QUANTUM MECHANICS - HOW WEIRD FOR BAYESIANS?

F.H. Fröhner
Kernforschungszentrum Karlsruhe
Institut für Neutronenphysik und Reaktortechnik
Postfach 3640, W-7500 Karlsruhe 1
Germany.

ABSTRACT. Quantum mechanics is spectacularly successful on the technical level. The meaning of its rules appears, however, shrouded in mystery even today, more than sixty years after its inception. Quantum-mechanical probabilities are often said to be "operator-valued" and therefore fundamentally different from "classical" probabilities, in disregard of the work of Cox (1946) – and of Schrödinger (1947) – on the foundations of probability theory. One central question concerns the superposition principle, i. e. the need to work with interfering wave functions, the absolute squares of which are the probabilities. Other questions concern the collapse of the wave function when new data become available. These questions are reconsidered from the Bayesian viewpoint. The superposition principle is found to be a consequence of an apparently little-known theorem for non-negative Fourier polynomials published by Fejér (1915). Combined with the classical Hamiltonian equations for point particles, it yields all basic features of the quantum-mechanical formalism. It is further shown that the correlations in the spin pair version of the Einstein-Podolsky-Rosen experiment can easily be calculated classically, in contrast to EPR lore. All this demystifies the quantum-mechanical formalism to quite some extent. Questions about the origin and the empirical value of Planck's quantum of action remain; finite particle size may be part of the answer.

1. The Riesz-Fejér Theorem and Quantum-Mechanical Probabilities

In his work on Fourier series L. Fejér (1915) published a proof given by F. Riesz of the following theorem (see Appendix): Each non-negative Fourier polynomial (truncated Fourier series) of order n (maximal wave number n) can be expressed as the absolute square of a Fourier polynomial of (at most) the same order,

$$0 \le \rho(x) \equiv \sum_{l=-n}^{n} c_l\, e^{ilx} = \Big| \sum_{k=-n}^{n} a_k\, e^{ikx} \Big|^2 \equiv \big|\psi(x)\big|^2 , \tag{1}$$

where the Fourier polynomial $\psi(x)$ is not restricted to non-negative values, in contrast to the Fourier polynomial $\rho(x)$. Our notation anticipates the obvious application to quantum-mechanical probability densities ρ and probability wave functions ψ (without excluding

A. Mohammad-Djafari and G. Demoments (eds.), Maximum Entropy and Bayesian Methods, 205–212.

application to other inherently positive quantities such as intensities of classical energy-carrying waves). Fourier techniques are most convenient whenever wave or particle propagation constrained by initial or boundary conditions is to be described. Constraints such as point sources, slits, scatterers etc. define, together with the wave equation for the Fourier components, eigenvalue problems whose eigenfunctions are all those waves which are possible under the given circumstances.

In quantum mechanics it is customary to introduce (infinite) Fourier series by the familiar device of the periodicity box. We note that

(a) infinite Fourier series can be approximated by finite Fourier polynomials to any desired accuracy if the order n is chosen high enough;

(b) the transition to Fourier integrals describing arbitrary nonperiodic processes is achieved if the box is made bigger and bigger.

In view of these uneventful generalisations we may consider the Riesz-Fejér theorem as equivalent to the wave-mechanical superposition principle: Probabilities are to be calculated as absolute squares of wave functions that can be expressed as linear superpositions of orthogonal functions. In Eq. 1 the orthogonal functions are standing waves in a (one-dimensional) periodicity box. Other possible orthogonal bases are generated by unitary transformations. Historically the superposition principle had been established first, as a rather puzzling empirical feature of the quantum world, before Born found that the absolute square of the wave function can be interpreted as a probability density.

If, on the other hand, one starts with probabilities, the superposition principle, far from puzzling, appears as a theorem, valid not only in quantum mechanics but *throughout probability theory* (cf. e. g. Feller 1966 on L^2 theory). The much discussed role of the phases of the superposed functions is also clarified: *They ensure faithful reproduction of the nonnegative probability density* $\rho(x)$ in Eq. 1. Furthermore, there is no reason to consider "operator-valued" quantum-mechanical probabilities as fundamentally different from "ordinary" ones. In fact, any such difference would contradict the results of Cox (1946), Schrödinger (1946) and Rényi (1954) who found that any formal system of logical inference must be equivalent to ordinary probability theory, with probability understood as a numerical scale of rational expectation (or incomplete knowledge) in the tradition of Bernoulli and Laplace (and Heisenberg 1930), – otherwise it is bound to contain inconsistencies.

