PAPER

Thermal properties of the Rényi entropies of free bosons and fermions

To cite this article: Joaquín E Drut and William J Porter 2017 *J. Phys. A: Math. Theor.* **50** 145304

View the [article online](#) for updates and enhancements.

Related content

- [Lattice methods for strongly interacting many-body systems](#)
Joaquín E Drut and Amy N Nicholson
- [Rényi entropies of generic thermodynamic macrostates in integrable systems](#)
Márton Mestyán, Vincenzo Alba and Pasquale Calabrese
- [A contour for the entanglement entropies in harmonic lattices](#)
Andrea Coser, Cristiano De Nobili and Erik Tonni

Recent citations

- [Entropy, purity, and fidelity in Majorana phase space](#)
Ria Rushin Joseph *et al*
- [Estimating the central charge from the Rényi entanglement entropy](#)
A. Bazavov *et al*

IOP | ebooks™

Bringing you innovative digital publishing with leading voices to create your essential collection of books in STEM research.

Start exploring the collection - download the first chapter of every title for free.

Thermal properties of the Rényi entropies of free bosons and fermions

Joaquín E Drut and William J Porter

Department of Physics and Astronomy, University of North Carolina, Chapel Hill, NC, 27599-3255, United States of America

E-mail: drut@email.unc.edu and wjporter@live.unc.edu

Received 18 November 2016, revised 1 February 2017

Accepted for publication 17 February 2017

Published 8 March 2017

CrossMark

Abstract

We generalize techniques previously used to compute ground-state properties of one-dimensional noninteracting quantum gases to obtain exact results at finite temperature. We compute the order- n Rényi entropy to all orders in the fugacity in one, two, and three spatial dimensions. In arbitrary spatial dimensions, we provide closed-form expressions for its virial expansion up to next-to-leading order. In all of our results, we find explicit volume scaling in the high-temperature limit.

Keywords: Rényi entropy, virial expansion, non-interacting quantum systems

(Some figures may appear in colour only in the online journal)

1. Introduction

The exciting prospect of quantum computation for condensed matter, nuclear, and high-energy physics has brought about considerable activity at the interface between those areas and that of quantum information [1]. This interest has been fueled even further by the discovery of direct connections between topological quantum phase transitions and the concept of entanglement entropy [2]. More recently, the realization of topological insulators in condensed matter systems has brought all of the above together and is at the moment one of the most active areas of research in physics (see e.g. [3]).

In the last few years, substantial work has been carried out to rigorously characterize the scaling of the Rényi and von Neumann entanglement entropies of noninteracting systems in the ground state [4]. A number of exact results and inequalities have been established for a variety of systems (e.g. in external traps, in varying dimensions, etc) in the ground state [5–12]. In contrast, the behavior of the Rényi entropy for such systems at finite temperature has been much less explored [13].

To help fill that gap, we generalize a technique previously applied with great success to degenerate noninteracting gases [14, 15]. Using this method, we perform calculations of the

Rényi entropies S_n to all orders in the fugacity $z = e^{\beta\mu}$, where β is the inverse temperature and μ the chemical potential. In addition, we present closed-form expressions of the contributions to S_n at leading and next-to leading order in z around $z = 0$, which are the first terms in the virial expansion; we compute those contributions for both bosons and fermions. This expansion is interesting because, even though it is only valid in a dilute regime (which implies high temperature in the scale set by the Fermi energy), it is non-perturbative in character, and it is therefore useful as a benchmark for other approaches toward calculating what has proven to be a challenging observable. Those approaches include, in particular, quantum Monte Carlo methods, of which a variety of flavors have been recently put forward [16–25].

It should be noted that we do not expect to see in our results any kind of peculiar behavior associated with phase transitions (such as anomalous area-law scaling). However, we emphasize that the results are exact, and for this reason they are both useful and interesting.

2. Formalism and results for fermions

2.1. Basics

We set the stage for our calculation of noninteracting fermions in this section. We focus on non-relativistic d -dimensional systems, such that the dispersion relation is $\varepsilon(\mathbf{p}) = \mathbf{p}^2/2m$, taking $m = 1$ in what follows. The grand-canonical partition function is

$$\mathcal{Z} = \det(\mathbb{1} + z \mathcal{U}) \quad (1)$$

where $\mathcal{U}_{\mathbf{p}\mathbf{p}'} = \delta^{(d)}(\mathbf{p} - \mathbf{p}') \exp(-\beta\varepsilon(\mathbf{p}))$, $z = \exp(\beta\mu)$ is the fugacity, β is the inverse temperature and μ is the chemical potential. The single-particle Green's function is

$$\mathcal{G} = \frac{z \mathcal{U}}{\mathbb{1} + z \mathcal{U}}, \quad (2)$$

which is diagonal in momentum space:

$$\mathcal{G}_{\mathbf{p}\mathbf{p}'} = \frac{z e^{-\beta\varepsilon(\mathbf{p})}}{1 + z e^{-\beta\varepsilon(\mathbf{p})}} \delta^{(d)}(\mathbf{p} - \mathbf{p}'), \quad (3)$$

while in coordinate space (in an infinite volume) it takes the form

$$\mathcal{G}_{\mathbf{x}\mathbf{x}'} = \int_{\mathbb{R}^d} \frac{d^d p}{(2\pi)^d} e^{i\mathbf{p} \cdot (\mathbf{x} - \mathbf{x}')} \frac{z e^{-\beta\varepsilon(\mathbf{p})}}{1 + z e^{-\beta\varepsilon(\mathbf{p})}}. \quad (4)$$

