Exact variances of von Neumann entropy over fermionic Gaussian states

Youyi Huang and Lu Wei
Department of Computer Science, Texas Tech University, Texas, USA
{youhuang, luwei}@ttu.edu

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Abstract—**We study the statistical behavior of quantum entanglement in bipartite systems over fermionic Gaussian states as measured by von Neumann entropy. The formulas of average von Neumann entropy with and without particle number constraints have been recently obtained, whereas the main results of this work are the exact yet explicit formulas of variances for both cases. For the latter case of no particle number constraint, the results resolve a recent conjecture on the corresponding variance. Different than the existing methods in computing variances over other generic state models, proving the results of this work relies on a new simplification framework. The framework consists of a set of new tools in simplifying finite summations of what we refer to as dummy summation and re-summation techniques.**

I. Introduction

Quantum entanglement is the most important feature in quantum mechanics. The understanding of the phenomenon of entanglement is crucial in realizing the revolutionary advances of quantum science. In the emerging field of quantum information processing, quantum entanglement is also the resource and medium that enable the underlying quantum technologies.

In this work, we study the statistical behavior of entanglement over the fermionic Gaussian states. In the past decades, considerable effort has been devoted to investigating the degree of entanglement as measured by different entanglement entropies over the well-known Hilbert-Schmidt ensemble [1]–[13]. In particular, these studies focus on the statistical behavior of entanglement entropies such as von Neumann entropy [1]–[8], quantum purity [9]–[11], and Tsallis entropy [12], [13]. Driven by the recent breakthrough in probability theory on the Bures-Hall ensemble [14]–[17], considerable progress has been made in understanding the von Neumann entropy [18]–[20] and quantum purity [21]–[23] over the Bures-Hall ensemble. Similar investigations are now being carried out over the fermionic Gaussian ensemble, which is a generic state model relevant for different quantum information processing tasks [24]–[29]. Very recently, the mean values of von Neumann entropy with and without particle number constraints over the fermionic Gaussian ensemble are obtained in [27] and [29], respectively. As an important step towards characterizing the statistical distribution of von Neumann entropy, we aim to derive the corresponding variances, which describe the fluctuation of the entropy around their mean values. The exact variance of von Neumann entropy over fermionic Gaussian states without particle number constraint has been conjectured in a prior work [30]. In the current work, we prove the conjecture as well as derive a variance formula for the case of fixed particle number.

II. Problem formulations

In this section, we introduce the formulation that leads to the fermionic Gaussian states with and without particle number constraints. A system of N fermionic degrees of freedom can be decomposed into two subsystems A and B of the dimensions m and n, respectively, with $m+n=N$. Without loss of generality, we assume $m \leq n$. In the present work, we consider two scenarios of fermionic Gaussian states – the fermionic Gaussian states with arbitrary number of particles and the fermionic Gaussian states with a fixed number of particles.

Case A: Arbitrary number of particles

A system of N fermionic modes can be formulated in terms of a set of fermionic creation and annihilation operators $\hat{a}_i$ and $\hat{a}_i^\dagger$, $i=1,\ldots,N$. Since the modes are fermionic, these operators obey the canonical anti-commutation relation [24], [29],

$$\{\hat{a}_i, \hat{a}_j^\dagger\} = \delta_{ij}\mathbb{I}, \qquad \{\hat{a}_i, \hat{a}_j\} = 0 = \{\hat{a}_i^\dagger, \hat{a}_j^\dagger\}, \tag{1}$$

where $\{\hat{A},\hat{B}\} = \hat{A}\hat{B}+\hat{B}\hat{A}$ denotes the anti-commutation relation and $\mathbb{I}$ is an identity operator. Equivalently, one can also describe these fermionic modes in terms of the Majorana operators γ_l, $l=1,\ldots,2N$, and

$$\hat{\gamma}_{2i-1} = \frac{\hat{a}_i^\dagger + \hat{a}_i}{\sqrt{2}}, \qquad \hat{\gamma}_{2i} = \imath\frac{\hat{a}_i^\dagger + \hat{a}_i}{\sqrt{2}} \tag{2}$$