With this understanding there is nothing strange about the "collapse of the wave function" when new data become available. Their utilisation by means of Bayes' theorem inevitably changes all prior probabilities to posterior ones. As this is not a physical but a *logical* change, questions about its sudden (superluminal) occurrence throughout physical space, or about the exact time of death of Schrödinger's cat, do not arise for Bayesians - who are quite prepared to reason even backwards in time.

2. Mechanics of Particles with Uncertain Initial Coordinates

Let us consider a classical particle. Its energy as a function of its location $\mathbf{x}$ and momentum $\mathbf{p}$ is given by the Hamilton function $H = H(\mathbf{x}, \mathbf{p})$; its motion is determined by Hamilton's canonical equations

$$\frac{d\mathbf{x}}{dt} = \frac{\partial H}{\partial \mathbf{p}} , \qquad (2) \qquad \frac{d\mathbf{p}}{dt} = -\frac{\partial H}{\partial \mathbf{x}} . \qquad (3)$$

For given initial phase space coordinates, $\{\mathbf{x}(0), \mathbf{p}(0)\}$, one obtains the trajectory in phase space, $\{\mathbf{x}(t), \mathbf{p}(t)\}$, by integration of the canonical equations, for $t < 0$ as well as for $t > 0$.

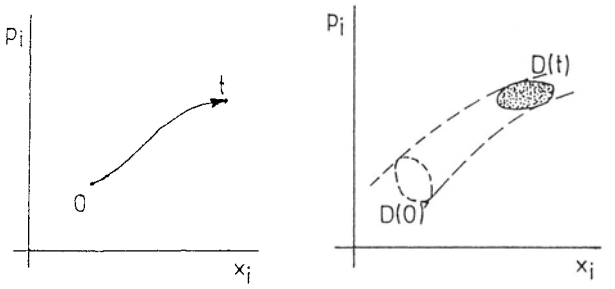

Fig. 1 – Classical particle trajectories in phase space without and with initial uncertainty

If the initial coordinates are uncertain, lying somewhere in a phase space domain $D(0)$, there is a multitude of possible trajectories (Fig. 1). At time t the possible values of $\mathbf{x}(t)$ and $\mathbf{p}(t)$ lie in a domain $D(t)$ that has the same size as $D(0)$: The canonical equations imply that the divergence in phase space is zero,

$$\sum_{i=1}^{3} \left(\frac{\partial}{\partial x_i} \frac{dx_i}{dt} + \frac{\partial}{\partial p_i} \frac{dp_i}{dt} \right) = 0 \tag{4}$$

(Liouville's theorem, valid already separately for each pair x_i, p_i). More generally the initial uncertainty can be described by a continuous probability density. Let us consider a time-dependent spatial probability density $\rho(\mathbf{x},t) = |\psi(\mathbf{x},t)|^2$ in a periodicity box so large that the Fourier polynomials of the Riesz-Fejér theorem can be replaced by Fourier integrals. The resulting wave function and its Fourier transform,

$$\psi(\mathbf{x},t) = (2\pi)^{-3/2} \int d^3k\, \varphi(\mathbf{k},0)\, e^{i(\mathbf{kx}-\omega t)}\,, \tag{5}$$

$$\varphi(\mathbf{k},t) = (2\pi)^{-3/2} \int d^3x\, \psi(\mathbf{x},0)\, e^{-i(\mathbf{kx}-\omega t)}\,, \tag{6}$$

both normalised to unity, are superpositions of waves propagating with phase velocities ω/k in directions $\mathbf{k}/k$. The resulting averages,

$$\langle \mathbf{x}(t) \rangle = \int d^3x \left|\psi(\mathbf{x},t)\right|^2 \mathbf{x} = \int d^3k\, \varphi(\mathbf{k},t)^* \frac{i\partial}{\partial \mathbf{k}} \varphi(\mathbf{k},t)\,, \tag{7}$$

$$\langle \mathbf{k}(t) \rangle = \int d^3k \left|\varphi(\mathbf{k},t)\right|^2 \mathbf{k} = \int d^3x\, \psi(\mathbf{x},t)^* \frac{\partial}{i\partial \mathbf{x}} \psi(\mathbf{x},t)\,, \tag{8}$$