To characterize the behavior of the entanglement entropy in the low- z regime, we need $\mathcal{G}$ in the virial expansion, which we write as

$$\mathcal{G}_{\mathbf{x}\mathbf{x}'} = \frac{z}{\lambda_T^d} \sum_{j=0}^{\infty} \mathcal{F}_{j,\mathbf{x}\mathbf{x}'} z^j, \quad (5)$$

where the thermal wavelength $\lambda_T = \sqrt{2\pi\beta}$ and the expansion coefficients are functions given by

$$\mathcal{F}_{j,\mathbf{x}\mathbf{x}'} = \frac{(-1)^j}{(j+1)^{d/2}} \exp\left(-\frac{\pi|\mathbf{x} - \mathbf{x}'|^2}{\lambda_T^2(j+1)}\right). \quad (6)$$

These functions will be essential in the virial expansion of the entanglement entropy, which we discuss below.

2.2. Rényi entropy

The Rényi entanglement entropy S_n for a subregion A is defined for positive integers n from the system's reduced density matrix $\hat{\rho}_A$ as

$$(1 - n)S_n = \ln \text{tr } \hat{\rho}_A^n. \quad (7)$$

By way of an auxiliary field decomposition, Grover showed that S_n may be computed as an expectation value taken over multiple copies (replicas) of a Hubbard-Stratonovich (HS) field (see [20]). Writing the reduced density operator as a superposition of operators corresponding to free particles in an HS field σ ,

$$\hat{\rho}_A = \int \mathcal{D}\sigma P_\sigma \hat{\rho}_{A,\sigma}, \quad (8)$$

with the normalized probability measure P_σ determined by the underlying dynamics, an explicit form for the operators $\hat{\rho}_{A,\sigma}$ may be derived by requiring them to reproduce the one-body physics. In particular, Grover showed

$$\hat{\rho}_{A,\sigma} = C_{A,\sigma} \exp(-\hat{\mathbf{c}}^\dagger \log(\mathcal{G}_{A,\sigma}^{-1} - \text{Id}_A) \hat{\mathbf{c}}), \quad (9)$$

where $\hat{\mathbf{c}}^{(\dagger)}$ are the fermionic annihilation (respectively, creation) operators, and

$$C_{A,\sigma} = \det(\text{Id}_A - \mathcal{G}_{A,\sigma}) \quad (10)$$

preserves the unit normalization. The identity operator (continuous or discrete) supported in the region A has been denoted by Id_A , and $\mathcal{G}_{A,\sigma}$ is the single-particle restricted Green's function in background field σ .

Using this form for the reduced density operator, it follows that the Rényi entropy can be written in path integral form as

$$(1 - n)S_n = \ln \int \mathcal{D}\sigma P[\sigma] \det \mathcal{M}_n[\sigma] \quad (11)$$

with $\sigma = (\sigma_1, \dots, \sigma_n)$, for normalized measure

$$\mathcal{D}\sigma P[\sigma] = \mathcal{D}\sigma_1 \dots \mathcal{D}\sigma_n P_{\sigma_1} \dots P_{\sigma_n}, \quad (12)$$

and with

$$\mathcal{M}_n[\sigma] = \prod_{k=1}^n (\text{Id}_A - \mathcal{G}_{A,\sigma_k}) \left[\text{Id}_A + \prod_{k=1}^n \frac{\mathcal{G}_{A,\sigma_k}}{\text{Id}_A - \mathcal{G}_{A,\sigma_k}} \right]. \quad (13)$$

Despite its amazingly general form, this expression has been found to be ill-suited for direct numerical calculations for systems with interactions of any appreciable strength, even in the case where $n = 2$ which requires no matrix inversion [24]. In spite of its complexity, numerous complementary approaches have been devised to compute the Rényi entropies for interacting systems [16–19, 21–25].

For the noninteracting case, the measure is trivial, and the entropy may be recast as

$$(1 - n)S_n = \ln \det \mathcal{M}_n \quad (14)$$

where $\mathcal{M}_n$ is given

$$\mathcal{M}_n = (\text{Id}_A - \mathcal{G}_A)^n + \mathcal{G}_A^n, \quad (15)$$

and multiplications prescribed above, in the case of continuous quantum numbers, are to be understood as

$$[\mathcal{O}_1 \mathcal{O}_2]_{xx'} = \int_A d^d y \mathcal{O}_{1,xy} \mathcal{O}_{2,yx'} \quad (16)$$

given operators $\mathcal{O}_1$ and $\mathcal{O}_1$ supported for $\mathbf{x}, \mathbf{x}' \in A$.

It is instructive to write down S_n above in terms of the eigenvalues λ of $\mathcal{G}_A$:

$$S_n = \frac{1}{1-n} \ln \det \mathcal{M}_n = \frac{1}{1-n} \sum_{\lambda} \ln [(1-\lambda)^n + \lambda^n], \quad (17)$$

where the eigenvalues λ lie in the closed segment $[0,1]$. We return to expressions of this form below.

