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Some generalizations of the Marcinkiewicz theorem and its implications to certain approximation schemes in many-particle physics*

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The Marcinkiewicz theorem states that the characteristic function of a probability distribution function cannot be an exponential of a polynomial of degree larger than 2. This theorem is generalized in the present paper to (i) probability distribution functions of many variables and to (ii) probability distribution functionals when the stochastic variables are both commuting (Bose) and anticommuting (Fermi). The consequences of this theorem to certain approximation schemes in many-particle physics, involving truncation of hierarchical equations, are pointed out. These follow when one observes that the hierarchical equations such as those of many-particle Green's functions can be generated from a single equation for a Green's functional whose structure is that of a characteristic functional of a probability distribution functional. The theorem implies that this would exhibit a nonpositive behavior when certain truncation schemes are employed. Specific examples illustrating our results are drawn from the theory of an electron gas, turbulence theory, and quantum optics.

I. INTRODUCTION

Marcinkiewicz[1] proved the following theorem (henceforth called the M theorem): The probability distribution function will violate its positive definiteness if its cumulant generating function is a polynomial of degree greater than 2.

This theorem was proved for single-variable distribution functions, and for more recent proofs and discussions of it, one may refer to the works of Linnik[2] and Richter.[3] The importance of this theorem in the physics of many-particle systems and field theories was first noted by Robinson.[4] One often employs the intuitive notation that the correlation between n events will be negligible if n is sufficiently large, and so one discards the correlation functions above some order (usually small for purposes of being practical) in dealing with the hierarchy of equations describing a system. A direct consequence of the M theorem is that such theories are inconsistent with the basic positive definiteness of the "probability distribution function" from which all the correlations of interest emerge. Only the "generalized free-field" model has zero cumulants of all orders greater than 2, corresponding to the "Gaussian" structure of the probability distribution. But schemes with only a finite number of nonzero cumulants are extensively employed in many-particle physics and relativistic field theory. Robinson[4] extended the M theorem to the case of Bose variables which obey the canonical commutation relations and indicated a proof for a relativistic field theory of the Wightman type. An account of this work may be found in a recent book by Emch.[5] Another interesting consequence of the M theorem for the Bose fields is that the Bogoliubov transformation can either be linear or involve an infinite series of operators, as was proved by 't Hooft and de Boer.[6]

In the theory of many-electron systems, the calculation of the pair correlation function is of great physical importance. In all the schemes proposed so far for calculating this there is the feature that it becomes *negative* at vanishing interparticle separations for interesting regions of density of the system. *It has been suggested that this is perhaps an indication of the failure of these schemes to maintain the positive definiteness of the basic many-particle probability distribution function.*[7] A similar difficulty in turbulence theory[8] appears in the computation of energy density in modes that are strongly excited at high Reynolds numbers. One usually attributes the failure of the "truncation" schemes to treat properly the secular properties of this system.[9] We may observe here that all these methods involve cumulants or linked diagrams of some low orders only and so the above failures possibly stem from the procedure itself as a direct consequence of the M theorem applied to these theories. It is our aim here to offer an extension of the M theorem to *probability functionals* from which, we may deduce that the failures alluded to above are a consequence of truncation. This is in the same spirit as Robinson's work.

In Sec. II we extend the M theorem to probability functions of finitely many variables, from which we deduce the corresponding theorem for proba-

bility functionals. We will also establish the M theorem for Fermi (anticommuting) variables. In Sec. III, a brief discussion of how the usual infinite chain of equations are recast in terms of a "generating functional" is presented and the M theorem is applied to the problems of many-particle systems and quantum optics. Section IV summarizes the results.

II. MARCINKIEWICZ'S THEOREM FOR GENERALIZED PROBABILITY FUNCTIONALS

We present the theorem in two parts—the M theorem for (i) a several-variable distribution function, and (ii) a probability functional of Bose fields and of Fermi fields.

Theorem I. If the cumulant generating function of a probability distribution in k variables is a multinomial of degree greater than 2, then the probability distribution will not be positive definite.

Proof. The proof consists in reducing the problem essentially to the one-variable case. We first prove this for the case of two variables and the same technique will be used to establish the theorem for finitely many-variable probability distribution functions. For simplicity we choose an infinite domain for the random variables.

The probability distribution function in two variables, $P_2(u_1, u_2)$, has the property

$$\int_{-\infty}^{\infty} P_2(u_1, u_2)\, du_2 = P_1(u_1), \tag{1}$$

where $P_1(u_1)$ is the probability distribution of the variable u_1. This is a special case of a more general principle. We want to prove that the cumulant generating function

$$E_2(x_1, x_2) = \int_{-\infty}^{\infty}\int P_2(u_1, u_2) \times \exp[i(x_1u_1 + x_2u_2)]\, du_1\, du_2 \tag{2}$$

cannot be expressed as

$$\exp\left(\sum_{i,j}^{N,M} a_{ij} x_1^i x_2^j\right) \quad \text{with } \infty > N+M > 2. \tag{3}$$

Let $x_1 = r_2\cos\theta_2$, $x_2 = r_2\sin\theta_2$, in (2). Then,

$$E_2(x_1, x_2) \equiv \tilde{E}_2(r_2, \theta_2) = \int_{-\infty}^{\infty}\int P_2(u_1, u_2) \times \exp[ir_2(\cos\theta_2 u_1 + \sin\theta_2 u_2)]\, du_1\, du_2.$$

Introduce new variables v_1, v_2 such that

$$\begin{aligned} u_1\cos\theta_2 + u_2\sin\theta_2 &= v_2, \\ -u_1\sin\theta_2 + u_2\cos\theta_2 &= v_1, \end{aligned} \tag{4}$$

so that

$$\tilde{E}_2(r_2, \theta_2) = \int_{-\infty}^{\infty}\int \tilde{P}_2(v_1, v_2; \theta_2)\exp(ir_2v_2)\, dv_1\, dv_2. \tag{5}$$

Note that

$$\int_{-\infty}^{\infty} \tilde{P}_2(v_1, v_2; \theta_2)\, dv_1 = \pi_2(v_2; \theta_2) \tag{6}$$

is also a probability distribution function. Suppose now that the left-hand side of Eq. (5) can be expressed as

$$\begin{aligned} \tilde{E}_2(r_2, \theta_2) &= \exp\left(\sum_{n}^{p} \alpha_n(\theta_2) r_2^n\right), \quad p > 2 \\ &= \int_{-\infty}^{\infty} \pi_2(v_2; \theta_2)\exp(ir_2v_2)\, dv_2. \end{aligned} \tag{7}$$

But this cannot be done in view of the M theorem applied to $\pi_2(v_2; \theta_2)$ for every θ_2 except for a set of measure zero. Hence the theorem is true for P_2.

This theorem can now be established for the case of k variables. The point to note here is that

$$\int_{-\infty}^{\infty}\cdots\int_{-\infty}^{\infty} \tilde{P}_k(v_1\cdots v_k; \theta_1\cdots\theta_{k-1})\, dv_1\cdots dv_{k-1} = \pi_k(v_k; \theta_1\cdots\theta_{k-1}) \tag{8}$$

is a probability distribution in v_k for fixed $(\theta_1\cdots\theta_{k-1})$. We will now prove the following theorem:

Theorem II. If $P_1[\rho]$ is a probability density functional, then

$$E_1[U] = \int P_1[\rho]\exp\left[i\int_{-\infty}^{\infty} U(t_1)\rho(t_1)\, dt_1\right] \mathfrak{D}\rho \tag{9}$$

cannot be expressed as

$$\exp\left(\sum_{\nu=1}^{N}\int\cdots\int_{-\infty}^{\infty} K_\nu(t_1\cdots t_\nu)U(t_1)\cdots \times U(t_\nu)\, dt_1\cdots dt_\nu\right), \tag{10}$$

with $N > 2$ without violating the positive definiteness of $P_1[\rho]$. We have here used a single variable t for simplicity; this has an obvious generalization.

Proof. By definition (see for instance, Ref. 10) a functional is defined as the limit

$$\lim_{n\to\infty} P_n(\rho_1, \rho_2, \ldots, \rho_n) = P_1[\rho],$$

where the discrete points $t_1\cdots t_n$ are replaced by a continuous variable t, and one defines a function $\rho(t)$ such that the variables $\rho_1, \rho_2, \ldots$ are $\rho(t_1), \rho(t_2), \ldots$, respectively, with the definition of the convergence of the limit either in the mean or in probability. Also, one employs *continuous functionals* defined by

$$\lim_{n\to\infty} P_1[\rho_n(t)] = P_1[\rho(t)]$$

whenever

$$\lim_{n\to\infty} \rho_n(t) = \rho(t).$$

One then defines the functional integration through

$$\lim_{n\to\infty} \int_{-\infty}^{\infty} \cdots \int d\rho_1 \cdots d\rho_n \to \int \mathfrak{D}\rho.$$

All these operations are assumed to have been performed in the foregoing manipulations. (Note: Similar definitions hold for functionals of several functions, $P[\rho, \xi, \ldots]$.)

To prove the statement of Theorem II, we first convert the functional relation to a statement about a multivariable function and then use Theorem I. To do this, we expand $\rho(x)$ in terms of a complete, biorthogonal set of functions $\{\phi_n\}, \{\psi_n\}$:

$$\rho(x) = \sum_n c_n \phi_n, \quad c_n = \langle \psi_n, \rho \rangle \equiv \int_{-\infty}^{\infty} \psi_n(t)\rho(t)\,dt,$$

since

$$\langle \psi_m, \phi_n \rangle = \delta_{m,n}.$$

The c_n's are now the required random variables. Also,

$$\mathfrak{D}\rho \to \lim_{n\to\infty} dc_1 \cdots dc_n,$$

$$\int_{-\infty}^{\infty} dt_1\, U(t_1)\rho(t_1) = \sum_n c_n U_n,$$

where

$$U_n = \langle U, \phi_n \rangle.$$

In terms of $\{\psi_n\}$, U has the expansion $\sum_n U_n \psi_n$. Thus, we have finally

$$E_1[U] = \tilde{E}_1(u_1, u_2, \ldots),$$

$$P_1[\rho] = \tilde{P}_1(c_1, c_2, \ldots),$$

and

$$\tilde{E}_1(u_1, u_2, \ldots) = \lim_{n\to\infty} \int \cdots \int dc_1 \cdots dc_n \times \exp\left(i \sum_{j=1}^{n} u_j c_j\right) \tilde{P}_n(c_1 \cdots c_n).$$

With a suitable definition of the existence of the limit and using Theorem I for finitely many mutually commuting variables, one arrives at the required theorem.

In the above theorems, the variables commute among themselves. In the quantum-mechanical theories, one encounters anticommuting variables and we will therefore extend the above theorems for such variables. In this case, one has to "order" the multiple integrations in some sequence by means of some convention.[11]

We will now restate Theorem II in a form applicable to random variables obeying either Bose or Fermi commutation relations, and in a form applicable to Green's-function theory of many-particle systems directly.[11]

Theorem II'. The generating functional

$$E_2[\xi, \xi^\dagger] = \int\int P_2[\psi, \psi^\dagger] \times \exp\left[i \int (\xi\psi + \psi^\dagger \xi^\dagger)\,dx\right] \mathfrak{D}\psi \mathfrak{D}\psi^\dagger \quad (11)$$

($P_2[\psi, \psi^\dagger]$ is the probability functional) cannot be expressed as

$$\exp\left(\sum_{n,m=1}^{N,M} \int \cdots \int \xi^\dagger(x_1)\cdots\xi^\dagger(x_n) K_{nm}(x_1 \cdots x_n; x_1' \cdots x_m') \times \xi(x_m') \cdots \xi(x_1')\,dx_1 \cdots dx_n\,dx_m' \cdots dx_1'\right) \quad (12)$$

with all $N+M>2$ without violating the positive definiteness of P_2. To keep the discussion quite general, here x_i stands for a multidimensional dependent variable such as the space-time variables, $(\vec{r}, t)$. If $\psi, \psi^\dagger$ obey the usual equal-time Bose commutation relation or Fermi anticommutation relation, so do the c-number variables, $\xi, \xi^\dagger$ correspondingly.

Proof. The case of Bose variables is easy to handle and proceeds as with the proof of Theorem II. In the case of Fermi variables, a little ingenuity is required, and we shall describe this here. As in the proof of Theorem II, we express $\psi(x), \psi^\dagger(x)$ in terms of a complete orthonormal set of functions $\{\psi_j\}$ (for simplicity we here use an orthonormal set instead of the more general set introduced earlier):

$$\psi(x) = \sum_j a_j \psi_j(x), \quad \psi^\dagger(x) = \sum_j a_j^\dagger \psi_j^*(x), \quad (13)$$

where $a_j, a_k^\dagger$ now obey the anticommutation relations:

$$[a_j, a_k]_+ = 0, \quad [a_j, a_k^\dagger]_+ = \delta_{j,k}. \quad (14)$$

Also,

$$\xi(x) = \sum_j \xi_j^\dagger \psi_j^*(x), \quad \xi^\dagger(x) = \sum_j \xi_j \psi_j(x) \quad (15)$$

where ξ_j and $\xi_k^\dagger$ also obey anitcommutation relations.

We now arrange the operators $a_j, a_k^\dagger$ in an arbitrary but fixed order of the labels. Define new operators,

$$b_j = \eta_j a_j = a_j \eta_j, \quad (16a)$$

$$b_j^\dagger = a_j^\dagger \eta_j = \eta_j a_j^\dagger, \quad \text{with } \eta_j = \exp\left(\pi i \sum_{k=1}^{j-1} a_k^\dagger a_k\right). \tag{16b}$$

Note that the operator

$$\exp(\pi i a_k^\dagger a_k) = (-1)^{a_k^\dagger a_k} = 1 - 2a_k^\dagger a_k .$$

The set of new operators $b_j, b_k^\dagger$ satisfy the simpler commutation relations:

$$[b_j, b_j^\dagger]_+ = 1, \quad b_j^2 = b_j^{\dagger 2} = 0,$$
$$[b_j, b_k]_- = 0, \quad [b_j, b_k^\dagger]_- = 0 \text{ for } j \neq k. \tag{17}$$

Thus b_j's form a *set of commuting Fermi operators*. Each single Fermi oscillator $b, b^\dagger$ can be identified with the Pauli spin-flip operators σ^-, σ^+ so that we obtain a system generated by a "multispinor." Also, the states of the modified Fermi operators generated from the vacuum may be identified with the states formed by coupling N spin-$\frac{1}{2}$ units. We get $N+1$ states of total spin $N/2$, which is symmetric in all the degrees of freedom and a number of other states of lower spin eigenvalue. It is enough to prove that

$$E_2(\cdots \xi_j, \xi_j^\dagger \cdots) = \left\langle \exp\left(i \sum_j \eta_j (\xi_j b_j^\dagger + b_j \xi_j^\dagger)\right)\right\rangle, \tag{18}$$

where $\langle \cdots \rangle$ denotes the average over the probability distribution function $\tilde{P}_2(\cdots b_j, b_j^\dagger \cdots)$, cannot be expressed as an exponential of a multinomial in $(\cdots \xi_j, \xi_j^\dagger \cdots)$ of degree greater than 2. To do this, we observe that if we define

$$\zeta_j = \eta_j \xi_j ,$$

then

$$E_2(\cdots \eta_j \xi_j, \eta_j \xi_j^\dagger \cdots) \equiv \left\langle \exp i \sum_j (\zeta_j a_j^\dagger + a_j \zeta_j^\dagger)\right\rangle \tag{18'}$$

where the ζ_j's are now suitable *commuting* Fermi variables. Let us assume that we can write E_2 in the form

$$E_2(\xi_1, \ldots, \xi_N^\dagger) = \exp[\mathcal{P}(\zeta_1, \ldots, \zeta_N^\dagger)], \tag{19}$$

where $\mathcal{P}$ is a multinomial in the variables. Consider the special case when

$$\zeta_1 = \zeta_1^\dagger = \cdots = x.$$

Then

$$E_2(x, \ldots, x) = \exp[Q(x)],$$

where

$$Q(x) = \mathcal{P}(x, \ldots, x).$$

But $E_2(x, \ldots, x)$ is the expectation value of the unitary O(3) operator, $\exp(2ixJ_1)$ where $J_1 = \frac{1}{2}\sum_1^N (b_j + b_j^\dagger)$. The spectrum of J_1 is of course the usual one consisting of $-\frac{1}{2}N, -\frac{1}{2}N+1, \ldots, \frac{1}{2}N-1, \frac{1}{2}N$. Hence, we also have

$$E_2(x) \equiv \sum_{r=-N/2}^{N/2} \pi_r \exp(2\pi i r x) = \exp Q(x).$$

Since x is assumed real in the above, we have

$$|E_2(x)| \leq E_2(0) = 1$$

and hence

$$1 > \exp\{\tfrac{1}{2}[Q(x) + Q^*(x)]\}.$$

Since $Q(x)$ is assumed to be a polynomial, we observe that $\frac{1}{2}[Q(x)+Q^*(x)]$ is also a polynomial, say $R(x)$. Hence, with the exception of the case where all $\pi_r = 0$ except one, we must have

$$R(x) < 0 \text{ for all nonzero real } x,$$
$$R(x=0) = 0.$$

But for a real polynomial this is impossible unless it is a monomial of even degree:

$$R(x) = -(ex)^{2\nu}, \quad \nu \text{ an integer}.$$

For sufficiently small x, if $E_2(x)$ can be approximated by a power series, then we must have the quadratic term necessarily since its coefficient is the expectation value of $\frac{1}{4}J_1^2$. Hence the only possibility is $R(x) = -(ex)^2$. This implies that we have at most $Q(x) = iS(x) - (ex)^2$, where $S(x)$ is an odd, real function of x. From an argument similar to the one used in proving the M theorem, we can further deduce that $S(x)$ must be linear in x and hence we get a Gaussian characteristic function at most. We thus establish that we cannot have $E_2(\xi_1 \cdots \xi_N^\dagger)$ expressed as an exponential of a multinomial in $\xi_1 \cdots \xi_N^\dagger$, except as a quadratic form.

We may mention in passing that a discrete variable version of the M theorem also exists, because we may express a probability distribution function $p(x)$ in the form

$$p(x) = \sum_n p_n \delta(x - x_n),$$

with

$$\sum_n p_n = 1, \quad 0 \leq p_n < 1$$

and hence $E(k) = \sum_n p_n \exp(ikx_n)$. The statement of the M theorem is then that $E(k)$ cannot be written as an exponential of a polynomial in k, of degree greater than 2. This may have relevance to the recent interest in binomial moments in particle physics.[12]

The implication of this theorem is clearly that one *cannot* set the cumulants as being nonzero up to a prescribed order larger than 2 and 0 beyond it

without violating the basic positive definiteness of the probability distribution function itself. Although the theorem does not indicate in which correlation function the difficulties will occur, we shall in Sec. III note certain examples in which the problems arise in low-order correlation functions of interest.

III. APPLICATIONS

A. Many-electron problem—remarks on Hartree-Fock (HF) theory and the random-phase approximation (RPA)

In Ref. 11, Martin and Schwinger discuss truncation procedures in detail for the system of equations obeyed by Green's functions of various orders for an interacting system of many identical particles obeying either Bose or Fermi statistics. It is clear from that discussion that HF scheme corresponds to $N=1, M=1$ or Gaussian approximation for $E_2[\xi, \xi^\dagger]$ in Eq. (12) and this clearly does not violate the positive definiteness of the probability functional, $P_2[\psi, \psi^\dagger]$. However, in RPA it amounts to keeping terms up to $N=M=2$ in Eq. (12), (with $K_{12}=0=K_{21}$). This scheme then must violate the positive definiteness of $P_2[\psi, \psi^\dagger]$. *To see that this indeed happens, one must examine the sequence of probabilities generated by the functional itself in detail and this is usually a difficult job.* However, the *pair correlation function is usually computed in the literature* as it is of great physical importance and *this is one of the elements defined by* $P_2[\psi, \psi^\dagger]$. It is found in the literature that (see Ref. 7 for a discussion of this and references to the literature) the pair correlation function (which is itself a probability) becomes negative for zero separation for densities corresponding to $r_s > 1$ in RPA. Various "improvements" have been made within such approximation schemes by many authors (notably Singwi and his coworkers) and essentially in our language, their attempts are all going into improving the probability functional by improving the calculation of K_{22} while still keeping all the rest of the cumulants zero. While an improvement in the computation of K_{22} improves the value of r_s (<4) up to which the pair correlation function is positive,[7] the problem still remains that this function becomes negative for larger r_s (>4). For values of r_s between 2 and 4, the theorem would imply that some other higher-order correlation functions would become negative. This observation holds for all the existing methods of computing the dielectric function for the many-electron system (from which the pair correlation function is deduced in the usual way) all of which amount to neglecting higher-order cumulants of order 3 or more. Incidentally, *the truncation procedures in many other areas will also have this difficulty if only one examines the various probabilities systematically. The theorem only states that some probability will become negative but does not indicate which one. Also, the truncation schemes may be a good physical approximation in some region of interest, but it would imply violation of a basic positivity requirement on the probability functional.*

B. Some theories of turbulence

Orszag[8] has surveyed some analytic theories of turbulence, in particular the formulation of the problem in terms of cumulants. He also develops the infinite hierarchy of equations for the various orders of velocity correlation functions to describe homogeneous turbulence; these can be reformulated also as a single functional differential equation. More recently, Martin *et al.*[9] have also examined this formulation, even though they had different reasons for so doing. In particular, Orszag has noted that truncation procedures lead to unphysical negative values for the energy spectrum and attributes this to irreversible relaxation effects caused by the neglect of cumulants of order 4 and more. (This is also noted by Martin *et al.*[9]) What this means in our formulation, is that such approximations make the probability functional negative and this reflects in the explicit computation of energy spectrum.

We may bring the attention of the reader to the paper of Martin *et al.*[9] where several physical theories of classical physics are reformulated in terms of the functional approach as well as to various other papers of Martin and co-workers who have also formulated many other quantum theories of many-particle systems in terms of functionals.[13] The theorem proved in this paper is of importance in connection with these formulations as it *signals a warning note* whenever truncation of some sort is used as an approximation scheme.

C. Quantum theory of partial coherence

In statistical optics the expectation values of the products of fields yield the higher-order coherence functions. The two-point coherence function, sometimes called the mutual intensity, is the fundamental function of the classical theory of partial coherence.[14] It obeys a wave equation in free space and its time-Fourier transform is the spectral density function and thus directly measured in terms of spectral profiles. Quantum theory of partial coherence yields absolutely no restrictions on the two-point function that is not already imposed by classical theory.[15]

Higher-order coherence functions become of importance in intensity correlations,[16] photoelectric counting,[17] and in nonlinear optics.[18] For a

Gaussian field the correlations of higher order can be determined by putting all the higher cumulants to be zero.[16] For non-Gaussian light (including phase-uncertain amplitude-fixed "laser" light) the higher cumulants do not vanish. These higher-order functions contain new spectral information.[19]

It would be tempting to characterize the light by a finite number of cumulants, say the fourth in addition to the second. However, the M *theorem forbids such a possibility* in classical optics. In quantum optics the corresponding ensemble weight functions are not necessarily positive[20] and one might consider this possibility. However, our generalization of the M theorem shows that even in quantum optics such a possibility is not realized. Once we go beyond the spectral profile, we have an unlimited number of new spectral densities.

IV. CONCLUDING REMARKS

The hierarchy of equations for various orders of correlation functions (or Green's functions) necessarily imply the existence of the "probability functional" (see Refs. 10 and 11 for instance) and hence the conclusion reached in this paper is of importance. The implication of this work is a negative one, and fills a gap that exists in the literature concerning the meaning of truncation schemes in many areas of physics (see Ref. 11). Furthermore, the futility of improving the theory within such a framework becomes transparent, unless one is seeking solutions in a region of interest where the violation of positive definiteness does not occur.

This work supplements that of Robinson's[4] by establishing the theorem of Marcinkiewicz for generalized probability functionals.

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