show that $|\varphi|^2$ is the probability density in $\mathbf{k}$ representation corresponding to the probability density $|\psi|^2$ in $\mathbf{x}$ representation. Furthermore, the factor $\mathbf{k}$ in $\mathbf{k}$ representation is replaced by the operator $-i\partial/\partial\mathbf{x}$ in $\mathbf{x}$ representation, and the factor $\mathbf{x}$ in $\mathbf{x}$ representation is replaced by the operator $i\partial/\partial\mathbf{k}$ in $\mathbf{k}$ representation. Similarly one finds

$$\langle \omega \rangle = \int d^3x\, \psi(\mathbf{x},t)^* \frac{i\partial}{\partial t} \psi(\mathbf{x},t) = \int d^3k\, \varphi(\mathbf{k},t)^* \frac{i\partial}{\partial t} \varphi(\mathbf{k},t) \tag{9}$$

which shows that ω is equivalent to the operator $i\partial/\partial t$ in both representations. The familiar wave-mechanical uncertainty relations for Fourier transforms are

$$\Delta x_i \, \Delta k_j \geq \frac{1}{2}\delta_{ij} \, , \qquad (i,j = 1,2,3) \, , \tag{10}$$

where Δx_i and Δk_j are root-mean-square deviations.

For a free particle, not influenced by forces, one finds from Eqs. 7 and 8 the expectation values (best estimates under quadratic loss)

$$\langle \mathbf{x}(t) \rangle = \int d^3k \, \varphi(\mathbf{k},0)^* \Big(\frac{i\partial}{\partial \mathbf{k}} \varphi(\mathbf{k},0) + \varphi(\mathbf{k},0) \frac{\partial \omega}{\partial \mathbf{k}} t \Big) = \langle \mathbf{x}(0) \rangle + \Big\langle \frac{\partial \omega}{\partial \mathbf{k}} \Big\rangle_{t=0} t \, , \tag{11}$$

$$\langle \mathbf{k}(t) \rangle = \int d^3k \, \varphi(\mathbf{k},0)^* \mathbf{k} \varphi(\mathbf{k},0) = \langle \mathbf{k}(0) \rangle \, , \tag{12}$$

describing linear translation with group velocity $\langle \partial\omega/\partial\mathbf{k} \rangle$. Their time derivatives,

$$\frac{d\langle \mathbf{x} \rangle}{dt} = \Big\langle \frac{\partial \omega}{\partial \mathbf{k}} \Big\rangle \, , \tag{13}$$

$$\frac{d\langle \mathbf{k} \rangle}{dt} = 0 \, , \tag{14}$$

can be compared with the expectation values

$$\frac{d\langle \mathbf{x} \rangle}{dt} = \Big\langle \frac{\partial H}{\partial \mathbf{p}} \Big\rangle \, , \tag{15}$$

$$\frac{d\langle \mathbf{p} \rangle}{dt} = 0 \, , \tag{16}$$

that follow from Hamilton's canonical equations for a free particle. Evidently we can take $\mathbf{k} \propto \mathbf{p}$ and $\omega \propto H$ (if we disregard uninteresting additive constants). Denoting the common proportionality constant by $\hbar$ we get de Broglie's particle-wave transcription,

$$H = \hbar\omega \, , \tag{17}$$

$$\mathbf{p} = \hbar\mathbf{k} \, , \tag{18}$$

and, from Eq. 10, Heisenberg's quantum-mechanical uncertainty relations,

$$\Delta x_i \, \Delta p_j \geq \frac{\hbar}{2}\delta_{ij} \, , \qquad (i,j = 1,2,3) \, , \tag{19}$$

comparable to Liouville's theorem – see Figs. 1 and 2. The equality sign applies if $|\psi|^2$ is a (three-dimensional) Gaussian, the *maximum entropy distribution* for given $\langle \mathbf{x} \rangle$ and $\langle \mathbf{x}^2 \rangle$. Expectation values of physical quantities that depend on both $\mathbf{x}$ and $\mathbf{p}$, such as the Hamilton function $H(\mathbf{p},\mathbf{x}) = \mathbf{p}^2/(2m) + V(\mathbf{x})$ of a particle with mass m moving in a potential $V(\mathbf{x})$, can be calculated from ψ or φ with the appropriate operators. For example, the best estimate of the orbital angular momentum with respect to the origin, $\mathbf{x} = 0$, is

$$\langle \mathbf{x} \times \mathbf{p} \rangle = \int d^3x \, \psi^* (\mathbf{x} \times \frac{\hbar}{i} \frac{\partial}{\partial \mathbf{x}}) \psi = \int d^3k \, \varphi^* \Big(\frac{i\partial}{\partial \mathbf{k}} \times \hbar\mathbf{k} \Big) \varphi \, . \tag{20}$$