The above results for noninteracting systems, or in general for quadratic Hamiltonians, were first derived by Peschel and colleagues in [27].

2.3. Fermionic Rényi entropy from the eigenvalue spectrum of restricted correlators

Inspired by [14, 15], we place the system in a finite box of volume $V = L^d$ and implement periodic boundary conditions. In principle, as soon as the eigenvalues λ of $\mathcal{G}_A$ are known, one can compute S_n ; however, $\mathcal{G}_A$ is a matrix with continuous indices, and therefore it is useful to obtain an expression in momentum space, where indices are discrete.

We begin by defining the Fredholm determinant $D_A(\lambda)$ in terms of the restricted finite-temperature correlator $\mathcal{G}_A$ and the identity operator on our subregion Id_A via

$$D_A(w) = \det(w \text{Id}_A - \mathcal{G}_A). \quad (18)$$

Note that this function vanishes whenever w equals an eigenvalue λ of $\mathcal{G}_A$. Using this fact, as previously done in [26], we write the n th order Rényi entropy as a contour integral

$$S_n = \oint_{\Gamma} \frac{dw}{2\pi i} f_n(w) \frac{d}{dw} \ln D_A(w) \quad (19)$$

where

$$f_n(w) = \frac{1}{1-n} \ln [(1-w)^n + w^n], \quad (20)$$

and the integration contour Γ encloses the segment $[0, 1] \subset \mathbb{R}$ of the complex- w plane (see equation (17) above). From this expression, we write

$$\ln \det(w \text{Id}_A - \mathcal{G}_A) = \omega(V) \ln w + \ln \det(\text{Id}_A - w^{-1} \mathcal{G}_A), \quad (21)$$

for some (infinite) constant ω that depends on the volume of space. Because the function f_n vanishes at $w = 0$ for $n \geq 2$, this term makes no contribution to the integral, and we may safely neglect it in derivations that follow and in the infinite-volume limit taken later. Expanding the Fredholm determinant on the right in powers of w^{-1} , we have

$$\ln \det(\text{Id}_A - w^{-1} \mathcal{G}_A) = - \sum_{s=1}^{\infty} \frac{\text{tr } \mathcal{G}_A^s}{w^s s}, \quad (22)$$

and writing out the trace in d spatial dimensions, we obtain

$$\text{tr } \mathcal{G}_A^s = \sum_{k_1 \in \mathbb{Z}^d} \dots \sum_{k_s \in \mathbb{Z}^d} F_{k_1 k_2} F_{k_2 k_3} \dots F_{k_s k_1} = \text{tr } F^s \quad (23)$$

for each positive integer s where the (infinite) overlap matrix F is comprised of discrete elements

$$F_{\mathbf{k}\mathbf{k}'} = \frac{1}{L^d} \frac{ze^{-\pi\mathbf{k}^2(\lambda_T/L)^2}}{1 + ze^{-\pi\mathbf{k}^2(\lambda_T/L)^2}} \int_A d^d x e^{-2\pi i \mathbf{x} \cdot (\mathbf{k} - \mathbf{k}')/L}. \quad (24)$$

We note that this matrix is identical to that used in [14, 15] save two crucial differences: the domain of the indices is not bounded as a result of all momentum states having nontrivial occupation at finite temperature; this noncompact support is thankfully accompanied by the additional Fermi-Dirac prefactor providing a point of connection between our generalization and this method's ground-state formulation (again, see [14, 15]). In the case of continuous indices, we find

$$S_n = \int_{\mathbb{R}^d} d^d k f_n(a(\mathbf{k})) \quad (25)$$

where the values $a(\mathbf{k})$ are the spectrum of the continuum limit of F , and we have indexed them by momenta.

In order to perform our numerical calculations for arbitrary fugacity, we diagonalize the matrix A defined above at fixed

$$\xi \equiv \lambda_T/L, \quad (26)$$

for some finite momentum cutoff Λ . Following that, we formally construct a (diagonal) matrix $M_n^{(\Lambda)}$ with elements $f_n(a(\mathbf{k}))\delta_{\mathbf{k}\mathbf{k}'}$ for values of the d -dimensional integer vectors satisfying $|\mathbf{k}|, |\mathbf{k}'| \leq \Lambda$ and perform the trace corresponding to the continuum limit via the limit of infinite cutoff and consequently the limit in which the matrix becomes infinite in linear extent N_Λ . That is, we compute the entropy in a finite volume via the limit

$$S_n^{(\Lambda)}(\xi) \equiv \frac{1}{N_\Lambda} \text{tr} M_n^{(\Lambda)} \xrightarrow{N_\Lambda \rightarrow \infty} \int_{\mathbb{R}^d} d^d k M_n(\mathbf{k}, \mathbf{k}). \quad (27)$$

In addition to the continuum limit, we perform the infinite volume limit by taking ξ to zero while fixing the region size L_A in units of the thermal wavelength, thus maintaining that we are in the dilute (high-temperature) regime.

