Random matrices and entanglement entropy of trapped Fermi gases

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We exploit and clarify the use of random matrix theory for the calculation of the entanglement entropy of free Fermi gases. We apply this method to obtain analytic predictions for Rényi entanglement entropies of a one-dimensional gas trapped by a harmonic potential in all the relevant scaling regimes. We confirm our findings with accurate numerical calculations obtained by means of an ingenious discretization of the reduced correlation matrix.

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I. INTRODUCTION

During the past decade entanglement became a very powerful tool for the study of many-body quantum systems, especially for the identification of critical and topological phases of matter (see, e.g., Refs. [1–3] as reviews). In this respect the most studied quantity is surely the (von Neumann or Rényi) entanglement entropy. In terms of the reduced density matrix $\rho_A = \mathrm{Tr}_{\bar{A}}\rho$ of a subsystem A ($\bar{A}$ denotes the complement of A), the order-q Rényi entropy is defined as

$$S_q = \frac{1}{1-q}\ln \mathrm{Tr}\rho_A^q, \quad (1)$$

that in the limit $q \to 1$ reduces to the most studied von Neumann entropy S_1. The knowledge of the Rényi entropies for arbitrary values of q contains much more information than the sole S_1 since from them one can extract the full spectrum of ρ_A [4].

From the definition and from the highly nonlocal character of Eq. (1), it can appear extremely difficult to calculate the entanglement entropy even for the simpler models. However, a number of advanced analytic techniques have been developed in such a way to have a rather precise characterization in many different classes of systems. These include one-dimensional conformal field theories [5–7], spin chains mappable to free fermions thanks to Toeplitz matrix techniques [7–12], higher-dimensional lattice fermions with Widom conjecture [13], holographic techniques [14], renormalization groups [15], and many more. The entanglement entropies are also a crucial concept to understand the scaling and the working [16] of matrix product states algorithms [17].

In this paper we discuss and develop the connection between the entanglement entropies and random matrix theory in free one-dimensional Fermi gases. A similar connection was first highlighted in lattice models in Ref. [18] and further developed in [10]. In two recent papers [19,20], random matrix theory has been used to calculate the particle number distribution (aka the full counting statistics) in a finite length interval, but not for the entanglement entropies. As we shall see, this approach makes it possible to clarify several concepts already present in the literature and provides also other results, such as the scaling of the entanglement entropy in a free fermion gas confined by a harmonic potential, a problem that so far has been studied only numerically [21].

The paper is organized as follows. In Sec. II we briefly review the standard methods for the calculation of the entanglement entropy in Fermi gases and we establish the correspondence with random matrix theory. In Sec. III we use this formalism to analytically calculate the entanglement entropies for a one-dimensional Fermi gas trapped in a harmonic potential for an interval symmetric with respect to the center of the trap. In the same section, we also confirm our findings by accurate numerical calculations. Finally, in Sec. IV we draw our conclusions and we discuss some possible generalizations and open issues. Some details about the density of eigenvalues of the overlap matrix have been relegated to the Appendix.

II. FREE FERMION GASES AND RANDOM MATRIX THEORY

Let us consider a system of N noninteracting spinless fermions with a discrete one-particle energy spectrum. The many-body wave function $\Psi(x_1,\ldots,x_N)$ is the Slater determinant built with the one-particle eigenstates, i.e.,

$$\Psi(x_1,\ldots,x_N) = \frac{1}{\sqrt{N!}}\det[\phi_k(x_n)], \quad (2)$$

where the normalized wave functions $\phi_k(x)$ are the occupied single-particle energy levels. The ground state $\Psi_0(x_1,\ldots,x_N)$ is obtained by filling the lowest N energy levels. The ground-state two-point correlation function is

$$C(x,y) \equiv \langle c^\dagger(x)c(y)\rangle = \sum_{k=1}^{N}\phi_k^*(x)\phi_k(y), \quad (3)$$

where $c(x)$ is the fermionic annihilation operator and the one-particle eigenfunctions $\phi_k(x)$ are ordered according to their energies. The Wick theorem makes it possible to write the reduced density matrix of a spatial subsystem A as [22]

$$\rho_A \propto \exp\left[-\int_A dy_1 dy_2 c^\dagger(y_1)\mathcal{H}(y_1,y_2)c(y_2)\right], \quad (4)$$

where $\mathcal{H} = \ln[(1-C)/C]$ and the normalization constant is fixed by requiring $\mathrm{Tr}\rho_A = 1$.

It is useful to define the correlation matrix restricted to the subsystem A,

$$C_A(x,y) \equiv I_A(x)C(x,y)I_A(y), \quad (5)$$

with $I_A(x)$ being the characteristic function of the subsystem; i.e.,

$$I_A(x) = \begin{cases} 1 & x \in A, \\ 0 & x \notin A. \end{cases} \quad (6)$$

A related quantity is the overlap matrix of the subsystem A defined as [23,24]

$$\mathbb{A}_{nm} = \int_A dz\, \phi_n^*(z)\phi_m(z), \quad n,m = 1,\dots,N. \quad (7)$$

As shown in Refs. [23,24], the overlap matrix and the restricted correlation matrix have the same spectrum although they act on different spaces. Using the quadratic form of the reduced density matrix (4), the Rényi entanglement entropies can be written in terms of the overlap or correlation matrices as

$$S_q = \frac{1}{1-q}\mathrm{Tr}\ln[\mathbb{A}^q + (1-\mathbb{A})^q], \quad (8)$$

$$S_q = \frac{1}{1-q}\mathrm{Tr}\ln\left[C_A^q + (1-C_A)^q\right]. \quad (9)$$

In terms of the eigenvalues a_i, common to the overlap and reduced correlation matrices, the entanglement entropy is

$$S_q = \sum_{i=1}^N e_q(a_i), \quad e_q(x) \equiv \frac{1}{1-q}\ln[x^q + (1-x)^q]. \quad (10)$$