Real expectation values imply Hermitean (self-conjugate) operators. If ψ is one of the eigenfunctions of the operator, the variance vanishes. If, for instance, ψ is an eigenfunction of the operator $H = i\hbar\partial/\partial t$, with eigenvalue E, satisfying the Schrödinger equation

$$H\psi = E\psi \tag{21}$$

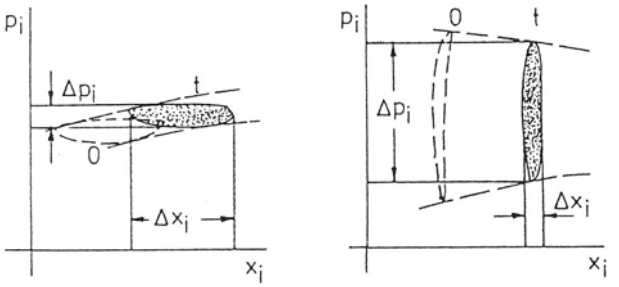

Fig. 2 – Phase space illustration of Heisenberg's uncertainty relations, Eq. 19. Left side: wave-like behaviour with well-defined momentum (wave length) but ill-defined location. Right side: particle-like behaviour with ill-defined momentum (wave length) but well-defined location.

(for given boundary conditions), one has $\langle H \rangle = E$ and var $H = \langle H^2 \rangle - \langle H \rangle^2 = 0$: The estimated energy is E without any uncertainty.

Thus we obtain, for a classical particle obeying Hamilton's canonical equations, the basic formal apparatus of quantum mechanics – complete with wave-particle duality, operator calculus including commutation rules, uncertainty relations and Schrödinger equation. All we had to do was to admit finite uncertainties of the phase space coordinates. The Riesz-Fejér theorem permits then unrestricted use of Fourier series – the proper tool for dealing with boundary conditions and similar constraints – in a way that guarantees the non-negativity of all probability densities. Planck's quantum of action appears naturally, as a "blurring" parameter, in such a probability theory of classical particles that move according to the Hamiltonian equations. Its role as a limit to attainable accuracies in phase space is clear from Heisenberg's uncertainty relations (see Fig. 2).

3. Spin Correlations

Generalisation to several indistinguishable particles and to additional attributes such as spins is straightforward. In the spin version of the famous Einstein-Podolsky-Rosen (1935) experiment one considers a particle with spin zero that decays into two particles, each with spin 1/2, flying in opposite directions. Because angular momentum is conserved, the spins of the two particles must be antiparallel, $\boldsymbol{\sigma}_1 = -\boldsymbol{\sigma}_2$. If one of the spin components of particle 1 is measured as pointing up, the same spin component of particle 2 is immediately known to be pointing down (which can be confirmed experimentally). More generally, one finds that the correlation of arbitrary spin coordinates $(\mathbf{a} \cdot \boldsymbol{\sigma}_1)$ and $(\mathbf{b} \cdot \boldsymbol{\sigma}_2)$ is given by

$$\langle (\mathbf{a} \cdot \boldsymbol{\sigma}_1)(\boldsymbol{\sigma}_2 \cdot \mathbf{b}) \rangle = -\mathbf{a} \cdot \mathbf{b} \; = -\cos(\mathbf{a}, \mathbf{b}) \; , \tag{22}$$

where $\mathbf{a}$ and $\mathbf{b}$ are unit vectors along two arbitrary analyser directions. This result is obtained quantum-mechanically if one describes the singlet state (total spin zero) by the antisymmetric fermion wave vector (wave function for the two discrete possibilities "spin up" and "spin down" of the two particles)

$$\psi = \frac{1}{\sqrt{2}} \left[\begin{pmatrix} 1 \\ 0 \end{pmatrix}_1 \begin{pmatrix} 0 \\ 1 \end{pmatrix}_2 - \begin{pmatrix} 0 \\ 1 \end{pmatrix}_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix}_2 \right] , \tag{23}$$

and the spin coordinates by Pauli matrices,

$$\boldsymbol{\sigma}_i = \{\sigma_{xi}, \sigma_{yi}, \sigma_{zi}\} = \left\{ \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}_i, \begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}_i, \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}_i \right\} \qquad (i = 1,2) \qquad (24)$$