From the above definitions, we note that for $\xi \ll 1$, the matrix elements of F become

$$F_{\mathbf{k}\mathbf{k}'} = \frac{(\xi\theta)^d}{(2\pi)^{d/2}} \frac{z}{1+z} + \mathcal{O}(\xi^{d+2}), \quad (28)$$

where we have written

$$\theta = \frac{L_A}{\lambda_T} \sqrt{2\pi}; \quad (29)$$

that is, they become momentum-independent to leading order as we take the continuum limit, so that in the this limit, F is a constant matrix. Working at leading order, we find that for fermions this gross degeneracy implies that the entropy takes a particularly simple form. Independent of the form of the cutoff, we find that for finite Λ the above trace gives

$$(\xi\theta)^{-d} S_n^{(\Lambda)}(\xi) \xrightarrow{\xi \rightarrow 0} \frac{1}{(2\pi)^{d/2}} \frac{n}{n-1} \frac{z}{1+z}, \quad (30)$$

a result independent of Λ .

2.4. Virial expansion of the entropy for fermions

Starting from equation (11), where the Green's function is an explicit function of the fugacity z , we expand to leading and next-to-leading order in z . In the interacting case, this involves expanding both the determinant present in the probability measure P , as well as the pure entanglement contribution coming from $\det \mathcal{M}_n$. In the noninteracting case, however, P is just a constant and therefore plays no role in the calculation, i.e. our starting point is actually equation (14). Thus, expanding that equation in powers of z , we obtain

$$(1-n)S_n = \text{tr} \ln \mathcal{M}_n|_{z=0} + z \text{tr} \left[\mathcal{M}_n^{-1} \frac{\partial \mathcal{M}_n}{\partial z} \right] \Big|_{z=0} + \frac{z^2}{2!} \left\{ \text{tr} \left[\mathcal{M}_n^{-1} \left(\frac{\partial^2 \mathcal{M}_n}{\partial z^2} \right) - \mathcal{M}_n^{-2} \left(\frac{\partial \mathcal{M}_n}{\partial z} \right)^2 \right] \right\} \Big|_{z=0} + O(z^3). \quad (31)$$

We continue by analyzing the z dependence of $\mathcal{M}_n$. At $z = 0$, the single-particle Green's function vanishes, which implies that the first term in the above expansion vanishes as well. From this, we find immediately that the limiting form of the operator $\mathcal{M}_n$, as well as its inverse (where it exists), is the identity, i.e.

$$\mathcal{M}_n|_{z=0} = \mathcal{M}_n^{-1}|_{z=0} = \text{Id}_A. \quad (32)$$

Therefore,

$$(1-n)S_n = z \text{tr} \left[\frac{\partial \mathcal{M}_n}{\partial z} \right] \Big|_{z=0} + \frac{z^2}{2!} \text{tr} \left[\frac{\partial^2 \mathcal{M}_n}{\partial z^2} - \left(\frac{\partial \mathcal{M}_n}{\partial z} \right)^2 \right] \Big|_{z=0} + O(z^3). \quad (33)$$

Further, we have for $n \geq 2$

$$\frac{\partial \mathcal{M}_n}{\partial z} \Big|_{z=0} = -n \frac{\partial \mathcal{G}_A}{\partial z} \Big|_{z=0}. \quad (34)$$

The peculiar structure of the operator under consideration, together with the behavior of the Green's function at $z = 0$, necessitates separating the second order contribution into cases $n = 2$ and $n > 2$. For $n = 2$, we find

$$\frac{\partial^2 \mathcal{M}_2}{\partial z^2} \Big|_{z=0} = \left[4 \left(\frac{\partial \mathcal{G}_A}{\partial z} \right)^2 - 2 \frac{\partial^2 \mathcal{G}_A}{\partial z^2} \right] \Big|_{z=0}, \quad (35)$$

with the general expression for $n > 2$ being different:

$$\frac{\partial^2 \mathcal{M}_n}{\partial z^2} \Big|_{z=0} = \left[n(n-1) \left(\frac{\partial \mathcal{G}_A}{\partial z} \right)^2 - n \frac{\partial^2 \mathcal{G}_A}{\partial z^2} \right] \Big|_{z=0}. \quad (36)$$

Therefore,

$$\left[\frac{\partial^2 \mathcal{M}_2}{\partial z^2} - \left(\frac{\partial \mathcal{M}_2}{\partial z} \right)^2 \right] \Big|_{z=0} = -2 \frac{\partial^2 \mathcal{G}_A}{\partial z^2} \Big|_{z=0}. \quad (37)$$

and

$$\left[\frac{\partial^2 \mathcal{M}_n}{\partial z^2} - \left(\frac{\partial \mathcal{M}_n}{\partial z} \right)^2 \right] \Big|_{z=0} = -n \left[\left(\frac{\partial \mathcal{G}_A}{\partial z} \right)^2 + \frac{\partial^2 \mathcal{G}_A}{\partial z^2} \right] \Big|_{z=0} \quad (38)$$

From the virial expansion of the free fermionic Green's function given in equation (5), we observe not only

$$\frac{\partial \mathcal{G}_{\mathbf{x}\mathbf{x}'}}{\partial z} \Big|_{z=0} = \lambda_T^{-d} \mathcal{F}_{0,\mathbf{x}\mathbf{x}'} \quad (39)$$

but also

$$\frac{\partial^2 \mathcal{G}_{\mathbf{x}\mathbf{x}'}}{\partial z^2} \Big|_{z=0} = 2\lambda_T^{-d} \mathcal{F}_{1,\mathbf{x}\mathbf{x}'}. \quad (40)$$

The restricted form of $\mathcal{G}_{\mathbf{x}\mathbf{x}'}$, therefore, translates into restricted forms of the $\mathcal{F}_{j,\mathbf{x}\mathbf{x}'}$ coefficients.

