Lawrence Berkeley National Laboratory
Recent Work

Title
COMPLEX BERNOULLI POLYNOMIALS FROM QUANTUM DISTRIBUTIONS

Permalink
https://escholarship.org/uc/item/9qp0g44m

Author
Elze, H.-T.

Publication Date
1986-05-01
Submitted to Journal of Physics, A

COMPLEX BERNOULLI POLYNOMIALS
FROM QUANTUM DISTRIBUTIONS

H.-T. Elze

May 1986

TWO-WEEK LOAN COPY

This is a Library Circulating Copy
which may be borrowed for two weeks.

Prepared for the U.S. Department of Energy under Contract DE-AC03-76SF0098
DISCLAIMER

This document was prepared as an account of work sponsored by the United States Government. While this document is believed to contain correct information, neither the United States Government nor any agency thereof, nor the Regents of the University of California, nor any of their employees, makes any warranty, express or implied, or assumes any legal responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by its trade name, trademark, manufacturer, or otherwise, does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof, or the Regents of the University of California. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof or the Regents of the University of California.
Complex Bernoulli Polynomials from Quantum Distributions

Hans-Thomas Elze

Nuclear Science Division
Lawrence Berkeley Laboratory
University of California
Berkeley, California 94720

May 12, 1986

Abstract:

Integral representations for Bernoulli polynomials of a complex argument are derived. We achieve this by contour integration of a class of integrals over Bose or Fermi distributions involving a complex parameter. It is illustrated how these integrals arise in the calculation of canonical partition functions involving complex "chemical potentials" at an intermediate step. We also find a relation between Bernoulli numbers and the \( \zeta \)-function and a special sum rule for the latter. Further applications are shortly mentioned.

\(^1\)Work supported by the Director, Office of High Energy and Nuclear Physics of the Department of Energy under Contract DE-AC03-76SF00098. The author also gratefully acknowledges support by a DAAD-NATO Postdoctoral Fellowship.
The purpose of this note is to derive integral representations for Bernoulli polynomials of a complex argument. As we shall see, they correspond to integrals as they may arise in the calculation of partition functions for quantum systems of massless particles. They particularly involve integrals over Bose or Fermi distributions with a complex "chemical potential" and we show how they can be calculated analytically. The derivation of our results will be a generalization of a previous calculation of the thermodynamical potential for the ideal relativistic Fermi gas [1]. To our knowledge it has not been given elsewhere.

Recently high-temperature expansions of partition functions for massive relativistic Bose and Fermi gases were studied extensively in ref.[2] (see also references therein) using a Zeta function regularization method to deal with various divergent series. Particular attention was given to the fact that the relevant "chemical potential" can become complex in physically interesting applications. As usual its real part is associated with a Lagrange multiplier which is introduced to ensure charge conservation on the average (grand canonical ensemble). A purely imaginary "chemical potential" can be produced by a background vacuum potential in a gauge theory at finite temperature [2,3,4].

In refs.[5,6] it was analyzed how imaginary chemical potentials are quite naturally involved in a canonical ensemble formalism [7] treating Abelian or non-Abelian charge conservation in quantum statistics exactly. The occurrence of complex chemical potentials can thus be understood in the framework of a mixed canonical/grand canonical ensemble [5,6]. There one implements some conservation laws exactly while others only in the sense of statistical averages depending on physical circumstance. This has important consequences for small systems as for example quark-gluon plasma droplets possibly formed in ultrarelativistic nucleus-nucleus collisions [8,9].

Having these remarks in mind, it seems worthwhile to present the calculation of a class of integrals over quantum distributions with a complex chemical potential [5]. We are interested in the integrals

\[ I_n(z)_{F,B} \equiv \int_0^\infty dx \, x^n \left\{ \frac{1}{e^{x-z} + 1} + (-1)^n \frac{1}{e^{x+z} + 1} \right\} , \quad n = 0, 1, 2, \ldots \quad (1) \]

where the "+" and "-" signs in the denominators correspond to the Fermi-Dirac and Bose-Einstein distributions respectively, and where \( z \) denotes a complex parameter. First, we observe that

\[ I_n(z)_{B} = -I_n(z + i\pi(2m + 1))_{F} , \quad m \in \mathbb{Z} \quad (2) \]

so that it suffices to study \( I_n F \) only (henceforth we drop the index \( F \)). Also

\[ I_n(z + 2m\pi i) = I_n(z) , \quad m \in \mathbb{Z} \quad (3) \]

so that in order to avoid possible poles in the integrand in eq.(1) we complete the definition of \( I_n \) by a restriction on the imaginary part of \( z \),

\[ -i\pi < \text{Im} \, z < +i\pi . \quad (4) \]
After a shift of variables we now obtain

\[ I_n(z) = \int_{-\infty}^{\infty} dx \frac{1}{e^x + 1} \left( x + \nu \right)^n + (-1)^{n+1} \int_{-\infty}^{\infty} dx \frac{1}{e^x + 1} \left( x - \nu \right)^n \cdot \frac{1}{e^x + 1} , \]  