with $\imath = \sqrt{-1}$ being the imaginary unit. Note that the Majorana operators are Hermitian satisfying the anti-commutation relation

$$\{\hat{\gamma}_l, \hat{\gamma}_k\} = \delta_{lk}\mathbb{I}. \tag{3}$$

By collecting the Majorana operators into a $2N$ dimensional operator-valued column vector $\gamma = (\hat{\gamma}_1,\ldots,\hat{\gamma}_{2N})^\dagger$, a fermionic Gaussian state is then written as the density operator of the form [28], [29]

$$\rho(\gamma) = \frac{\mathrm{e}^{-\gamma^\dagger Q\gamma}}{\mathrm{tr}(\mathrm{e}^{-\gamma^\dagger Q\gamma})}, \tag{4}$$

where the coefficient matrix Q is a $2N\times 2N$ imaginary anti-symmetric matrix as the consequence of the anti-communication relation (3). There always exsits an orthogonal matrix M that diagnoses the coefficient matrix Q by transforming γ into another Majorana basis $\mu = (\hat{\mu}_1, \ldots, \hat{\mu}_{2N})^\dagger = M\gamma$ [29]. A fermionic Gaussian state is labelled by its anti-symmetric covariance matrix [29]

$$J = -\imath \tanh(Q) = M^T J_0 M, \tag{5}$$

where $\tanh(x)$ denotes the hyperbolic tangent function [31], the matrix J_0 takes the block diagonal form

$$J_0 = \begin{pmatrix} \tanh(\lambda_1)\mathbb{A} & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ldots & \tanh(\lambda_N)\mathbb{A} \end{pmatrix}, \tag{6}$$

and

$$\mathbb{A} = \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix}. \tag{7}$$

We consider the von Neumann entropy as the measure of entanglement between the two subsystems. By restricting the matrix J to the entries from subsystems A, the restricted matrix J_A becomes the $2m \times 2m$ left-upper block of J. The von Neumann entropy of a fermionic Gaussian state of case A can be represented in terms of the real positive eigenvalues $x_i, i = 1, \ldots, m$ of $\imath J_A$ as [27], [29], [30]

$$S = -\sum_{i=1}^{m} v(x_i), \tag{8}$$

where

$$v(x) = \frac{1-x}{2} \ln \frac{1-x}{2} + \frac{1+x}{2} \ln \frac{1+x}{2}. \tag{9}$$

The resulting joint probability density of the eigenvalues $x_i, i = 1, \ldots, m$ is proportional to [27]

$$\prod_{1 \le i < j \le m} \left(x_i^2 - x_j^2\right)^2 \prod_{i=1}^{m} \left(1 - x_i^2\right)^{n-m}, \qquad x_i \in [0, 1], \tag{10}$$

which is obtained by recursively applying the result in [32, Proposition A.2].

Case B: Fixed number of particles

For a fermionic Gaussian state $|F\rangle$ with a fixed particle number p, $m \le p \le n$, the corresponding covariance matrix H can be expressed via the commutator of fermionic creation and annihilation operators as [25], [26], [29]

$$H_{ij} = -\imath \langle F | \hat{a}_i^\dagger \hat{a}_j - \hat{a}_j \hat{a}_i^\dagger | F \rangle. \tag{11}$$

Recall the canonical anti-commutation relation (1), the entries of the matrix H are then of the form

$$H_{ij} = -2\imath G_{ij} + \imath \delta_{ij} \mathbb{I}, \tag{12}$$

where $G_{ij} = \langle F | \hat{a}_i^\dagger \hat{a}_j | F \rangle$ denotes the entries of an $N \times N$ matrix G of a fermionic system of N modes. There exists a unitary transformation U that diagonalizes G into the form $U^\dagger G U$, where the first p diagonal elements are equal to 1 and the rest are 0. Therefore, one can write

$$G = U_{N \times p} U_{N \times p}^\dagger. \tag{13}$$

A fermionic Gaussian state of dimension $N = m + n$ with p particles can be fully characterized by the matrices H and G. The von Neumann entropy of the fermionic system in the case B can be represented as [25], [26], [29]