We evaluate the required traces according to

$$\text{tr } \mathcal{O}_A = \int_A d^d y \mathcal{O}_{A,yy} \quad (41)$$

for the d -dimensional case, and we have chosen the region A to be the rectangular prism defined by the vectors $\mathbf{x}_1$ and $\mathbf{x}_2$ via $A = [x_{1(1)}, x_{2(1)}] \times \cdots \times [x_{1(d)}, x_{2(d)}] \subseteq \mathbb{R}^d$. Putting the above contributions together up to second order in z , we find that the second Rényi entropy is

$$S_2(z, \theta) = (2 \text{tr } \mathcal{F}_{0,A}) z + (2 \text{tr } \mathcal{F}_{1,A}) z^2 + O(z^3), \quad (42)$$

while for $n > 2$ Rényi entropies we obtain

$$\begin{aligned} S_n(z, \theta) &= \frac{n}{n-1} (\text{tr } \mathcal{F}_{0,A}) z \\ &\quad + \frac{n}{2(n-1)} (\text{tr } \mathcal{F}_{0,A}^2 + 2 \text{tr } \mathcal{F}_{1,A}) z^2 + O(z^3). \end{aligned} \quad (43)$$

For the coefficients, we obtain the following closed-form expressions:

$$\text{tr } \mathcal{F}_{0,A} = (2\pi)^{-d/2} \theta_1 \theta_2 \cdots \theta_d \quad (44)$$

$$\text{tr } \mathcal{F}_{1,A} = -\frac{1}{2^{d/2}} \text{tr } \mathcal{F}_{0,A} = -\frac{1}{2^{d/2} \pi^{d/2}} \theta_1 \theta_2 \cdots \theta_d \quad (45)$$

$$\text{tr } \mathcal{F}_{0,A}^2 = \prod_{k=1}^d \left[\frac{1}{2\sqrt{\pi}} \theta_k \text{erf } \theta_k + \frac{1}{2\pi} (e^{-\theta_k^2} - 1) \right]. \quad (46)$$

In each case above, we have introduced dimensionless length variables θ_k defined for each k by

$$\theta_k = \frac{\sqrt{2\pi}}{\lambda_T} (x_{2(k)} - x_{1(k)}). \quad (47)$$

Equations (42) and (43) are our main result for the virial expansion for fermions. Plots of the first of these results are given in figure 1, where we display the second Rényi entropy $S_2(z, \theta)$ for dimensions $d = 1, 2$, and 3 . We note that for the second entropy, both virial coefficients display explicit volume scaling so that to quadratic order in the fugacity, $S_2(z, \theta)/\theta^d$ is a function of the fugacity and spatial dimension alone. In figure 2, we show the $n = 3$ case for

Figure 1. Analytic results to all orders in z (solid lines) along with first- (dot-dashed) and second-order (dashed) virial expansions for the second Rényi entropy $S_2(z, \theta)$ for fermions versus fugacity, shown for dimensions $d = 1, 2$, and 3 (from top to bottom). Note that this case ($n = 2$) has no dependence on θ at the orders shown.

Figure 2. Third Rényi entropy S_3 of noninteracting fermions as a function of the fugacity and for several values of the dimensionless region size θ and for dimensions 1, 2, and 3 (top to bottom panels). The dashed lines show, for each dimension, the leading order results, which are proportional to θ^d , colored lines represent the second-order results for various subsystem sizes, and solid extended lines show the result of analytic calculations to all orders in the fugacity.

several values of the dimensionless region size θ and for dimensions 1, 2, and 3. In contrast to the $n = 2$ case, $n > 2$ does have non-trivial volume effects at second order in z .

3. Formalism and results for bosons

3.1. Basics

Continuing with our focus on non-relativistic systems, the partition function for noninteracting bosons is

$$\mathcal{Z} = [\det(\mathbb{1} - z\mathcal{U})]^{-1}, \quad (48)$$

such that the single-particle Green's function is

$$\mathcal{G} = \frac{z\mathcal{U}}{\mathbb{1} - z\mathcal{U}}, \quad (49)$$

which takes the momentum-space form

$$\mathcal{G}_{pp'} = \frac{ze^{-\beta\varepsilon(\mathbf{p})}}{1 - ze^{-\beta\varepsilon(\mathbf{p})}} \delta^{(d)}(\mathbf{p} - \mathbf{p}'), \quad (50)$$

and the coordinate-space form $\mathcal{G}_{xx'}$ can be obtained by Fourier transforming, as shown above in the fermion case. With this as a starting point, we may formally expand in powers of z :