(5)

thus shifting the integration from the real axis to the lower and upper horizontal lines in Fig.1. Choosing closed contours as indicated in Fig.1 and applying Cauchy’s theorem yields

\[ I_n(z) = \sum_{\nu=0}^{n} \binom{n}{\nu} \left( 1 + (-1)^{n+\nu+1} \right) \int_{0}^{\infty} dx \frac{x^{n-\nu}}{e^x + 1} \]

\[ + (-1)^n \int_{-\nu}^{\nu} dx \left( x - \nu \right)^n \left\{ \frac{1}{e^{-x} + 1} + \frac{1}{e^{x} + 1} \right\} , \]

(6)

where we also used a substitution \( x \rightarrow -x \) for the first term in the second integral and suitably rearranged terms. Since \((e^{-x} + 1)^{-1} + (e^{x} + 1)^{-1} = 1\), we finally can perform all integrations:

\[ I_n(z) = \frac{z^{n+1}}{n+1} + \sum_{\nu=0}^{n} \binom{n}{\nu} \left( 1 + (-1)^{n+\nu+1} \right) \left( 1 - 2^{-n+\nu} \right) \Gamma(n-\nu+1) \zeta(n-\nu+1) ; \]

(7)

\( \Gamma \) and \( \zeta \) denote the conventional Gamma and Riemann’s Zeta functions and we used a known result for the first integral on the rhs. of eq.(6) [10]. Note that for \( \text{Im} z = 0 \) eq.(7) simply reproduces the result of ref.[11].

In order to find the advertised relation between \( I_n \) and the Bernoulli polynomials we quickly recalculate \( I_n \) for \( \text{Re} z = 0 \) by using a series expansion of the integrand in eq.(1), which is well-behaved in this case, and integrating term by term. Let \( \alpha \) be real, then according to eq.(1)

\[ I_n(i\alpha) = 2n! \sum_{\nu=1}^{\infty} \frac{(-1)^{\nu+1}}{\nu^{n+1}} \times \begin{cases} \cos \alpha \nu, & n \text{ odd} \\ i \sin \alpha \nu, & n \text{ even} \end{cases} \]

(8)

Both series are known to be summable into polynomial form and they constitute Fourier expansions of Bernoulli polynomials in particular [11]. Combining both cases from eq.(8), we obtain

\[ I_n(i\alpha) = i^{n+1} \frac{(2\pi)^{n+1}}{n+1} B_{n+1}((\pi + \alpha)/2\pi) . \]

(9)

We conclude from eqs.(7,9) and by uniqueness of the polynomials involved:

\[ I_n(z) = i^{n+1} \frac{(2\pi)^{n+1}}{n+1} B_{n+1}((\pi - iz)/2\pi) ; \]

(10)

here it is important to remember that \( z \) is restricted to the strip \(-i\pi < \text{Im} z < i\pi\. Due to eq.(3), however, it is obvious how to calculate \( I_n(z) \) in a neighbouring strip. Eq.(10) presents our main new result.
We remark here that the author of ref. [2] also in principle calculated the real part of $I_n(z)$ using a similar series expansion as in eq.(8), but he did not comment upon the questionable convergence of his series. From eqs.(7,10) we learn that considering the real part only necessarily forced him to introduce new polynomials depending on $Re \ z$ and $Im \ z$ separately, which can be avoided as we have shown.