$$S = -\sum_{i=1}^{m} v(2y_i - 1), \qquad y_i \in [0, 1], \tag{14}$$

where y_i, $i = 1, \ldots, m$ are the eigenvalues of the restricted $m \times m$ matrix $G_A = U_{m \times p} U_{m \times p}^\dagger$. The eigenvalue distribution of the random matrix $U_{m \times p} U_{m \times p}^\dagger$ is the well-known Jacobi unitary ensemble [33], [34]. We denote x_i, $i = 1, \ldots, m$ the eigenvalues of the $m \times m$ left-upper block of matrix $\imath H$. Changing the variables $x_i = 2y_i - 1$ in (14) leads to the von Neumann entropy (8) of case B. The resulting joint probability density of the eigenvalues $x_i, i = 1, \ldots, m$ is proportional to [35]

$$\prod_{1 \le i < j \le m} (x_i - x_j)^2 \prod_{i=1}^{m} (1 + x_i)^{p-m} (1 - x_i)^{n-p}, x_i \in [-1, 1]. \tag{15}$$

It is important to point out that the joint probability densities (10) and (15) of the considered two cases can be compactly represented by a single joint density as

$$f_{\mathrm{FG}}(x) \propto \prod_{1 \le i < j \le m} \left(x_i^\gamma - x_j^\gamma\right)^2 \prod_{i=1}^{m} (1 - x_i)^a (1 + x_i)^b, \tag{16}$$

where for the case A we have

$$\gamma = 2, \quad a = b = n - m \ge 0, \quad x \in [0, 1], \tag{17}$$

and for the case B we have

$$\gamma = 1, \quad a = n - p \ge 0, \quad b = p - m \ge 0, \quad x \in [-1, 1]. \tag{18}$$

We omit the normalizations of the density (16) as they will not be made use of in the subsequent calculations. Note that the variance computation for an arbitrary γ in (16) appears difficult, where one has to consider the case $\gamma = 2$ in (17) and the case $\gamma = 1$ in (18) separately.

III. Variance formulas

We now introduce the exact mean and variance formulas of von Neumann entropy for both case A and case B. The mean values have been recently computed [27], [29] as summarized in Proposition 1 and Proposition 2 for case A in (17) and case B in (18), respectively. The corresponding variance formulas are presented in Proposition 3 and Proposition 4 below, which are the main results of the work[1].

Proposition 1 ([27]): For subsystem dimensions $m \le n$, the mean value of the von Neumann entropy (8) of fermionic

[1]Proofs to the Proposition 3 and Proposition 4 can be found in the full version [36].

Gaussian states with arbitrary number of particles (17) is given by

$$\mathbb{E}[S] = \left(m+n-\frac{1}{2}\right)\psi_0(2m+2n) + \left(\frac{1}{4}-m\right)\psi_0(m+n) + \left(\frac{1}{2}-n\right)\psi_0(2n) - \frac{1}{4}\psi_0(n) - m, \tag{19}$$

where

$$\psi_0(x) = \frac{\mathrm{d}\ln\Gamma(x)}{\mathrm{d}x} \tag{20}$$

is the digamma function.

Proposition 2 ([29]): For subsystem dimensions $m \leq n$, the mean value of the von Neumann entropy (8) of fermionic Gaussian states with a fixed particle number (18) is given by

$$\mathbb{E}[S] = -\frac{m(m+n-p)}{m+n}\psi_0(m+n-p) + (m+n) \times \psi_0(m+n+1) - \frac{mp}{m+n}\psi_0(p+1) - n\psi_0(n+1) - m. \tag{21}$$

Proposition 3: For subsystem dimensions $m \leq n$, the variance of the von Neumann entropy (8) of fermionic Gaussian states with arbitrary number of particles (17) is given by

$$\mathbb{V}[S] = \left(\frac{1}{2}-m-n\right)\psi_1(2m+2n) + \left(n-\frac{1}{2}\right)\psi_1(2n) + \left(\frac{m(2m+n-1)}{2m+2n-1}-\frac{1}{8}\right)\psi_1(m+n) + \frac{1}{8}\psi_1(n) - \frac{1}{2}(\psi_0(2m+2n)-\psi_0(2n)), \tag{22}$$

where

$$\psi_1(x) = \frac{\mathrm{d}^2\ln\Gamma(x)}{\mathrm{d}x^2} \tag{23}$$

is the trigamma function.

Proposition 4: For subsystem dimensions $m \leq n$, the variance of the von Neumann entropy (8) of fermionic Gaussian states with a fixed particle number (18) is given by

$$\mathbb{V}[S] = c_0\psi_1(m+n-p) - (m+n)\psi_1(m+n) + n\psi_1(n) + c_1\psi_1(p) + c_2(\psi_0(m+n-p)-\psi_0(p))^2 + c_3(\psi_0(m+n-p)-\psi_0(p)) - \psi_0(m+n), + \psi_0(n) + c_4 \tag{24}$$

where the coefficients c_i are summarized in Table I below with $(a)_n = \Gamma(a+n)/\Gamma(a)$ denoting the Pochhammer symbol.

The sketch of proof to Proposition 3 and Proposition 4 will be presented in appendices. Note that a special case of equal subsystem dimensions $m = n$ of Proposition 3 has been proved very recently in [30] by utilizing an existing simplification framework developed in [6]–[8], [20], [23], [30], [37]. However, for the general case of subsystem dimensions $m \leq n$, the existing framework is not sufficient to simplify some of the summations in the variance calculation. This difficulty is resolved by developing a new simplification framework, which is the key technical contribution of the work. The proposed new framework consists of two new tools of dummy summation and re-summation techniques. The new framework gives rise to six lemmas as summarized in Appendix B that convert the summations involved into simplifiable ones within the existing simplification framework, leading to the desired closed-form variance formulas in Proposition 3 and Proposition 4.

TABLE I
COEFFICIENTS OF VON NEUMANN ENTROPY VARIANCE IN PROPOSITION 4

c_0	=	$\frac{m(m+n-p)(m^2+2mn+n^2-np-1)}{(m+n-1)_3}$
c_1	=	$\frac{mp(m^2+mn+np-1)}{(m+n-1)_3}$
c_2	=	$\frac{mnp(m+n-p)}{(m+n)(m+n-1)_3}$
c_3	=	$-\frac{m(m+1)(m+n-2p)}{(m+n)(m+n)_2}$
c_4	=	$-\frac{m(2m+n+2)}{(m+n)(m+n)_2}$

IV. SIMULATIONS AND ASYMPTOTIC RESULTS

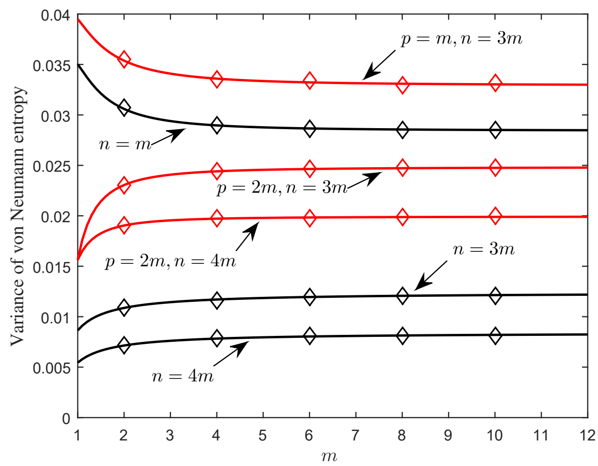

Fig. 1. Variance of von Neumann entropy: analytical results versus simulations. The black curves represent the obtained analytical result (22) for the cases $n = m$, $n = 3m$, and $n = 4m$. The red curves are drawn by the result (24) for the cases $p = m, n = 3m$; $p = 2m, n = 3m$; and $p = 2m, n = 4m$. The diamond scatters represent numerical simulations.

To illustrate the derived results (22) and (24), we plot in Figure 1 the exact variance of von Neumann entropy as compared with numerical simulations[2]. We define

$$f_1 = \frac{m}{n+m} \tag{25}$$

$$f_2 = \frac{p}{n+m}, \tag{26}$$

[2]The simulations performed in figures 1–3 utilize the Mathematica codes provided by Santosh Kumar based on the log-gas approach as discussed in [18, Appendix B].

it is observed in Figure 1 that the variance in case A approaches to a constant when system dimensions m and n increase with a fixed f_1, while the variance in case B follows the same behavior when the dimensions m, n, p increase with both f_1 and f_2 kept fixed. This phenomenon can be analytically established by the asymptotic results of variances in the literature. For case A, in the asymptotic regime [27]

$$m\to\infty,\quad n\to\infty,\quad 0<f_1\leq\frac{1}{2}, \tag{27}$$

one has [27]

$$\mathbb{V}[S]=\frac{1}{2}\left(f_1+f_1^2+\ln(1-f_1)\right)+o\left(\frac{1}{m+n}\right), \tag{28}$$

whereas for case B, in the asymptotic regime [29]

$$m\to\infty,\quad p\to\infty,\quad n\to\infty,\quad 0<f_1\leq f_2\leq\frac{1}{2}, \tag{29}$$

one has [29]

$$\begin{aligned}\mathbb{V}[S]=&\ f_1+f_1^2+\ln(1-f_1)+f_1f_2(1-f_1)(1-f_2)\\&\times\ln^2\frac{1-f_2}{f_2}+f_1^2(2f_2-1)\ln\frac{1-f_2}{f_2}\\&+o\left(\frac{1}{(m+n)^2}\right).\end{aligned} \tag{30}$$

The above asymptotic variances (28) and (30) can be directly recovered by the results in Proposition 3 and Proposition 4, respectively. Moreover, the correction terms of any order can be simply obtained from our exact variance formulas upon using the asymptotic behavior of polygamma functions

$$\psi_0(x)=\ln(x)-\frac{1}{2x}-\sum_{l=1}^{\infty}\frac{B_{2l}}{2lx^{2l}},\qquad x\to\infty, \tag{31}$$

$$\psi_1(x)=\frac{1+2x}{2x^2}+\sum_{l=1}^{\infty}\frac{B_{2l}}{x^{2l+1}},\qquad x\to\infty, \tag{32}$$

where B_k is the k-th Bernoulli number [31]. For example, utilizing the next order of correction, the asymptotic result (30) is refined to

$$\begin{aligned}\mathbb{V}[S]=&f_1^2+f_1+\ln(1-f_1)+f_1^2(2f_2-1)\ln\frac{1-f_2}{f_2}+f_1\\&\times f_2(1-f_1)(1-f_2)\ln^2\frac{1-f_2}{f_2}+\frac{1}{12(m+n)^2}\\&\times\left(\frac{f_1^2}{(f_2-1)^2}+\frac{f_1^2}{f_2^2}+12f_1^2-12f_1+\frac{1}{(f_1-1)^2}\right.\\&+\frac{f_1-3f_1^2}{f_2-1}+\frac{3f_1^2-f_1}{f_2}-1+\frac{2(f_1-1)f_1}{(f_2-1)f_2}\\&\times\left(12f_2^3-18f_2^2+4f_2+1\right)\ln\frac{1-f_2}{f_2}+12(f_1-1)\\&\left.\times f_1(f_2-1)f_2\ln^2\frac{1-f_2}{f_2}\right)+o\left(\frac{1}{(m+n)^4}\right).\end{aligned} \tag{33}$$

To understand the distribution of the von Neumann entropy, simple approximations can now be constructed by using the

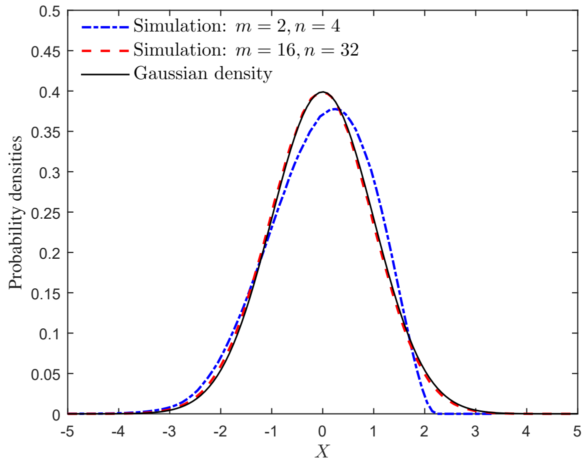

Fig. 2. Probability densities of standardized von Neumann entropy for case A: a comparison of Gaussian density (35) to simulation results. The dash-dot curve in blue and the dashed curve in red refer to the standardized von Neumann entropy (34) of subsystem dimensions $m=2$, $n=4$, and $m=16$, $n=32$, respectively. The solid black curve represents the Gaussian density (35).

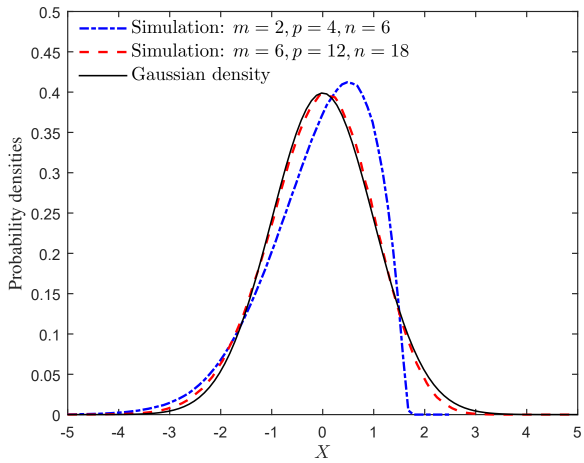

Fig. 3. Probability densities of standardized von Neumann entropy for case B: a comparison of Gaussian density (35) to simulation results. The dash-dot curve in blue and the dashed curve in red refer to the standardized von Neumann entropy (34) of dimensions $m=2$, $p=4$, $n=6$, and $m=6$, $p=12$, $n=18$, respectively. The solid black curve represents the Gaussian density (35).

obtained mean and variance formulas. We first standardize the von Neumann entropy as

$$X=\frac{S-\mathbb{E}[S]}{\sqrt{\mathbb{V}[S]}}, \tag{34}$$

where the random variable X is of zero mean and unit variance. We now compare the distribution of X with a standard Gaussian distribution

$$\phi(x)=\frac{1}{\sqrt{2\pi}}\mathrm{e}^{-\frac{1}{2}x^2},\qquad x\in(-\infty,\infty). \tag{35}$$

In figures 2–3, we plot the simulation results of the standardized von Neumann entropy X as compared with a standard Gaussian. Specifically, the ratios (25)–(26) are fixed to $f_1 = 1/3$ for case A in Figure 2 and $f_1 = 1/4$, $f_2 = 1/2$ for case B in Figure 3. It is observed from the figures that the Gaussian density captures accurately the distribution of the standardized von Neumann entropy X for moderately large dimensions. We also observe that the true distribution of X is non-symmetric and appears to be left-skewed when the subsystem dimensions are small as seen from the dash-dot blue curves. In comparison, when the subsystem dimensions become larger, the distribution of X appears to be closer to the Gaussian distribution. In fact, the Gaussian density as a limiting behavior of von Neumann entropy has been conjectured for different random matrix models of Hilbert-Schmidt ensemble [7], Bures-Hall ensemble [20], and fermionic Gaussian ensemble of an arbitrary number of particles [30]. Here, as motivated by the simulations in Figure 3, one is also tempted to conjecture that under the asymptotic regime (29), the standardized von Neumann entropy (34) of fermionic Gaussian states with a fixed particle number (18) converges in distribution to a standard Gaussian.

V. Conclusion

In this work, we compute the exact yet explicit variance formulas of von Neumann entanglement entropy over fermionic Gaussian states with and without particle number constraints. The obtained formulas provide insights into the fluctuations of von Neumann entropy. An essential ingredient in obtaining the results is a new simplification framework of dummy summation and re-summation techniques. The new framework may also be useful in computing higher order moments of von Neumann entropy and other entanglement indicators over the fermionic Gaussian ensemble.

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