2 \geq 0, 1 - f(y)^2 \geq 1, 1 - f(z)^2 \geq 0, \tag{9}$$

in particular f must be real-valued, and of the principal 3×3 minors

$$1 - f(x)^2 - f(y)^2 - f(z)^2 \geq 0.$$

The latter condition also ensures nonnegativity of the complete 4×4 determinant. Thus the convex set of all normalised, (trivially) continuous ω-nonnegative-definite functions on $\hat{G}$ coincides with the unit ball $B = \left\{(\xi, \eta, \zeta) \in \mathbb{R}^3 : \xi^2 + \eta^2 + \zeta^2 \leq 1\right\}$. Recalling that the convex set of density operators on $\mathbb{C}^2$ is also affinely equivalent to the unit ball in $\mathbb{R}^3$ by expressing the corresponding density matrix as $\frac{1}{2}(I + \xi\sigma_x + \eta\sigma_y + \zeta\sigma_z)$ we recover the quantum Bochner theorem in this case.

Similarly, to determine the convex set of all normalised nonnegative-definite functions f on $\hat{G}$, we require that the matrix

$$\begin{bmatrix} 1 & f(x) & f(y) & f(z) \\ f(x) & 1 & f(z) & f(y) \\ f(y) & f(z) & 1 & f(x) \\ f(z) & f(y) & f(x) & 1 \end{bmatrix}$$

be nonnegative. Applying the Schur criterion in the same way we find again that (9) holds and f is real valued. But the condition on the principal 3×3 minors is now

$$1 + 2f(x)f(y)f(z) - f(x)^2 - f(y)^2 - f(z)^2 \geq 0, \tag{10}$$

whereas nonnegativity of the whole determinant gives

$$\begin{aligned} & 1 - 2f(x)^2 - 2f(y)^2 - 2f(z)^2 + 8f(x)f(y)f(z) + f(x)^4 + f(y)^4 + f(z)^4 \\ & -2f(y)^2f(z)^2 - 2f(x)^2f(z)^2 - 2f(x)^2f(y)^2 \\ \geq\ & 0, \end{aligned}$$

that is

$$\begin{aligned}
&(1+f(x)+f(y)+f(z))(1+f(x)-f(y)-f(z))(1-f(x)+f(y)-f(z))\\
&(1-f(x)-f(y)+f(z))\\
\geq\ & 0.
\end{aligned}$$

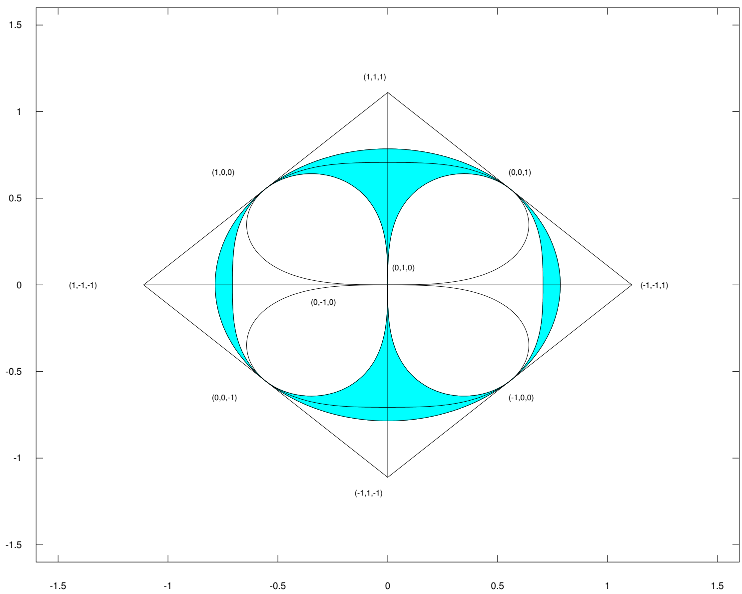

Fig. 1.

The latter condition when combined with (9) is equivalently that $(f(x), f(y), f(z))$ belong to the simplex bounded by the regular tetrahedron T in $\mathbb{R}^3$ whose vertices are the points $(1,1,1)$, $(1,-1,-1)$, $(-1,1,-1)$ and $(-1,-1,1)$. Condition (10) holds automatically for all such points. Thus the convex set of normalised, continuous nonnegative-definite functions on $\hat{G}$ is affinely equivalent to the convex set of probability measures on the 4-point set G in accordance with Bochner's theorem for the lcAg G.

The midpoints of the edges of the tetrahedron T are the points $(\pm 1, 0, 0,)$, $(0, \pm 1, 0)$ and $(0, 0, \pm 1)$ of B. Thus T is *escribed* to B in the sense that its edges are tangent to the unit sphere; see Figure 1. Note that neither of T or B is contained in the other. The set of pure states which correspond in this way to classical probability measures (that is, the analogues of the pure Gaussian states which have nonnegative Wigner densities) is coextensive with the region of the unit sphere in $\mathbb{R}^3$ which remains after the excision of the four mutually tangent small circles which are external to T cut by the faces

$$-\xi+\eta+\zeta=1,\ \xi-\eta+\zeta=1,\ \xi+\eta-\zeta=1,\ \xi+\eta+\zeta=-1$$

of T.

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REFERENCES

[1] S. Bochner: Lectures on Fourier Integrals. Princeton University Press 1959.

[2] C. D. Cushen: Quasi-characteristic functions of canonical observcables in quantum mechanics. Nottingham PhD Thesis 1970.

[3] A. S. Holevo: Veroiatnostnye i statistichneskie aspekty kvantovoi teorii. Nauka, Moscow 1980, English translation Probabilistic and statistical aspects of quantum theory, North Holland 1982.

[4] R. L. Hudson: When is the Wigner quasi-probability density nonnegative? Rep. Math. Phys. *6* (1974), 249–252.

[5] I. I. Gikhman and A. V. Skorohod: Introduction to the Theory of Random Processes. Philadelphia 1969.

[6] J. von Neumann: Die Eindeutigkeit der Schrõdingerschen Operatoren. Math. Ann. *104* (1931), 570–578.

[7] J. C. T. Pool: Mathematical aspects of the Weyl correspondence. J. Math. Phys. *7* (1966), 66–76.

[8] W. Rudin: Fourier Analysis on Groups. Interscience New York 1962.

[9] E. Wigner: On the quantum correction to thermodynamic equilibrium. Phys. Rev. *40* (1932), 749–759.

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