As a first application we obtain from eqs.(7,10) the following formula relating Bernoulli numbers to the $\Gamma$– and $\zeta$–functions ($k = 1, 2, 3, \ldots$)

$$B_k \equiv B_k(0) = (-2)^{-k} + (-2)^{-k} \sum_{\nu=0}^{k-1} \frac{k-1}{\nu} \left( i\pi \right)^{\nu-k} \left( 1 + (-1)^{k+\nu} \right) \left( 1 - 2^{-k+\nu+1} \right) \Gamma(k - \nu) \frac{\zeta(k - \nu)}{\nu},$$

(11)

which, of course, is real, since only terms even in $\nu - k$ contribute to the rhs. sum. Using the relations $B_{2k} = -2k\zeta(1 - 2k)$ and $\zeta(1 - 2k) = 2(2\pi i)^{-2k}\Gamma(2k)\zeta(2k)$ [10,11] we find from eq.(11) an interesting sum rule for the $\zeta$-function ($k = 1, 2, 3, \ldots$)

$$\left(4k\right)^{-1} = -\sum_{\nu=0}^{k-1} \frac{2k-1}{2\nu} \left( i\pi \right)^{2\nu-2k} \left( 1 - 2^{-2k+2\nu+1} \right) \frac{\Gamma(2k - 2\nu)}{\nu},$$

(12)

where by "*" we indicate that for $\nu = 0$ one has to replace $1 \rightarrow 2$ in the bracket.

Finally, we consider the generating function $Z$ [5,6] for charged bosons or fermions defined by

$$Z(T, V, z) \equiv Tr e^{-\beta \hat{H} + z(\hat{N}_p - \hat{N}_a)} ;$$

(13)

here the trace refers to the Hilbert space of many-particle states and $\hat{H}$, $\hat{N}_p$, $\hat{N}_a$ denote the Hamiltonian, particle number, and antiparticle number operators respectively; the variables are the temperature $T$ ($\beta \equiv T^{-1}$), volume $V$, and there is a complex parameter ("chemical potential") $z$. It is essentially from $Z$ that one can calculate by a group-theoretical projection technique [5,6,7] the canonical ensemble partition function respecting an exact internal symmetry. For example, one can thus enforce the constraint of Gauss' law upon the physical states of the system in a non-Abelian gauge theory. - Evaluation of the rhs. of eq.(13) in the particle number representation gives $Z$ for non-interacting particles in $d$ space dimensions

$$\ln Z^\pm(T, V, z)_d = \pm \sum_k \left( \ln(1 \pm e^{-\beta \epsilon_k + z}) + \ln(1 \pm e^{-\beta(\epsilon_k - z)}) \right)$$

$$= gVT^d \frac{2^{1-d} \pi^{-d/2}}{d \Gamma(d/2)} \int_0^\infty dx \ x^d \left\{ \frac{1}{e^{x-z} \pm 1} \right. + \left. \frac{1}{e^{x+z} \pm 1} \right\} ,$$

(14)

where the "+" ("−") sign applies for fermions (bosons) and $g$ counts any internal degeneracy of states. We also used the continuum approximation replacing the sum over states with energy $\epsilon_k$ by a $d \times d$-dimensional phase-space integral with $\epsilon(k) = k$ in the ultrarelativistic limit and performed a partial integration. Via eqs.(1,2,9)
for an even number of space-time dimensions we then arrive at the simple result 
\((d + 1 = 2, 4, 6, \ldots)\):

\[
\ln \tilde{Z}^{\pm}(T, V, z)_d = 4gVT^d \frac{i^{d+1} \pi^{1+d/2}}{d(d+1) \Gamma(d/2)} \times \left\{ \begin{array}{ll}
B_{d+1}((\pi - iz)/2\pi) & \text{(fermions)} \\
- B_{d+1}(-iz/2\pi) & \text{(bosons)}
\end{array} \right.
\]

(15)

here again eq.(4) applies. For \(d + 1\) odd a power series in \(\exp - z\) \((Re z \geq 0)\) has to be added because of the wrong "+" sign in eq.(14) as compared to eq.(1).

In conclusion we remark that the result in eq.(15) can be improved to include finite size corrections and thus opens the way to treat these quantum gases consistently in a canonical ensemble formalism. Presently we are studying such an extension and its application to small quark-gluon plasma droplets. It would also be most desirable to obtain similar results for cases where the single-particle energy spectrum contains a mass gap, eventually allowing e.g. a study of Bose condensation [12] away from the infinite volume limit and related phenomena.

\textit{Figure caption}  \textit{Fig.1} The contours employed for the evaluation of eq.(5).

\textbf{References}


This report was done with support from the Department of Energy. Any conclusions or opinions expressed in this report represent solely those of the author(s) and not necessarily those of The Regents of the University of California, the Lawrence Berkeley Laboratory or the Department of Energy.

Reference to a company or product name does not imply approval or recommendation of the product by the University of California or the U.S. Department of Energy to the exclusion of others that may be suitable.