where the subscripts 1 and 2 refer to particles 1 and 2, and the subscripted matrix operators act only on column vectors with the same subscript. Expectation values are calculated as $\langle \ldots \rangle \equiv \psi^\dagger \ldots \psi$ which yields Eq. 22, and also

$$\langle \mathbf{a} \cdot \boldsymbol{\sigma}_1 \rangle = 0 \,, \qquad (25)$$

$$\langle (\mathbf{a} \cdot \boldsymbol{\sigma}_1)^2 \rangle = 1 \,, \qquad (26)$$

$$\langle \sigma_{x1}^2 \rangle = \langle \sigma_{y1}^2 \rangle = \langle \sigma_{z1}^2 \rangle = \langle \boldsymbol{\sigma}_1^2 \rangle / 3 = 1 \qquad (27)$$

(similarly for $\mathbf{b}$ and $\boldsymbol{\sigma}_2$). Because of $\operatorname{var} x \equiv \langle (x - \langle x \rangle)^2 \rangle$, $\operatorname{cov}(x,y) \equiv \langle (x - \langle x \rangle)(y - \langle y \rangle) \rangle$, one recognises (26) as the variance of $(\mathbf{a} \cdot \boldsymbol{\sigma}_1)$, and (22) as the covariance of the spin coordinates $(\mathbf{a} \cdot \boldsymbol{\sigma}_1)$ and $(\mathbf{b} \cdot \boldsymbol{\sigma}_2)$. The latter is numerically equal to the correlation coefficient, $r(x,y) \equiv \operatorname{cov}(x,y) / \sqrt{\operatorname{var} x \operatorname{var} y}$.

It is often stated that the correlation (22) cannot be obtained classically. Its confirmation by experiment is then taken as evidence that the spin coordinates cannot exist simultaneously before a measurement reveals one of them, in accordance with N. Bohr's (1935) epistemological interpretation of quantum mechanics but at variance with the ontological view of Einstein, Podolsky and Rosen (1935). Since, however, the quantum-mechanical result (22) does not contain Planck's constant one expects that a classical derivation is possible – as, for instance, in the case of the Rutherford scattering formula. Let us therefore consider the spin $\boldsymbol{\sigma}_1 = -\boldsymbol{\sigma}_2$ as an ordinary vector, for which all orientations are equally possible. Expectation values are then to be calculated classically as

$$\langle \ldots \rangle \equiv \int_0^\infty d\sigma_1 \, \rho(\sigma_1) \int_{-1}^{+1} \frac{d(\cos\vartheta)}{2} \int_0^{2\pi} \frac{d\varphi}{2\pi} \ldots \,, \qquad (28)$$

where $\rho(\sigma_1)$ is the probability density of the length $\sigma_1 = |\boldsymbol{\sigma}_1|$ of both spin vectors and ϑ, φ are the polar angle and azimuth of $\boldsymbol{\sigma}_1$. Without any difficulty one finds

$$\langle (\mathbf{a} \cdot \boldsymbol{\sigma}_1)(\boldsymbol{\sigma}_2 \cdot \mathbf{b}) \rangle = -\langle (\mathbf{a} \cdot \boldsymbol{\sigma}_1)(\boldsymbol{\sigma}_1 \cdot \mathbf{b}) \rangle = -\frac{\langle \boldsymbol{\sigma}_1^2 \rangle}{3} (\mathbf{a} \cdot \mathbf{b}) \qquad (29)$$

which, with $\langle \boldsymbol{\sigma}_1^2 \rangle / 3 = 1$ (cf. Eq. 27), is equal to the quantum-mechanical result. Hence the correlation measurements alone do not rule out the ontological viewpoint, i. e. reality of unobserved spin components. On the other hand, if one treats the quantum-mechanical spin eigenvalues, $+1$ or -1, measured along $\mathbf{a}$ and $\mathbf{b}$, as determined by hidden variables, one gets the inequalities derived by Bell (1964) that are, in fact, contradicted by experiment. That Bell's inequalities are only valid for a certain class of hidden-variable models, and hence less general than is commonly believed, was pointed out by Jaynes (1989).

4. Summary

The formalism of quantum mechanics, in the traditional axiomatic presentation, seems mysterious. It emerges naturally, however, if one handles phase space uncertainties for classical point particles wave-mechanically, by means of the Riesz-Fejér superposition theorem,

– which by the way dispels any doubts about the *linearity* of the theory. Planck's quantum of action appears automatically, as a "blurring" parameter. The *nonlocality* (instantaneous collapse of the wave function throughout physical space if new information is taken into account) follows from Born's interpretation of $|\psi|^2$ as a probability density and from the Bayesian scheme for the updating of knowledge. There is no reason to doubt that physical quantities, such as the spin coordinates in the spin version of the Einstein-Podolsky-Rosen experiment, have a *reality independent of the observer*, in obvious contrast to eigenfunction expansions and eigenvalues that reflect his choice of measurement. From this viewpoint *quantum mechanics looks much like an error propagation formalism for uncertainty-afflicted physical systems that obey the classical equations of motion.*

What remains mysterious, however, is the *irreducible uncertainty* enforced by the empirical finite and universal value of the blurring parameter $\hbar$. That this value is the same for electrons, nucleons, photons etc. is not too surprising since their mutual interactions conserve energy and momentum. Its role as a limit to the attainable information and control in microphysics has been clear ever since Heisenberg (1930) discussed his uncertainty relations: Phase space trajectories and orbits are always affected by a non-removable minimum blur. As finite particle size would produce a similar blur, one is tempted to ask if quantum mechanics can perhaps be viewed as a kind of minimum information (maximum entropy) generalisation of probabilistic Hamiltonian mechanics *from mass points to particles with finite extension* (spatial distribution) *and internal motion* (momentum distribution, spin). How this conjecture compares with others, such as zitterbewegung, granular space-time structure, or superstrings, remains to be seen.

Appendix: Proof of the Riesz-Fejér Theorem

The proof presented by L. Fejér (1915) as due to F. Riesz is given here in slightly different notation. Consider the real Fourier polynomial

$$\rho(x) = \rho(x)^* = \sum_{l=-n}^{n} c_l\, e^{ilx} \,, \qquad (c_l = c_{-l}^*) \tag{A1}$$

Defining the polynomial $g(z)$ as

$$g(z) \equiv c_n^* + \ldots + c_1^* z^{n-1} + c_0 z^n + c_1 z^{n+1} + \ldots + c_n z^{2n} \tag{A2}$$

one can write $\rho(x) = e^{-nix} g(e^{ix})$. If the Fourier polynomial is non-negative, this becomes

$$\rho(x) = |g(e^{ix})|. \tag{A3}$$

The polynomial $g(z)$ is of degree $2n$ if $c_n \neq 0$, so that $g(0) \neq 0$. If z_k is a solution of $g(z) = 0$,

$$g(z_k) = c_n^* + \ldots + c_n z_k^{2n} = 0 \,, \tag{A4}$$

then $1/z_k^*$ is another solution,

$$g(\frac{1}{z_k^*}) = [(c_n^* + \ldots + c_n z_k^{2n}) z_k^{-2n}]^* = 0 \,. \tag{A5}$$

One concludes that each root z_k is accompanied by another root $1/z_k^*$. (Recall that $z = 0$ is not a root.) On the unit circle, $z = e^{i\varphi}$, both roots coincide. If the root z_k is of multiplicity m one has $2m$ roots on the unit circle. Thus a complete set of independent roots contains, for instance, those within the unit circle and half of those on the unit circle itself, with due account of multiple roots. One gets

$$g(z) = c_n \prod_{k=1}^{n} (z - z_n)(z - \frac{1}{z_k^*}) \tag{A6}$$

and, with $z = e^{ix}$,

$$\rho(x) = |g(e^{ix})| = \left| \sqrt{c_n} \prod_{k=1}^{n} \frac{e^{ix} - z_k}{\sqrt{z_k}} \right|^2 . \tag{A7}$$

This is the absolute square of a Fourier polynomial of the same order as $\rho(x)$ so we can write

$$\rho(x) = \sum_{l=-n}^{n} c_l e^{ilx} = |\psi(x)|^2 , \qquad -\pi < x \leq \pi \tag{A8}$$

$$\psi(x) = e^{i\alpha} \sqrt{\left| \frac{c_n}{z_1 \ldots z_n} \right|} \prod_{k=1}^{n} (e^{ix} - z_k) , \qquad (\alpha \text{ arbitrary}) , \tag{A9}$$

which completes the (constructive) proof that each non-negative Fourier polynomial can be written as the absolute square of an unrestricted Fourier polynomial of (at most) the same order (same highest harmonic), with an arbitrary phase factor.

ACKNOWLEDGMENTS. It is a pleasure to thank R. Balian for valuable discussions.

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