At this point there are two possible roads for a numerical evaluation of the entropy. The first possibility is to explicitly construct the overlap matrix, find its eigenvalues numerically, and from them compute S_q. This numerical approach has been effectively applied for the determination of the entanglement entropy of Fermi gases in many equilibrium [21,23–29] and nonequilibrium situations [29–32], as well as to the related statistics of particle number in the subsystem [19,20,33–37] (we mention that the entanglement entropies of trapped lattice gases were numerically studied in [38]). A second possibility is to extract the spectrum from the reduced correlation matrix. While at first this can sound awkward, because we should work with a continuous kernel, some very effective discretizations have been developed [39], which allow a much faster computation of the entropies especially when the integrals defining the elements of the overlap matrix (7) cannot be analytically performed. In Fig. 1 we report the numerically evaluated entanglement entropy S_1 for the model studied in this paper which is a Fermi gas trapped in a harmonic potential. We only consider the case in which the subsystem is the symmetric interval $A = [-\ell,\ell]$. We calculated the spectrum of C_A by using the Gauss-Legendre discretization proposed in Ref. [39]. We found that in order to achieve a precision of about 10^{-8} on the entropy, the discretized matrix should have a dimension growing linearly in N, which is the same as the overlap matrix, but its elements must not be calculated by numerical integration. The main reason for this high efficiency is that convergence is exponential in the number of steps on Gauss-Legendre discretization [39]. We checked for several values of N that the spectrum of the reduced correlation matrix obtained in this way is the same as the one of the overlap matrix, but its numerical determination is much faster. Obviously, every time the overlap matrix is analytically evaluable (as, e.g., in the cases considered in [24]), there is no advantage in this procedure and the overlap matrix method remains favorable. We mention that the results reported in Fig. 1 are equivalent to those already reported in Ref. [21].

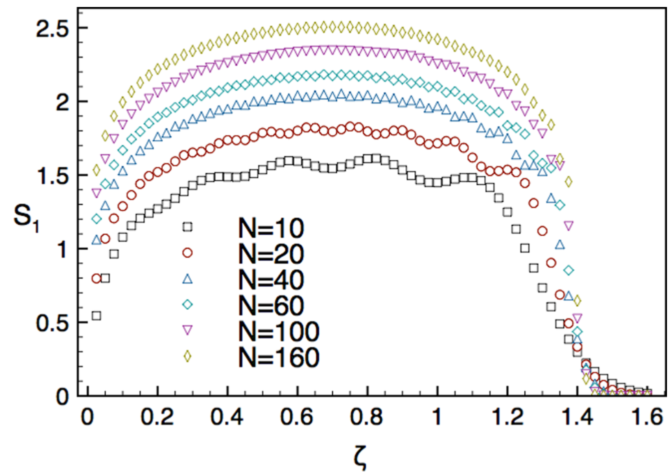

FIG. 1. (Color online) Entanglement entropy S_1 for a Fermi gas with N particles trapped in a harmonic potential. We consider the bipartition in which the subsystem A is the interval $A = [-\ell,\ell]$. We report the entanglement entropy as function of $\zeta = \ell/\sqrt{N}$ for different values of N. The reported data are obtained from an ingenious discretization of Eq. (9).

A. The connection with random matrix theory

The connection with random matrix theory [19,20] starts from the definition of the characteristic polynomial of $\mathbb{A}$ (or C_A),

$$D_A(\lambda) = \prod_{i=1}^N (\lambda - a_i) = \det[\lambda\mathbb{I} - \mathbb{A}], \quad (11)$$

which is a standard tool in the analytic calculation of the entanglement entropy [8,10]. This characteristic polynomial $D_A(\lambda)$ can be straightforwardly written as a random matrix average. Indeed, by definition we have [using the completeness of the eigenfunctions $\phi_m(z)$ on the full line]

$$\begin{aligned} D_A(\lambda) &= \det\left[\lambda\int_{-\infty}^{\infty} dz\phi_n^*(z)\phi_m(z) - \int_A dz\phi_n^*(z)\phi_m(z)\right] \\ &= \det\left\{\int_{-\infty}^{\infty} dz[\lambda - I_A(z)]\phi_n^*(z)\phi_m(z)\right\}. \end{aligned} \quad (12)$$

At this point we can use the Cauchy-Binet identity,

$$\begin{aligned} &\int dx_1\cdots dx_N \det[f_i(x_j)]\det[g_k(x_l)]\prod_{i=1}^N h(x_i) \\ &= N!\det\left[\int dx h(x) f_i(x) g_j(x)\right], \end{aligned} \quad (13)$$

to rewrite $D_A(\lambda)$ as

$$D_A(\lambda) = \frac{1}{N!}\int dx_1\cdots dx_N \det[\phi_i(x_j)]\det[\phi_k(x_l)] \times \prod_{i=1}^{N}[(\lambda - I_A(x_i)] = \int dx_1\cdots dx_N |\Psi_0(x_1,\ldots,x_N)|^2 \prod_{i=1}^{N}[\lambda - I_A(x_i)], \tag{14}$$

where we recognized $\Psi_0(x_1,\ldots,x_N) = \det[\phi_k(x_n)]/\sqrt{N!}$. Thus, every time $|\Psi_0(x_1,\ldots,x_N)|^2$ corresponds to a random matrix average $\langle\cdot\rangle_{\rm RM}$, when the x_i are related to eigenvalues of a random matrix (see below), the above equation is equivalent to

$$D_A(\lambda) = \left\langle \prod_{i=1}^{N}[\lambda - I_A(x_i)]\right\rangle_{\rm RM}. \tag{15}$$

We list and analyze in the following a number of interesting random matrix averages for one-dimensional Fermi gases, but first we proceed to further simplifications and interpretation of the above average. We also remove the subscript RM from the averages.

To this aim, let us introduce the operator counting particle number in the subsystem A [here $\hat{n}(x) = c^\dagger(x)c(x)$ is the particle density],

$$N_A = \sum_{i=1}^{N} I_A(x_i) = \int_A \hat{n}(x)dx, \tag{16}$$

and its generating function

$$\chi(s) \equiv \langle e^{-sN_A}\rangle = \left\langle \prod_{i=1}^{N} e^{-sI_A(x_i)}\right\rangle. \tag{17}$$

[Often $\chi(is)$ is called generating function, but this is not important for what follows.] Since

$$e^{-sI_A(x)} = \begin{cases} e^{-s} & x\in A, \\ 1 & x\notin A, \end{cases} \tag{18}$$

we have

$$e^{-sI_A(x)} = e^{-s}I_A(x) + [1 - I_A(x)] = 1 - (1-e^{-s})I_A(x), \tag{19}$$

and then

$$\chi(s) = \left\langle \prod_{i=1}^{N}[1-(1-e^{-s})I_A(x_i)]\right\rangle = (1-e^{-s})^N \left\langle \prod_{i=1}^{N}\left[\left(\frac{1}{1-e^{-s}}\right) - I_A(x_i)\right]\right\rangle. \tag{20}$$

Setting

$$\lambda = \frac{1}{1-e^{-s}} \Rightarrow e^{-s} = \frac{\lambda-1}{\lambda}, \tag{21}$$

we have

$$\left\langle \left(\frac{\lambda-1}{\lambda}\right)^{N_A}\right\rangle = \frac{1}{\lambda^N}\left\langle \prod_{i=1}^{N}(\lambda - I_A(x_i))\right\rangle. \tag{22}$$

Thus, plugging the above equation into Eq. (15), we have

$$D_A(\lambda) = \lambda^N \chi\left(e^{-s} = 1 - \frac{1}{\lambda}\right) = \lambda^N \left\langle \left(\frac{\lambda-1}{\lambda}\right)^{N_A}\right\rangle. \tag{23}$$

This is a very compact expression for the characteristic polynomial valid for arbitrary number of particles N and arbitrary random matrix average. Although it appeared (in a more or less explicit form) a few times in the literature, its general validity has not been appreciated enough.

In order to calculate the entropies, let us introduce the resolvent

$$F(\lambda) = \sum_{i=1}^{N}\frac{1}{\lambda - a_i} = {\rm Tr}\frac{1}{\lambda\mathbb{I} - \mathbb{A}}, \tag{24}$$

which is related to $D_A(\lambda)$ as

$$F(\lambda) = \frac{D_A'(\lambda)}{D_A(\lambda)} = \frac{d}{d\lambda}\ln D_A(\lambda). \tag{25}$$

Using Eq. (23) for $D_A(\lambda)$ we have after simple algebra

$$F(\lambda) = \frac{N}{\lambda} + \frac{1}{\lambda(\lambda-1)}\frac{\langle N_A(1-\frac{1}{\lambda})^{N_A}\rangle}{\langle(1-\frac{1}{\lambda})^{N_A}\rangle}. \tag{26}$$

Given that the entropies are given by Eq. (10), we immediately have

$$S_q = \int_C \frac{d\lambda}{2\pi i} e_q(\lambda)\, F(\lambda), \tag{27}$$

where the contour C in the complex λ plane goes counterclockwise over the rectangle: $[0,1]\times[-\epsilon,\epsilon]$, as shown in Fig. 2, with $\epsilon \to 0^+$ eventually. Note that the function $e_q(\lambda)$ has branch cuts for $\text{Re}(\lambda) < 0$ and $\text{Re}(\lambda) > 1$ (this is equivalent to the analogous formulas for spin chains [8,10]). Substituting the definition of $F(\lambda)$ from Eq. (24) on the right-hand side

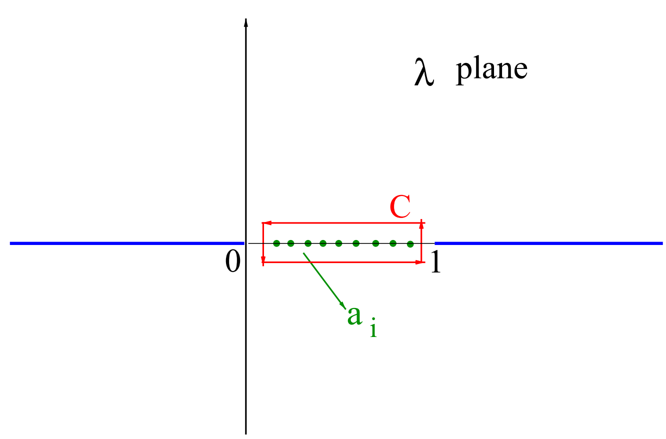

FIG. 2. (Color online) The rectangular counterclockwise contour C in the complex λ plane encloses the poles at a_i's shown by dots. The left vertical line of C is to right of $\lambda = 0$ and the right vertical line is to the left of $\lambda = 1$.

of Eq. (27) and calculating the residues around the poles $0 \leqslant a_i \leqslant 1$, gives this result immediately.

Plugging the expression of $F(\lambda)$ from Eq. (26) into Eq. (27), one arrives at a rather compact exact expression for the entropy, valid for all N,

$$S_q = \frac{1}{(1-q)}\frac{1}{2\pi i}\int_C \frac{d\lambda}{\lambda(\lambda-1)}\ln[\lambda^q+(1-\lambda)^q] \times \frac{\langle N_A(1-\frac{1}{\lambda})^{N_A}\rangle}{\langle(1-\frac{1}{\lambda})^{N_A}\rangle}. \tag{28}$$

The term N/λ in Eq. (25) does not contribute to the entropy S_q because, inside the integration contour, it provides an analytic function with zero residue. By writing further, $1-1/\lambda = e^{-s}$, one can write a slightly more compact expression for the ratio

$$\frac{\langle N_A(1-\frac{1}{\lambda})^{N_A}\rangle}{\langle(1-\frac{1}{\lambda})^{N_A}\rangle} = -\frac{\partial}{\partial s}\ln[\langle e^{-sN_A}\rangle]. \tag{29}$$

Finally, these expressions allow us to derive the asymptotic large N density of eigenvalues $\rho(a)$ of the overlap matrix (or reduced correlation matrix) which is defined by the implicit relation

$$N\int da\frac{\rho(a)}{\lambda-a} = F(\lambda), \tag{30}$$

leading to

$$\rho(a) = -\frac{1}{\pi}\lim_{\epsilon\to 0^+}\mathrm{Im}F(a+i\epsilon). \tag{31}$$

We discuss explicitly the density of eigenvalues $\rho(a)$ for a trapped Fermi gas in the Appendix.

B. Gaussian distribution

An immediate consequence of the exact formula in Eq. (28) is the well-known relation [33,40–43] between the variance of N_A and entropies in the case the random variable N_A is a *pure* Gaussian with mean $\langle N_A\rangle$ and variance V_{N_A}, i.e.,

$$N_A = \langle N_A\rangle + \sqrt{V_{N_A}}\,\mathcal{N}(0,1), \tag{32}$$

where $\mathcal{N}(0,1)$ is a standard normal Gaussian variable with zero mean and unit variance. Indeed, using the Gaussian property of $\mathcal{N}(0,1)$, it follows immediately that

$$\langle e^{-sN_A}\rangle = e^{-s\langle N_A\rangle + \frac{s^2}{2}V_{N_A}}. \tag{33}$$

Taking logarithm and deriving with respect to s as in Eq. (29) we obtain

$$\frac{\langle N_A(1-\frac{1}{\lambda})^{N_A}\rangle}{\langle(1-\frac{1}{\lambda})^{N_A}\rangle} = \langle N_A\rangle + V_{N_A}\ln\left(1-\frac{1}{\lambda}\right). \tag{34}$$

Plugging this expression in Eq. (28) gives

$$S_q = \frac{1}{(1-q)}\frac{1}{2\pi i}\int_C \frac{d\lambda}{\lambda(\lambda-1)}\ln[\lambda^q+(1-\lambda)^q] \times\left[\langle N_A\rangle + V_{N_A}\ln\left(1-\frac{1}{\lambda}\right)\right]. \tag{35}$$

The contour integral with the constant term $\langle N_A\rangle$ vanishes since the integrand in analytic inside the contour (which does not include the poles at $\lambda=0$ and $\lambda=1$). This leaves us with

$$S_q = \frac{V_{N_A}}{(1-q)}\frac{1}{2\pi\, i}\int_C\frac{d\lambda}{\lambda(\lambda-1)} \times\ln[\lambda^q+(1-\lambda)^q]\ln\left(1-\frac{1}{\lambda}\right), \tag{36}$$

which is an exact expression for entropy when N_A is a pure Gaussian. The contour integral in Eq. (36) can be performed exactly in the limit $\epsilon\to 0^+$. The contributions from the vertical portions vanish as $\epsilon\to 0^+$ and the contributions from the horizontal portions gives a real integral over $\lambda\in[0,1]$ as follows:

$$S_q = -\frac{V_{N_A}}{\pi(1-q)}\int_0^1\frac{dx}{x(x-1)} \times\ln[x^q+(1-x)^q]\,\mathrm{Im}\left[\ln\left(1-\frac{1}{x+i\epsilon}\right)\right]_{\epsilon\to 0^+}. \tag{37}$$

Using $\mathrm{Im}[\ln(1-\frac{1}{x+i\epsilon})]_{\epsilon\to 0^+}=\pi$ then gives the final result for the entropy, given that N_A is a pure Gaussian,

$$S_q = -\frac{V_{N_A}}{(1-q)}\int_0^1\frac{dx}{x(x-1)}\ln[x^q+(1-x)^q] = \frac{\pi^2}{6}\left(1+\frac{1}{q}\right)V_{N_A}. \tag{38}$$

Although this relation between entropy and fluctuations is well known in the literature [33,43], we find the above derivation very instructive from the random matrix point of view.

C. Examples of random matrix ensembles and corresponding fermionic systems

For a Fermi gas in a ring of length L with periodic boundary conditions, the normalized one-particle wave functions are plane waves $\phi_k(x)=e^{2\pi ikx/L}/\sqrt{L}$ and the corresponding many-body wave function Ψ_0 gives the circular unitary ensemble (CUE). This random matrix ensemble has been already studied in the context of the entanglement entropy of spin chains [10,18] and the these results have been exported to the Fermi gas in [25]. In the case when A is an interval of length ℓ embedded in a finite system of length L, the leading and subleading behavior for the entropy has been obtained in [25]. The asymptotic large N behavior of the entropies for fixed ratio ℓ/L and at finite density $n=N/L$ (obtained by means of the Fisher-Hartwig conjecture) is [23,25]

$$S_q = \frac{1}{6}\left(1+\frac{1}{q}\right)\ln\left(2N\sin\pi\frac{\ell}{L}\right)+E_q+o(N^0), \tag{39}$$

and the constant E_q is given by [8]

$$E_q = \left(1+\frac{1}{q}\right)\int_0^\infty\frac{dt}{t}\left[\frac{1}{1-q^{-2}} \times\left(\frac{1}{q\sinh t/q}-\frac{1}{\sinh t}\right)\frac{1}{\sinh t}-\frac{e^{-2t}}{6}\right]. \tag{40}$$

Random matrix techniques are instead a needed tool to access some of the corrections to the above leading behavior; see

Ref. [10]. More general results for the case when A is composed of disjoint intervals are also known [25].

It is important to mention that the functional dependence of the entanglement entropy (39) over ℓ and L is a general prediction of conformal field theory [6,45]. Indeed, from the well-known infinite system result

$$S_q = \frac{1}{6}\left(1+\frac{1}{q}\right)\ln \ell + E_q, \tag{41}$$

one obtains Eq. (39) with the replacement $\ell \to N \sin \pi\ell/L$, as a consequence of the mapping from the plane to a cylinder of circumference L [6]. This simple result is indeed valid for a general correlation function of primary operators (in conformal field theory the entanglement entropies for integer q are correlation functions of the so-called twist fields [45,46]). This is a very powerful prediction for the finite size-scaling function of the entanglement entropy for homogeneous systems whose analog in the presence of a harmonic potential will be calculated in the following section.

For a gas of spinless fermions confined in the interval $[0,L]$ by a hard-wall potential, the one-particle wave functions are $\phi_k(x) = \sqrt{\frac{2}{L}}\sin[\pi k \frac{x}{L}]$. In this case the corresponding random matrix ensemble is $O^+(2N)$ symmetric [18], but the consequences of this correspondence have not been studied in great detail yet. The asymptotic large N behavior of the entanglement entropy has been obtained by using a generalization of the Fisher-Hartwig conjecture (for spin chains in [11] and for Fermi gases in [25]). For the Fermi gas this asymptotic result reads

$$S_q = \frac{1}{12}\left(1+\frac{1}{q}\right)\ln\left(4N\sin\pi\frac{\ell}{L}\right) + \frac{E_q}{2} + o(N^0), \tag{42}$$

where E_q is the same constant in Eq. (40). Also in this case, the system being homogeneous, the finite-size scaling function can be entirely obtained from boundary conformal field theory [6,45].

III. ENTANGLEMENT ENTROPY FOR A QUADRATIC TRAPPING POTENTIAL

Let us now consider free fermions in an external harmonic potential (trap)

$$V(x) = \tfrac{1}{2}m\omega^2 x^2. \tag{43}$$

For simplicity in the following, we set $\hbar = m = \omega = 1$. The dependence over the trap frequency ω can easily be restored using trap size-scaling arguments [44]. The single-particle wave functions are

$$\phi_n(x) = \frac{H_{n-1}(x)}{\sqrt{\pi^{1/2}2^{n-1}(n-1)!}}e^{-x^2/2}, \quad n = 1,\ldots N, \tag{44}$$

where $H_n(x)$ are the Hermite polynomials. The many-body ground-state wave function is

$$\Psi_0(x_1,\ldots,x_N) = Z_N^{-1}\prod_{i<j}(x_i-x_j)e^{-\sum_{i=1}^N x_i^2/2}, \tag{45}$$

with Z_N a normalization constant. Note that $|\Psi_0(x_1,\ldots,x_N)|^2$ can be interpreted as the joint distribution of N real eigenvalues $(x_1,\ldots,x_N)$ drawn from the famous Gaussian unitary ensemble (GUE) [47]. Using Christoffel-Darboux formula, the two-point function (3) is

$$C(x,y) = \frac{N^{1/2}}{\sqrt{2}}\frac{\phi_{N+1}(x)\phi_N(y) - \phi_N(x)\phi_{N+1}(y)}{x-y}, \tag{46}$$

which is the well-known GUE kernel.

The generating function for the particle number can be read from Eqs. (11) and (23) and it is

$$\chi(s) \equiv \langle e^{-sN_A}\rangle = \det[\mathbb{I} + (e^{-s}-1)\mathbb{A}], \tag{47}$$

which, expanded to $O(s^2)$, yields the particle variance for an arbitrary subsystem A,

$$V_{N_A} = \int_A dx\, C(x,x) - \int_A dx \int_A dy\, |C(x,y)|^2, \tag{48}$$

which is $V_{N_A} = \mathrm{Tr}[C_A - C_A^2] = \mathrm{Tr}[\mathbb{A} - \mathbb{A}^2]$.

For the harmonic potential, the entanglement entropy has been studied numerically in [20,21] for several bipartition of the systems. The particle-number variance has been studied numerically in the above papers, but in the case when A is a symmetric interval with respect to the center of the trap of length 2ℓ, i.e., $A = [-\ell,\ell]$, random matrix theory allowed for a full large N asymptotic analytical prediction for arbitrary value of ℓ. Three different scaling regimes have been identified, which are [19]

$$V_{N_A} \simeq \begin{cases} \frac{1}{\pi^2}\ln[N\zeta(2-\zeta^2)^{3/2}], & \sqrt{2}-\zeta \sim O(1), \\ \tilde{V}_2[\sqrt{2}N^{2/3}(\zeta-\sqrt{2})], & \zeta-\sqrt{2} \sim O(N^{-\frac{2}{3}}), \\ \exp[-2N\phi(\zeta)], & \zeta-\sqrt{2}\sim O(1), \end{cases} \tag{49}$$

where we introduced $\zeta = \ell/\sqrt{N}$ (notice that, in random matrix literature, lengths are always normalized to $\sqrt{N}$ as, e.g., in Ref. [19]) and the functions

$$\tilde{V}_2(s) = 2\int_s^\infty K_{\mathrm{Ai}}(x,x) - 2\int_{[s,\infty]^2} dx dy |K_{\mathrm{Ai}}(x,y)|^2,$$
$$\phi(\zeta) = \frac{\zeta\sqrt{\zeta^2-2}}{2} + \ln\frac{\zeta-\sqrt{\zeta^2-2}}{\sqrt{2}}, \tag{50}$$

where $K_{\mathrm{Ai}}(x,y)$ is the Airy kernel,

$$K_{\mathrm{Ai}}(x,y) = \frac{\mathrm{Ai}(x)\mathrm{Ai}'(y) - \mathrm{Ai}(y)\mathrm{Ai}'(x)}{x-y}. \tag{51}$$

We mention that while the scaling behavior of the variance in the intermediate edge regime in Eq. (49) was well known [48] (see also [20]), the full scaling function $\tilde{V}_2(s)$ (and, in particular, its asymptotic behaviors for both negative and positive arguments) was computed explicitly only recently in [19].

In the following we generalize the findings of Ref. [19] to the entanglement entropy of a bipartite system in the case when A is a symmetric interval around the center of the trap.

A. Bulk regime: $\zeta \sim 1/N \ll 1$

We first consider the so-called bulk regime when $\zeta \sim 1/N \ll 1$, i.e., when the box size scales as the typical distance between eigenvalues of GUE in the bulk, i.e., far away from the edges $\zeta = \sqrt{2}$ of the semicircle. It is called bulk regime because the condition $\zeta \ll 1$ ensures that the gas is almost homogeneous on these length scales.

In this regime, when $N \to \infty$, $\zeta \to 0$ but keeping the product

$$z = \frac{2\sqrt{2}N\zeta}{\pi} \tag{52}$$

fixed, it has been proved [48–51] that the random variable N_A is indeed a *pure* Gaussian with mean $\langle N_A \rangle \approx z$ and the variance

$$V_{N_A} \approx V(z), \tag{53}$$

where the scaling function $V(z)$ for all z was first computed by Dyson and Mehta [52] and is given by (see, e.g., Appendix A.38 in Mehta's book [47])

$$V(z) = z - 2\int_0^z dr\,(z-r)\left[\frac{\sin(\pi r)}{\pi r}\right]^2. \tag{54}$$

This function has the asymptotics

$$\begin{aligned} V(z) &\to z - \frac{1}{2}z^2 + O(z^3), \quad \text{as} \quad z \to 0, \\ &\to \frac{1}{\pi^2}\ln(2\pi z) + \frac{(1+\gamma_E)}{\pi^2} + O(1/z), \quad \text{as } z \to \infty, \end{aligned} \tag{55}$$

where $\gamma_E = 0.577\,215\ldots$ is the Euler constant. Thus, in this range when $z \gg 1$, or equivalently $1/N \ll \zeta \ll 1$, the variance behaves as

$$V_{N_A} = \frac{1}{\pi^2}\ln(2\sqrt{2}N\zeta) + C_{\rm DM} + O(1/z), \tag{56}$$

where the constant $C_{\rm DM}$ is known as the Dyson-Mehta constant (see A.38 in the book [47]) and is given by

$$C_{\rm DM} = \frac{(1+\gamma_E+\ln 2)}{\pi^2} = 0.230\,036\ldots \tag{57}$$

At this point, one would be tempted to use the fact that, in this bulk limit, N_A is a pure Gaussian and, hence, Eq. (38) should be valid. We anticipate that this is not the case, but before let us see what the prediction for the entropy under this assumption would be. In this case also S_q becomes a function of the single scaling variable z [cf. Eq. (52)] given by

$$S_q \stackrel{?}{=} \frac{\pi^2}{6}\left(1+\frac{1}{q}\right)V(z), \tag{58}$$

with $V(z)$ given in Eq. (54) for all z. In particular, for large z, i.e., when $\zeta \gg 1/N$ but still $\zeta \ll 1$, using the large z asymptotics of $V(z)$ in Eq. (56), one would get

$$S_q \stackrel{?}{=} \frac{1}{6}\left(1+\frac{1}{q}\right)\ln(2\sqrt{2}N\zeta) + C_q + \cdots, \tag{59}$$

where the constant C_q is

$$C_q = \frac{\pi^2}{6}\left(1+\frac{1}{q}\right)C_{\rm DM}. \tag{60}$$

Notice the very simple dependence on q of this constant compared with the fairly more complicated one in the case of homogeneous systems [cf. Eq. (40)].

The reasoning above has an obvious flaw. Indeed, even if in the bulk regime the distribution of N_A becomes Gaussian, by no means does this imply that the full entropy is given by Eq. (59): The leading term in N of the entropy is clearly correct, but non-Gaussian corrections to the distribution of N_A, when integrated to calculate the entropy in Eq. (28), can give rise to terms of the order $O(N^0)$, which add up to C_q in Eq. (59). Indeed, these higher cumulants of N_A have been calculated for a homogenous Fermi gas in [33] and their general relation with the entropies have been studied in Refs. [33,41–43].

However, the subleading $O(N^0)$ term can be obtained by a general physical requirement. Indeed, close to the center of the trap, the system is almost homogeneous with density $n(0) = N^{1/2}\sqrt{2}/\pi$. Thus, we expect the entanglement entropy to have the same value as a uniform system [cf. Eq. (39)], which for small ℓ is

$$S_q = \frac{1}{6}\left(1+\frac{1}{q}\right)\ln\left(2\frac{N}{L}\pi\ell\right) + E_q + \cdots. \tag{61}$$

Replacing now the density N/L with $n(0) = N^{1/2}\sqrt{2}/\pi$, we have the prediction

$$S_q = \frac{1}{6}\left(1+\frac{1}{q}\right)\ln(2\sqrt{2}N^{1/2}\ell) + E_q + \cdots, \tag{62}$$

which has the same leading term as Eq. (59), but presents a different additive constant. The two values C_q and E_q are indeed relatively close; for example, at $q = 1$ they are $C_1 = 0.756\,788\ldots$ and $E_1 = 0.726\,067\ldots$.

In order to confirm the correctness of the previous reasoning, we compute numerically the entanglement entropy in this bulk regime. In Fig. 3 we report the result for $q = 1$ (but we checked also for other values of q). It is evident that the data in this regime converges quickly (increasing N) to Eq. (62). It is also clear that changing the constant term from E_1 to C_1 moves the curve up of about 0.03, which is a very visible shift on the vertical scale, as shown explicitly in Fig. 3.

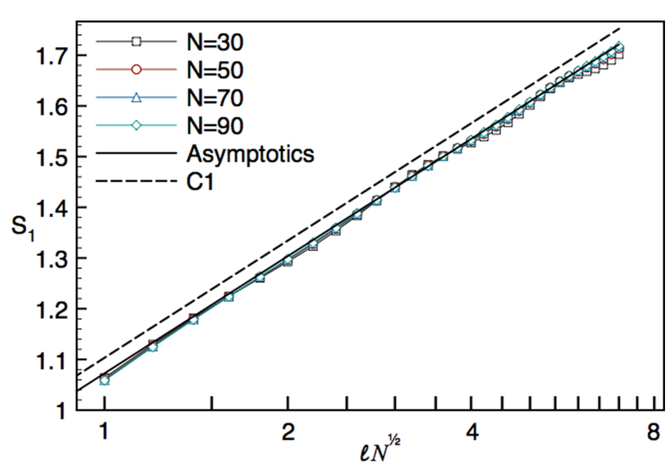

FIG. 3. (Color online) Numerical evaluation of the entanglement entropy S_1 from the discretization of Eq. (9) for several values of N and ℓ in the bulk regime $\ell \ll \sqrt{N}$. By increasing N the data approach the asymptotic prediction (62) in a nonmonotonic way. The dotted line is Eq. (59), in which the additive constant has not been fixed to its correct value.

While the prediction in this bulk regime has been obtained on the sole basis of a scaling argument, this will not be the case for the intermediate regime described in the following section. However, having established the correct scaling behavior of the entanglement entropy in this regime, where the final result was known *a priori*, will be a very useful guide in the following section.

B. Intermediate regime: $\zeta \sim O(1) < \sqrt{2} - O(N^{2/3})$

The question we answer in this section is what happens when one relaxes the upper limit $\zeta \ll 1$, to $\zeta \sim O(1) < \sqrt{2} - O(N^{2/3})$, i.e., still far from the edge-scaling regime. In this regime, the full large deviation function associated with the distribution of N_A was computed recently in [19] using a Coulomb gas method. From this large deviation function, the variance of N_A can then be read off and it was found to be a function of the single scaling variable [19]

$$\Delta = N\,\zeta(2-\zeta^2)^{3/2}. \qquad (63)$$

The regime $\zeta \sim O(1) < \sqrt{2} - O(N^{2/3})$ translates into the regime $\Delta \gg 1$ and it was shown recently [19] that the variance V_{N_A} of N_A behaves as

$$V_{N_A} = \frac{1}{\pi^2}\ln(\Delta) + C_{\rm DM} + O(1/\Delta). \qquad (64)$$

While the leading term was found analytically in Ref. [19], the subleading constant $C_{\rm DM}$ was found, by fitting numerical data, to be the same as the Dyson-Mehta constant in Eq. (57); see also [21]. Note that, in the limit $\zeta \ll \sqrt{2}$, using Eq. (63), the result in Eq. (64) reduces precisely to the bulk result in Eq. (56), as it should.

The question is as follows: Can we use this result for the variance to compute the entropy S_q? The main point is that the distribution of N_A may no longer be a pure Gaussian and the entropy may have non-Gaussian corrections. Had the distribution been purely Gaussian with variance V_{N_A} given in Eq. (64), we could use Eq. (38) to obtain the prediction

$$S_q \stackrel{?}{=} \frac{1}{6}\left(1+\frac{1}{q}\right)\ln[N\,\zeta(2-\zeta^2)^{3/2}] + C_q + \cdots, \qquad (65)$$

where the constant C_q is given in Eq. (60). The prediction in Eq. (65) is valid assuming N_A is *purely* Gaussian with variance V_{N_A} given in Eq. (64). However, the distribution of N_A in this intermediate regime is not purely Gaussian and there are logarithmic corrections [19]. While these logarithmic corrections do not modify the leading term on the right-hand side of Eq. (65), they are expected to modify the subleading ζ-independent constant term C_q (as in the bulk regime). However, we can fix the constant term by requiring that, for small ζ, Eq. (65) reduces to the bulk one (62), obtaining

$$S_q = \frac{1}{6}\left(1+\frac{1}{q}\right)\ln[N\,\zeta(2-\zeta^2)^{3/2}] + E_q + o(N^0). \qquad (66)$$

This new prediction is one of the main results of this paper. Equation (66) is indeed an expansion for $\Delta \gg 1$ of the scaling function for the entropy, in which Δ has been replaced with its actual value (63).

In Ref. [21], on the basis of the numerical data, it was conjectured that the Rényi entanglement entropies could have

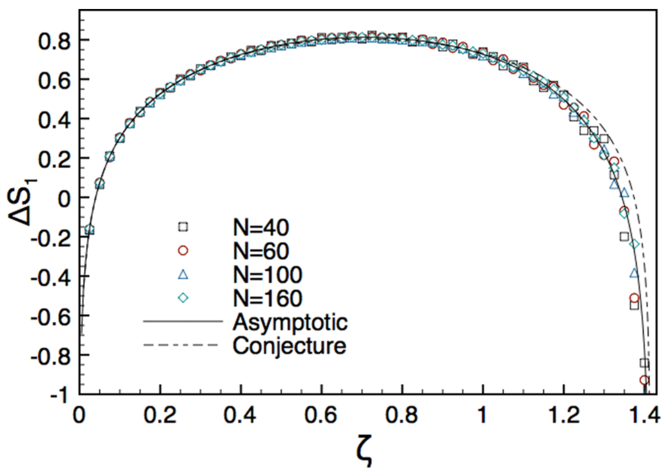

FIG. 4. (Color online) Subtracted von Neumann entanglement entropy $\Delta S_1 = S_1 - (\ln N)/3$ as function of $\zeta = \ell/\sqrt{N}$ for several values of N up to $N = 160$. By increasing N the data approach the asymptotic curve (66) in a nonuniform way as function of ζ. The dashed line is the conjecture in Eq. (67), which is very close to the actual asymptotic curve everywhere except close to the edge.

been described by the asymptotic form

$$S_q \approx \frac{1}{6}\left(1+\frac{1}{q}\right)\ln\left(\frac{4N}{\pi}\sin\frac{\pi\zeta}{\sqrt{2}}\right) + E_q + \cdots. \qquad (67)$$

The two scaling curves are indeed very close to each other, but the numerical data for $q = 1$ fit slightly better the random matrix prediction (66) compared to the above conjecture (which, however, is very accurate; see Fig. 4). In Figs. 4 and 5 we report (for $q = 1$ and $q = 2$) the subtracted entropy

$$\Delta S_q = S_q - \frac{1}{6}\left(1+\frac{1}{q}\right)\ln N, \qquad (68)$$

which, in the limit of large N, is a scaling function of $\zeta = \ell/\sqrt{N}$. Increasing N, the numerical data approach the random matrix prediction (66). For $q = 1$ the agreement is

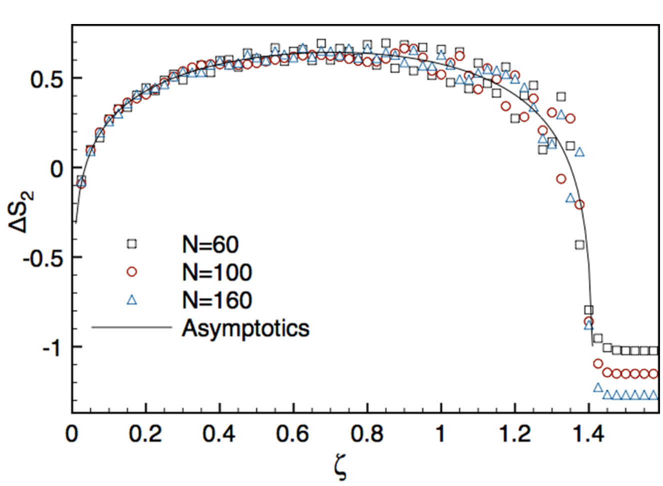

FIG. 5. (Color online) Subtracted second-order Rényi entropy $\Delta S_2 = S_2 - (\ln N)/4$ as function of $\zeta = \ell/\sqrt{N}$ for several values of N up to $N = 160$. The nonuniform approach to the asymptotic result (66) is more evident than in the case $q = 1$.

very clear, while for $q = 2$ there are oscillating corrections to this asymptotic form (especially close to the edge), which make the distinction between Eq. (66) and the conjecture (67) impossible. As noticed already in Ref. [21] the approach to the asymptotic result is nonuniform and gets very bad close to the edge, but, as we show in the next section, following Refs. [19,20], this apparently strange behavior can be understood in terms of the different scaling at the edge.

We have been also trying to describe, at least phenomenologically, the corrections to the asymptotic scaling behavior in the regime with $\Delta \gg 1$ by subtracting from the numerical data the asymptotic prediction (66). However, as it should be already clear from Fig. 5 with $q = 2$, at least two different kinds of corrections affect the data. The first is present also for small ζ in the form of small oscillations around the asymptotic value. This is reminiscent of the nowadays well-understood "unusual corrections" to the scaling [9,10,53–55], which have been discussed in many different situations in homogeneous systems in which case they scale like $N^{-2/q}$ (for periodic systems). The second corrections instead originate from the edge $\ell \sim \sqrt{2N}$ and its form is derived in the next section. However, in the intermediate regime with $\zeta \sim O(1)$, a quantitative description of the corrections to the scaling eludes our understanding because the two effects are mixed up even for large, but finite, N.

C. Edge regime

Close to the edge and in the limit of large N, the GUE kernel (46) tends to the Airy kernel [cf. Eq. (51)] in terms of the scaling variable [56,57],

$$s = \sqrt{2}N^{2/3}(\zeta - \sqrt{2}). \tag{69}$$

Since we are considering a symmetric interval with respect to the center of the trap, there are two edges which contribute identically to the entanglement entropy. Thus, the large N limit in the edge-scaling regime is simply the limit of Eq. (9), i.e. [58],

$$S_q = \frac{2}{1-q}\mathrm{Tr}\ln[(P_s K_{\mathrm{Ai}} P_s)^q + (1 - P_s K_{\mathrm{Ai}} P_s)^q], \tag{70}$$

where P_s is the projector on the interval $[s,\infty]$. This expression can be readily calculated from the spectrum of the operator $P_s K_{\mathrm{Ai}} P_s$, obtained by a proper discretization following Ref. [39] (this procedure has been already applied for $q = 1$ in Ref. [20]). In Fig. 6 we report the obtained exact scaling curve for S_q as a function of s and for various values of q. It is evident that the scaling curves present oscillations whose amplitude grows with increasing q. This behavior explains why in the intermediate regime, the data for S_1 in Fig. 4 are much better described by the asymptotic curve than the data for S_2 in Fig. 5. The behavior of the amplitude of the oscillations is reminiscent of the one of the unusual corrections to the scaling [9,10,25], but, their origin being different, if there is any connection between the two is still to be understood. Furthermore a similar behavior has been observed also close to the boundary of a hard-wall trap [25], but in that case the theory of soft edge does not apply and the calculation of the asymptotic curve needs different methods.

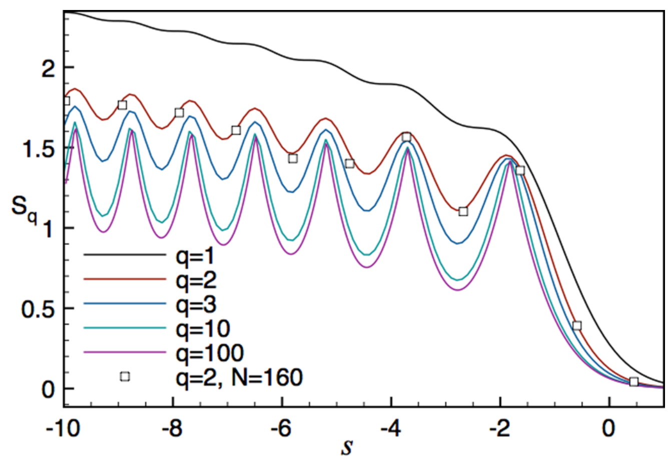

FIG. 6. (Color online) Universal scaling of the Rényi entanglement entropy (always for $A = [-\ell,\ell]$ in a trapped gas) close to the edge. We report the asymptotic curves in Eq. (70) as function of the scaling variable s in Eq. (69) for different values of q. We only report the numerical data for $N = 160$ and $q = 2$.

Finally, we also checked that in the edge regime the numerical data approach the asymptotic result. This was already discussed in Ref. [20] for $q = 1$. Thus, in Fig. 6 we limit to reporting a few data for $q = 2$ and $N = 160$. The agreement between the numerics and the prediction (70) is very good already for $N = 160$. We checked also other values of q, but we do not report them in order to have a readable figure.

D. Beyond the edge

There is clearly a third regime for $\zeta > \sqrt{2}$, in which the leading order of the entropy S_q vanishes for large N. Thus, S_q is exponentially small. For the sake of completeness, in this section we report the calculation the entropy in this regime.

In order to compute the leading correction we again start from Eq. (23). When $N_A = N$, i.e., all particles are inside the interval $[-\zeta, +\zeta]$, we have $D_A(\lambda) = (\lambda - 1)^N$ and hence $\rho(a) = \delta(a - 1)$. