Complex Probabilities on R^N as Real Probabilities on C^N and an Application to Path Integrals

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We establish a necessary and sufficient condition for averages over complex-valued weight functions on R^N to be represented as statistical averages over real, non-negative probability weights on C^N. Using this result, we show that many path integrals for time-ordered expectation values of bosonic degrees of freedom in real-valued time can be expressed as statistical averages over ensembles of paths with complex-valued coordinates, and then speculate on possible consequences of this result for the relation between quantum and classical mechanics.

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For a wide range of quantum mechanical systems, if real-valued time is analytically continued to imaginary values, the weight assigned to each path in the path-integral formula for time-ordered vacuum expectation values becomes real and non-negative, permitting interpretation as a probability density. Paths distributed according to this probability density can then be generated by the Metropolis method, one version of which makes use of the Langevin equation.

For the Langevin equation applied to paths for imaginary time path integrals, however, the coefficients entering the equation are themselves analytic functions of the action occurring in the path weight. As a consequence of this analyticity, the Langevin equation can be analytically continued, at least formally, to complex-valued weights [1], among which are those of the original path integral with real-valued time. For complex path weights, the coefficients in the analytically continued Langevin equation and the coordinates in the path ensembles the equation generates are complex.

Numerical tests and some analytic results concerning the Langevin equation with complex coefficients yield a complicated picture [2]. For some systems the method gives accurate answers, for others values of the coordinates blow up as the equation's running time is increased, and in still other applications averages over complex Langevin trajectories converge but to wrong answers. A question which follows from these results is whether the failure of the Langevin equation for many complex-valued path weights is simply a limitation of the Langevin equation or, alternatively, arises from the nonexistence of equivalent real, non-negative weights on complex-valued trajectories. More generally, with no reference to the Langevin equation, under what circumstances can averages over complex weights on real coordinates be realized as statistical averages over real, non-negative weights on complex coordinates? The main result addressing this problem so far is a proof [3] that an average over real coordinates of a complex polynomial multiplied by a complex Gaussian can be realized as an average over a real, non-negative weight on complex coordinates.

In this Letter, by an explicit construction unrelated to the Langevin equation, we establish a necessary and sufficient condition for averages on R^N over complex weight functions, with no explicit restriction on functional form, to be represented as averages over real, non-negative probability densities on C^N. For the particular case of $N = 1$, we show this condition is fulfilled for all complex weights normalized to a total integral of 1.

As an application of our result for general N, we show that real-time path integrals for many systems with bosonic degrees of freedom can be represented as averages over ordinary statistical ensembles of paths through complex space. Among the systems which can be represented in this way are scalar field theories, in any space-time dimension, with self-interaction ϕ^p, p even, field theories, in any dimension, with bosonic degrees of freedom which range only over a bounded region, and therefore lattice gauge field theories over any compact gauge group. We then briefly speculate on possible consequences of this result for the relation between quantum and classical mechanics.

The systems we consider all have time reduced to a finite, discrete lattice of points. We do not examine the existence of limits as the time lattice spacing is taken to zero. We also do not discuss algorithms for actually generating averages over the probability densities on C^N which we prove exist.

For $c(x_1, \ldots, x_N)$ a complex-valued weight function on $(x_1, \ldots, x_N) \in R^N$, $t(z_1, \ldots, z_N)$ a real, non-negative weight on $(z_1, \ldots, z_N) \in C^N$, and $p(r_1, \ldots, r_N)$ a real, non-negative weight on $(r_1, \ldots, r_N) \in [0, \infty)^N$, define the expectation values

$$\langle f \rangle_c = Z_c^{-1} \prod_j \left(\int_{-\infty}^{\infty} dx_j \right) f(x_1, \ldots, x_N) c(x_1, \ldots, x_N), \quad (1a)$$

$$\langle f \rangle_t = Z_t^{-1} \prod_j \left(\int_0^{2\pi} d\theta_j \int_0^{\infty} r_j dr_j \right) f(z_1, \ldots, z_N) \times t(z_1, \ldots, z_N), \quad (1b)$$

$$\langle f \rangle p = Z_p^{-1} \prod_j \left(\int_0^{\infty} dr_j \right) f(r_1, \ldots, r_N) p(r_1, \ldots, r_N), \quad (1c)$$

with z_j given by $r_j \exp(i\theta_j)$ in Eq. (1b). We require $c(x)$, $t(z)$, and $p(r)$ to have nonzero total integrals, then choose Z_c, Z_t, and Z_p to give $\langle 1\rangle_c$, $\langle 1\rangle_t$, and $\langle 1\rangle_p$ all the value 1.

We will show that for any $c(x_1, \ldots, x_N)$, a necessary and sufficient condition for the existence of a $t(z_1, \ldots, z_N)$ with the same moments

$$\langle x_1^{m_1} \cdots x_N^{m_N}\rangle_c = \langle z_1^{m_1} \cdots z_N^{m_N}\rangle_t \tag{2}$$

for all integer $m_j \geq 0$, is that there exists a $p(r_1, \ldots, r_N)$ satisfying the bound

$$|\langle x_1^{m_1} \cdots x_N^{m_N}\rangle_c| \leq \langle r_1^{m_1} \cdots r_N^{m_N}\rangle_p \tag{3}$$

for all integer $m_j \geq 0$.

For notational simplicity, we consider first a detailed proof for $N = 1$, then briefly summarize the generalization to arbitrary N.

To show that Eq. (2) implies Eq. (3) for some $p(r)$, we take absolute values of both sides of Eq. (2) and obtain

$$\left| Z_c^{-1} \int_{-\infty}^{\infty} x^m c(x)dx \right| \leq Z_t^{-1} \int_0^{\infty} r^m p(r)dr, \tag{4a}$$

$$p(r) = r \int_0^{2\pi} d\theta t(z). \tag{4b}$$

But Z_p is identical to Z_t. Thus Eqs. (4) imply Eq. (3).

We now assume Eq. (3) and construct a $t(z)$ which satisfies Eq. (2). For z given by $r\exp(i\theta)$ as before and a real parameter $\lambda > 1$, Eq. (3) implies we can define the functions

$$q_\lambda(\theta) = \sum_{m\geq 0} \frac{\exp(-im\theta)\langle x^m\rangle_c}{\lambda^m \langle r^m\rangle_p} - 1. \tag{5a}$$

$$s_\lambda(\theta) = \{1 + 2\mathrm{Re}[q_\lambda(\theta)]\}. \tag{5b}$$

Equations (5) imply for $m \geq 0$

$$\int_0^{2\pi} \frac{d\theta}{2\pi} \exp(im\theta) s_\lambda(\theta) = \frac{\langle x^m\rangle_c}{\lambda^m \langle r^m\rangle_p}. \tag{6}$$

With the definitions

$$\langle f\rangle_{\lambda t} = Z_{\lambda t}^{-1} \int_0^{2\pi} d\theta \int_0^{\infty} dr r f(z) t_\lambda(z), \tag{7a}$$

$$t_\lambda(z) = r^{-1} p(\lambda^{-1} r) s_\lambda(\theta), \tag{7b}$$

and $Z_{\lambda t}$ chosen to make $\langle 1\rangle_{\lambda t} = 1$, Eqs. (6) and (7) then yield

$$\langle z^m\rangle_{\lambda t} = \langle x^m\rangle_c, \tag{8}$$

which is Eq. (2) for $N = 1$.

By a choice of λ we can ensure that $t_\lambda(z)$ is non-negative. From Eq. (7b) it follows that $t_\lambda(z)$ is non-negative if $s_\lambda(\theta)$ is non-negative. Equations (3) and (5) then yield

$$s_\lambda(\theta) \geq 1 - 2|q_\lambda(\theta)|, \tag{9a}$$

$$\geq 1 - 2 \sum_{m\geq 1} \frac{|\langle x^n\rangle_c|}{\lambda^m \langle r^n\rangle_p}, \tag{9b}$$

$$\geq \frac{\lambda - 3}{\lambda - 1}. \tag{9c}$$

Equation (9c) implies that for $\lambda \geq 3$, $t_\lambda(z)$ is non-negative.

Consider now arbitrary N. The proof that Eq. (2) implies Eq. (3) for some $p(r_1, \ldots, r_N)$ for arbitrary N is an immediate extension of the $N = 1$ proof. The proof that Eq. (3) implies Eq. (2) requires very little more effort. For general N, $q_\lambda(\theta)$ of Eq. (5a) becomes

$$q_\lambda(\theta_1, \ldots, \theta_N) = \sum_{m_i\geq 0} \frac{\exp(-i\sum_i m_i\theta_i)\langle x_1^{m_1} \ldots x_N^{m_N}\rangle_c}{\lambda \sum_i m_i \langle r_1^{m_1} \ldots r_N^{m_N}\rangle_p} - 1. \tag{10}$$

Equation (9c), ensuring the positivity of $s_\lambda(z_1, \ldots, z_N)$ and therefore of $t_\lambda(z_1, \ldots, z_N)$, becomes

$$s_\lambda(\theta_1, \ldots, \theta_N) \geq 3 - \frac{2\lambda^N}{(\lambda - 1)^N}, \tag{11}$$

the right side of which is positive for

$$\lambda \geq \frac{1}{1 - (\frac{2}{3})^{1/N}}. \tag{12}$$

Returning to the case of $N = 1$, we now show that a $p(r)$ exists, fulfilling Eq. (3) for any $c(x)$ with $\langle 1\rangle_c$ of 1 [4]. To do this, we make use of a theorem giving conditions for the existence of a $p(r)$ such that for all non-negative integers m

$$\langle r^m\rangle_p = s_m, \tag{13}$$

for a specified sequence of real numbers $s_0, s_1, \ldots$. From the s_m, for any non-negative integer n, define the $(n + 1) \times (n + 1)$ matrices

$$H_{ij}^{2n} = s_{i+j}, \tag{14a}$$

$$H_{ij}^{2n+1} = s_{i+j+1}, \tag{14b}$$

with $0 \leq i, j \leq n$. Then according to a result of Stieltjes [5] a $p(r)$ obeying Eq. (13) exists if for all non-negative n

$$\det(H^n) > 0. \tag{15}$$

For any $c(x)$, we will construct a sequence $s_0, s_1, \ldots$, obeying both Eqs. (3) and (15). Choose s_0 to be 1. Now suppose $s_0, s_1, \ldots, s_k$, have been found obeying Eqs. (3) and (15) for all $n \leq k$. By isolating the dependence of $\det(H^{k+1})$ on s^{k+1}, it is not hard to show that a positive real bound b exists, such that Eq. (15) is fulfilled for $n = k + 1$ for any $s_{k+1} > b$. We choose s_{k+1} to be the greater of $|\langle x^{k+1}\rangle_c|$ and b. By induction, the resulting sequence $s_0, s_1, \ldots$ obeys Eqs. (3) and (15) for all m. It follows that a $p(r)$ exists fulfilling Eq. (13) and thus also Eq. (3).

The result we have just proved cannot be extended automatically to $N > 1$ since, for $N > 1$, the analog of Eq. (15) is not a sufficient condition for the existence of a $p(r_1, \ldots, r_N)$ fulfilling the analog of Eq. (13) [6].

For each $c(x_1, \ldots, x_N)$ obeying Eq. (3) for some $p(r_1, \ldots, r_N)$, the non-negative, real $t_\lambda(z_1, \ldots, z_N)$ we construct satisfying Eq. (2) is only one representative of a large family of such functions fulfilling Eq. (2). At the very least, given any $p(r_1, \ldots, r_N)$ obeying Eq. (3), an infinite family of distinct $p'(r_1, \ldots, r_N)$ which also obey Eq. (3) can be constructed by shifting some part of the weight carried by $p(r_1, \ldots, r_N)$ out to larger values of $r_1, \ldots, r_N$. For example, for positive $a_1, \ldots, a_N$, define $p'(r_1, \ldots, r_N)$ to be zero except on the region $r_1 \geq a_1, \ldots, r_N \geq a_N$, where it is given by $p(r_1 - a_1, \ldots, r_N - a_N)$. Each moment of $p'(r_1, \ldots, r_N)$ is greater than the corresponding moment of $p(r_1, \ldots, r_N)$, and thus satisfies Eq. (3). By means of Eqs. (10)–(12), $p'(r_1, \ldots, r_N)$ can therefore be turned into a new $t'_\lambda(z_1, \ldots, z_N)$ with moments satisfying Eq. (2).

An expression for $q_\lambda(\theta_1, \ldots, \theta_N)$ somewhat simpler than Eq. (10) can be found if $p(r_1, \ldots, r_N)$ in Eq. (3) is a product $\hat{p}(r_1) \cdots \hat{p}(r_N)$ with moments $\langle r^m \rangle_{\hat{p}}$ which, for any $R > 0$ and integer $m \geq 0$, obey

$$\langle r^m \rangle_{\hat{p}} \geq b_R R^m \tag{16}$$

for some $b_R > 0$ independent of m. Then with the definition

$$f_\lambda(y) = \sum_{m \geq 0} \frac{y^m}{\lambda^m \langle r^m \rangle_{\hat{p}}}, \tag{17}$$

Eq. (10) takes the form

$$q_\lambda(\theta_1, \ldots, \theta_N) = \langle f_\lambda[x_1 \exp(-i\theta_1)] \cdots f_\lambda[x_N \exp(-i\theta_N)] \rangle_c - 1. \tag{18}$$

For many quantum mechanical systems, a finite volume, lattice approximation to the path integral in real-valued time leads to an expectation value fulfilling Eq. (3) and therefore representable as an ordinary statistical average over an ensemble of random paths through complex space. Among the systems which obey Eq. (3) for some $p(x_1, \ldots, x_N)$ are scalar field theories, in any space-time dimension, with self-interaction ϕ^p, p even, field theories, in any dimension, with bosonic degrees of freedom which range only over a bounded region, and therefore lattice gauge field theories over any compact gauge group. In addition, of course, for any system for which the real-valued time path integral is correctly handled by the complex Langevin equation, the probability distribution $t(z_1, \ldots, z_N)$, defined implicitly by the Langevin trajectory, fulfills Eq. (2). Since Eq. (2) implies Eq. (3), such a system then has a $p(r_1, \ldots, r_N)$ fulfilling Eq. (3).

As an example of a proof of Eq. (3), consider the path integral for a single anharmonic oscillator with time reduced to a periodic lattice of points labeled by a positive integer $t \leq T$. With x_t the position at time t, the time-ordered expectation of a polynomial $f(x_1, \ldots, x_T)$ becomes $\langle f \rangle_c$ of Eq. (1a) with

$$c(x_1, \ldots, x_T) = \exp\left\{ i \sum_t \left[\mu \frac{(x_t - x_{t+1})^2}{2\delta} - \kappa x_t^4 \delta \right] \right\}, \tag{19}$$

where μ is the particle's mass, κ the anharmonic spring constant, and δ the lattice spacing. Rotating each integral over real x_t to an integral over $\exp(-i\pi/8) y_t$ with y_t real, taking the absolute value of both sides of the rotated version of Eq. (1a), and using the inequality

$$(y_t - y_{t+1})^2 \leq 2(y_t^2 + y_{t+1}^2), \tag{20}$$

we obtain

$$|\langle x_1^{m_1} \cdots x_N^{m_N} \rangle_c| \leq \frac{Z_{\hat{p}}^T}{|Z_c|} \prod_t \langle r_t^{m_t} \rangle_{\hat{p}}, \tag{21a}$$

$$\hat{p}(r) = \exp\left(\frac{\sqrt{2} r^2}{\mu \delta} - \kappa r^4 \delta \right), \tag{21b}$$

with $\langle \cdots \rangle_{\hat{p}}$ given by Eq. (1c) for $N = 1$. Equation (21a) then gives Eq. (3) with

$$p(x_1, \ldots, x_T) = \prod_t \hat{p}\left(\frac{x_t}{\lambda} \right), \tag{22a}$$

$$\lambda = \max\left[1, \frac{Z_{\hat{p}}}{|Z_c|^{1/T}} \right]. \tag{22b}$$

The proof of Eq. (3) for an anharmonic oscillator extends easily to a ϕ^p field theory, p even, for any dimension of space-time and to bosonic field theories, in any dimension, with degrees of freedom bounded by some positive real B. In a proof of Eq. (3) for bounded degrees of freedom, $\hat{p}(r)$ in Eq. (21b) becomes $\delta(r - B)$.

Finally, we speculate briefly on the possibility that the degrees of freedom of the real world might actually be complex valued, distributed according to a probability which, as we have shown possible in many cases, yields averages agreeing with those of conventional quantum mechanics. A version of this idea suggested by the complex Langevin equation is considered in Ref. [7]. A problem encountered immediately by this proposal is that the macroscopic world, governed nearly by classical mechanics, exhibits only real-valued positions. This problem would be solved if, within the statistical ensemble of paths through complex space, the paths for macroscopic variables happened nearly to obey classical mechanics and to have only small imaginary parts. A formulation of quantum mechanics incorporating this feature would, potentially, be capable of resolving many of the puzzles in the interpretation of quantum mechanics [8,9]. A discussion of the proposed resolution of these problems by decoherence criteria [10,11] and of the difficulties which these encounter appears in Ref. [12].

The speculation we offer here, in effect, is that quantum mechanics is a version of ordinary statistical mechanics but for paths through a complex-valued coordinate space. Although this prospect may sound implausible, the harmonic oscillator provides a simple model of how such behavior might conceivably come about.

Assume periodic boundary conditions for time period $T = 2M + 1$ and Fourier transform the oscillator coordinate x_t at integer time t according to the convention

$$x_t = \sum_{0 \le k \le M} \left[a_k \cos\left(\frac{2\pi kt}{T}\right) + b_k \sin\left(\frac{2\pi kt}{T}\right) \right], \tag{23}$$

with real coefficients a_k and b_k, b_0 identically 0. The time-ordered expectation of a polynomial $f(a_0, \ldots, a_M, b_1, \ldots, b_M)$ is $\langle f \rangle_c$ of Eq. (1a) for

$$c(a_0, \ldots, a_M, b_1, \ldots, b_M) = \exp\left[i \sum_{0 \le k \le M} (a_k^2 + b_k^2) s_k \right], \tag{24}$$

where s_k is

$$s_k = \frac{2\mu}{\delta}[1 - \cos(k)] - \kappa\delta, \tag{25}$$

and δ is the time lattice spacing.

In Eq. (1a) expressed as integrals over real a_k and b_k, for s_k positive the integrals can be rotated, respectively, to $\sqrt{i}c_k$ and $\sqrt{i}d_k$ with real c_k and d_k. For s_k negative, the a_k and b_k integrals can be rotated, respectively, to $\sqrt{-i}c_k$ and $\sqrt{-i}d_k$. If μ, however, is given a microscopic positive imaginary part ϵ and a correctly chosen real part, there will be a single k for which s_k has no real part and a microscopic positive imaginary part. For this k the integrals over a_k and b_k can be left pure real. Inverting the Fourier transform of Eq. (23), a statistical ensemble of complex-valued trajectories x_t results with real, nonnegative probability weight. A typical trajectory in this ensemble consists of the sum of a real part, with amplitude of order $\epsilon^{-1/2}$, oscillating at the frequency predicted by classical mechanics, and a complex part independent of ϵ.

The preceding construction is, effectively, an application to the harmonic oscillator path integral of the method of steepest descent. A similar construction can be carried out for a free scalar field theory in any dimension of space-time. For more complicated field theories, the method of steepest descent can also be applied to obtain a $t(x_1, \ldots, x_N)$ which includes real-valued trajectories obeying the classical equations of motion, but the $t(x_1, \ldots, x_N)$ produced in this way will only approximately fulfill Eq. (2). Whether for interacting systems $t(x_1, \ldots, x_N)$ can be found which fulfill Eq. (2) and include real-valued trajectories obeying classical equations of motion is an open question.

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[1] John Klauder, in *Recent Developments in High-Energy Physics*, edited by H. Mitter and C. B. Lang (Springer, Vienna, 1983); Phys. Rev. A **29**, 2036 (1984).
[2] J. Ambjorn, M. Flensburg, and C. Petersen, Phys. Lett. **159B**, 335 (1985); J. R. Klauder and W. P. Petersen, J. Stat. Phys. **39**, 53 (1985); J. Ambjorn and S. K. Yang, Phys. Lett. **165B**, 140 (1985); J. Ambjorn, M. Flensburg, and C. Peterson, Nucl. Phys. **B275[FS17]**, 375 (1986); B. Söderberg, Nucl. Phys. **B295[FS21]**, 396 (1988); L. L. Salcedo, Phys. Lett. B **304**, 125 (1993); S. Lee, Nucl. Phys. **B41[FS]**, 827 (1994); H. Gausterer, J. Phys. A **27**, 1325 (1994).
[3] L. L. Salcedo, J. Math. Phys. (N.Y.) **38**, 1710 (1997).
[4] I am grateful to L. L. Salcedo for suggesting the proof of the existence of $p(r)$ for $N = 1$.
[5] N. I. Akhiezer, *The Classical Moment Problem* (Hafner, New York, 1965).
[6] C. Berg, Proc. Symp. Appl. Math. **37**, 110 (1987).
[7] A. A. Migdal, Sov. Phys. Usp. **29**, 389 (1986).
[8] J. S. Bell, *Speakable and Unspeakable in Quantum Mechanics* (Cambridge University Press, Cambridge, 1987).
[9] D. Weingarten, Nuovo Cimento Soc. Ital. Fis. **22B**, 293 (1974).
[10] D. Weingarten, Neils Bohr Institute Report No. NBI-HE-73-3, 1973.
[11] R. B. Griffiths, J. Stat. Phys. **36**, 219 (1984); R. Omnes, J. Stat. Phys. **53**, 893 (1988); M. Gell-Mann and J. B. Hartle, in *Complexity, Entropy, and the Physics of Information*, edited by W. Zurek (Addison-Wesley, Reading, MA, 1990), p. 425.
[12] S. Goldstein, Phys. Today **51**, No. 3, 42 (1998); **51**, No. 4, 38 (1998).