$$\mathcal{G}_{xx'} = \frac{z}{\lambda_T^d} \sum_{j=0}^{\infty} \mathcal{B}_{j,xx'} z^j \quad (51)$$

where, not surprisingly, we find

$$\mathcal{B}_{j,xx'} = (-1)^j \mathcal{F}_{j,xx'}. \quad (52)$$

3.2. Rényi entropy

With the replacement of the bosonic Green's function defined above for the fermionic equivalent used earlier, the auxiliary-field decomposition of the reduced density matrix becomes

$$\hat{\rho}_{A,\sigma} = B_{A,\sigma} \exp\left(-\hat{\mathbf{b}}^\dagger \log(\mathcal{G}_A^{-1} + \text{Id}_A) \hat{\mathbf{b}}\right) \quad (53)$$

where

$$B_{A,\sigma} = [\det(\text{Id}_A + \mathcal{G}_A)]^{-1} \quad (54)$$

and we have introduced the bosonic annihilation (creation) operators $\hat{\mathbf{b}}^{(\dagger)}$.

From this expression for the reduced density operator, the Rényi entropy for bosons can be expressed in path integral form as

$$(1 - n)S_n = \ln \int \mathcal{D}\sigma P[\sigma] \det \mathcal{N}_n[\sigma] \quad (55)$$

with

$$\begin{aligned} \mathcal{N}_n[\sigma] &= \prod_{k=1}^n (\text{Id}_A + \mathcal{G}_{A,\sigma_k})^{-1} \\ &\times \left[\text{Id}_A - \prod_{k=1}^n \frac{\mathcal{G}_{A,\sigma_k}}{\text{Id}_A + \mathcal{G}_{A,\sigma_k}} \right]^{-1} \end{aligned} \quad (56)$$

and where the probability $P[\sigma]$ is now generated by the product measure of the single-field densities coming from the underlying dynamics of the bosonic degrees of freedom.

Interestingly, the above expressions extend Grover's Monte Carlo method to interacting bosons. However, stability of the latter requires a repulsive interaction, which would give a sign problem. Therefore, the above is not (at the moment) of practical interest for Monte Carlo methods. It does, however, provide a starting point for formal analyses. In particular, in the noninteracting case the entropy becomes

$$(1 - n)S_n = -\ln \det \mathcal{N}_n \quad (57)$$

where

$$\mathcal{N}_n = (\text{Id}_A + \mathcal{G}_A)^n - \mathcal{G}_A^n. \quad (58)$$

3.3. Bosonic Rényi entropy from the spectrum of restricted correlators

In close analogy to the fermionic case, we again place the system in a finite box and impose periodic boundary conditions. We define the Fredholm determinant $D_A(\lambda)$ in terms of the restricted bosonic correlator as

$$D_A(w) = \det(w \text{Id}_A - \mathcal{G}_A), \quad (59)$$

and write the n th order Rényi entropy as a contour integral

$$S_n = \oint_{\Sigma} \frac{dw}{2\pi i} g_n(w) \frac{d}{dw} \ln D_A(w) \quad (60)$$

where now

$$g_n(w) = \frac{1}{1-n} \ln \left[\frac{1}{(1+w)^n - w^n} \right], \quad (61)$$

and the integration contour Σ is defined to contain the segment $[0, \infty) \subset \mathbb{R}$ of the complex- w plane.

Again, writing out the trace in d spatial dimensions, we obtain an expression

$$\text{tr } \mathcal{G}_A^s = \sum_{k_1 \in \mathbb{Z}^d} \dots \sum_{k_s \in \mathbb{Z}^d} B_{k_1 k_2} B_{k_2 k_3} \dots B_{k_s k_1} = \text{tr } B^s \quad (62)$$

for each positive integer s where the (again infinite) matrix B differs from the matrix F in an obvious way:

$$B_{kk'} = \frac{1}{L^d} \frac{z e^{-\pi k^2 \xi^2}}{1 - z e^{-\pi k^2 \xi^2}} \int_A d^d x e^{-2\pi i x \cdot (k - k')/L}. \quad (63)$$

Evaluating the limit as before, we obtain a continuum limit valid to all orders in the fugacity:

$$(\xi \theta)^{-d} S_n^{(\Lambda)}(\xi) \xrightarrow{\xi \rightarrow 0} \frac{1}{(2\pi)^{d/2}} \frac{n}{n-1} \frac{z}{1-z}. \quad (64)$$

3.4. Virial expansion of the entropy for bosons

Again, we find that a zero fugacity, the single-particle Green's function vanishes. Hence, once again in this limit, $\mathcal{N}_n$ and its inverse are the identity. Therefore, the virial expansion of S_n in the bosonic case simplifies to

$$(n-1)S_n = z \operatorname{tr} \left[\frac{\partial \mathcal{N}_n}{\partial z} \right] \Big|_{z=0} + \frac{z^2}{2!} \operatorname{tr} \left[\frac{\partial^2 \mathcal{N}_n}{\partial z^2} - \left(\frac{\partial \mathcal{N}_n}{\partial z} \right)^2 \right] \Big|_{z=0} + O(z^3). \quad (65)$$

We easily obtain for orders $n \geq 2$

$$\frac{\partial \mathcal{N}_n}{\partial z} \Big|_{z=0} = n \frac{\partial \mathcal{G}_A}{\partial z} \Big|_{z=0}. \quad (66)$$

Similar operator structure requires we again treat separately the second order contribution into cases of $n = 2$ and $n > 2$. For $n = 2$, we get

$$\frac{\partial^2 \mathcal{N}_2}{\partial z^2} \Big|_{z=0} = 2 \frac{\partial^2 \mathcal{G}_A}{\partial z^2} \Big|_{z=0} \quad (67)$$

and with the expression for $n > 2$ being

$$\frac{\partial^2 \mathcal{N}_n}{\partial z^2} \Big|_{z=0} = \left[n(n-1) \left(\frac{\partial \mathcal{G}_A}{\partial z} \right)^2 + n \frac{\partial^2 \mathcal{G}_A}{\partial z^2} \right] \Big|_{z=0}. \quad (68)$$

From the virial expansion given above for the bosonic correlator, we find that for the second order entropy the expansion becomes

$$S_2(z, \theta) = (2 \operatorname{tr} \mathcal{B}_{0,A}) z + (2 \operatorname{tr} \mathcal{B}_{1,A} - 2 \operatorname{tr} \mathcal{B}_{0,A}^2) z^2 + O(z^3) \quad (69)$$

$$= (2 \operatorname{tr} \mathcal{F}_{0,A}) z - (2 \operatorname{tr} \mathcal{F}_{1,A} + 2 \operatorname{tr} \mathcal{F}_{0,A}^2) z^2 + O(z^3), \quad (70)$$

and for the entropies of order $n > 2$, we have

$$S_n(z, \theta) = \frac{n}{n-1} (\operatorname{tr} \mathcal{B}_{0,A}) z + \frac{n}{2(n-1)} (2 \operatorname{tr} \mathcal{B}_{1,A} - \operatorname{tr} \mathcal{B}_{0,A}^2) z^2 + O(z^3) \quad (71)$$

$$= \frac{n}{n-1} (\operatorname{tr} \mathcal{F}_{0,A}) z - \frac{n}{2(n-1)} (\operatorname{tr} \mathcal{F}_{0,A}^2 + 2 \operatorname{tr} \mathcal{F}_{1,A}) z^2 + O(z^3). \quad (72)$$

Equations (69) and (71) are our main result for the virial expansion for bosons. As could be anticipated, the leading-order result is the same for bosons and fermions. This is expected, as it corresponds to the single-particle contributions, and therefore the statistics plays no role.

In figure 3 we show our results for bosons for the $n = 2$ case. As in the fermionic case, there is no dependence on θ for $n = 2$. In figure 4, we show the $n = 3$ case for several values of the dimensionless region size θ and for dimensions 1, 2, and 3. In contrast to the $n = 2$ case, $n > 2$ does have non-trivial volume effects at second order in z .

Figure 3. Exact results (solid) along with first- (dot-dashed) and second-order (dashed) virial expansions of the second Rényi entropy $S_2(z, \theta)$ for bosons shown (from top to bottom) for dimensions $d = 1, 2$, and 3 versus fugacity z .

Figure 4. Third Rényi entropy S_3 of noninteracting bosons as a function of the fugacity and for several values of the dimensionless region size θ and for dimensions 1, 2 and 3 (top to bottom panels). The dashed lines show, for each dimension, the leading order results, which are proportional to θ^d .

4. Summary and conclusions

We have performed a semi-analytic calculation to all orders in the fugacity $z = e^{\beta\mu}$ of the Rényi entanglement entropy of noninteracting quantum gases in arbitrary spatial dimensions. We provide an analytic expression in the continuum, high-temperature limit $L \rightarrow \infty$, $\lambda_T/L \rightarrow 0$, at fixed λ_T/L_A . In addition, we have calculated the leading and next-to-leading order terms in the virial expansion.

As expected, we found volume scaling for our exact results as well as at both orders in the virial expansion. In [28], the same leading scaling was found via a different analysis. At leading order (where the statistics is irrelevant) our result is the same for bosons and fermions. For fermions, the two-particle, i.e. z^2 , contributions decrease the entanglement entropy relative to the leading-order result, while the opposite happens for bosons; this appears to be true for all n .

In all cases, we find that the convergence properties of the virial expansion, as estimated from considering the two orders computed here, improve when going to higher dimensions. Indeed, in the scale shown in our plots the results for $d = 1$ are much less promising in this regard than $d = 3$.

With the rapid development in the area of Monte Carlo calculations of the entanglement properties of many-body systems, having non-perturbative results available is of great value as a benchmark. In this work we have aimed to provide such results.

Acknowledgments

The authors are grateful to L Rammelmüller for thought-provoking discussions and proofreading. This material is based upon work supported by the National Science Foundation under Grants No. PHY1306520 (Nuclear Theory program) and No. PHY1452635 (Computational Physics program).

References

- [1] Amico L, Fazio R, Osterloh A and Vedral V 2008 *Rev. Mod. Phys.* **80** 517
 Horodecki R, Horodecki P, Horodecki M and Horodecki K 2009 *Rev. Mod. Phys.* **81** 865
 Eisert J, Cramer M and Plenio M B 2010 *Rev. Mod. Phys.* **82** 277
- [2] Osterloh A, Amico L, Falci G and Fazio R 2002 *Nature* **416** 608–10
 Vidal G, Latorre J I, Rico E and Kitaev A 2003 *Phys. Rev. Lett.* **90** 227902
 Kitaev A and Preskill J 2006 *Phys. Rev. Lett.* **96** 110404
 Levin M and Wen X-G 2006 *Phys. Rev. Lett.* **96** 110405
- [3] Barkeshli M and Sau J D 2015 arXiv:1509.07135
 Xu Y, Miotkowski I, Liu C, Tian J, Nam H, Alidoust N, Hu J, Shih C-K, Hasan M Z and Chen Y P 2014 *Nat. Phys.* **10** 956
- [4] Gioev D and Klich I 2006 *Phys. Rev. Lett.* **96** 100503
 Leschke H, Sobolev A V and Spitzer W 2014 *Phys. Rev. Lett.* **112** 160403
- [5] Peschel I and Eisler V 2009 *J. Phys. A: Math. Theor.* **42** 504003
- [6] Süsstrunk R and Ivanov D A 2012 *Europhys. Lett.* **100** 60009
- [7] Ivanov D A and Abanov A G 2013 *J. Phys. A: Math. Theor.* **46** 375005
 Eisler V and Peschel I 2013 *J. Stat. Mech.* **P04028**
- [8] Ossipov A 2014 *Phys. Rev. Lett.* **113** 130402
 Pouranvari M and Yang K 2014 *Phys. Rev. B* **89** 115104
- [9] Calabrese P, Le Doussal P and Majumdar S N 2015 *Phys. Rev. A* **91** 012303
 Drut J E and Porter W J 2015 *Phys. Rev. Lett.* **114** 050402
- [10] Peschel I and Eisler V 2012 *J. Phys. A: Math. Theor.* **45** 155301

- [11] Mondragon-Shem I and Hughes T L 2014 *J. Stat. Mech.* [P10022](#)
Eisler V and Peschel I 2014 *J. Stat. Mech.* [P04005](#)
You W-L 2014 *J. Phys. A: Math. Theor.* **47** 255301
- [12] Chen X and Fradkin E 2013 *J. Stat. Mech.* [P08013](#)
Storms M and Singh R R P 2014 *Phys. Rev. E* **89** 012125
- [13] Pastur L and Slavin V 2014 *Phys. Rev. Lett.* **113** 150404
Bernigau H, Kastoryano M J and Eisert J 2015 *J. Stat. Mech.* [P02008](#)
Schliemann J 2014 *J. Stat. Mech.* [P09011](#)
- [14] Calabrese P, Mintchev M and Vicari E 2011 *J. Stat. Mech.* [P09028](#)
- [15] Vicari E 2012 *Phys. Rev. A* **85** 062104
Eisler V and Peschel I 2012 *Europhys. Lett.* **99** 20001
Calabrese P, Mintchev M and Vicari E 2012 *J. Phys. A: Math. Theor.* **45** 105206
Calabrese P, Mintchev M and Vicari E 2012 *Europhys. Lett.* **97** 20009
- [16] Buividovich P V and Polikarpov M I 2008 *Nucl. Phys. B* **802** 458
- [17] Melko R G, Kallin A B and Hastings M B 2010 *Phys. Rev. B* **82** 100409
Hastings M B, González I, Kallin A B and Melko R G 2010 *Phys. Rev. Lett.* **104** 157201
Isakov S V, Hastings M B and Melko R G 2011 *Nat. Phys.* **7** 772
Singh R R P, Hastings M B, Kallin A B and Melko R G 2011 *Phys. Rev. Lett.* **106** 135701
Inglis S and Melko R G 2013 *Phys. Rev. E* **87** 013306
- [18] Humeniuk S and Roscilde T 2012 *Phys. Rev. B* **86** 235116
- [19] McMinis J and Tubman N M 2013 *Phys. Rev. B* **87** 081108
- [20] Grover T 2013 *Phys. Rev. Lett.* **111** 130402
- [21] Broecker P and Trebst S 2014 *J. Stat. Mech.* [P08015](#)
- [22] Wang L and Troyer M 2014 *Phys. Rev. Lett.* **113** 110401
- [23] Luitz D J, Plat X, Laflorencie N and Alet F 2014 *Phys. Rev. B* **90** 125105
- [24] Assaad F F, Lang T C and Toldin F P 2014 *Phys. Rev. B* **89** 125121
Assaad F F 2015 *Phys. Rev. B* **91** 125146
- [25] Drut J E and Porter W J 2015 *Phys. Rev. B* **92** 125126
Drut J E and Porter W J 2016 *Phys. Rev. E* **93** 043301
- [26] Jin B-Q and Korepin V E 2004 *J. Stat. Phys.* **116** 79
- [27] Chung M-C and Peschel I 2001 *Phys. Rev. B* **64** 064412
Cheong S-A and Henley C L 2004 *Phys. Rev. B* **69** 075111
Peschel I 2003 *J. Phys. A: Math. Gen.* **36** L205
- [28] Leschke H, Sobolev A V and Spitzer W 2016 *J. Phys. A: Math. Theor.* **49** 30LT04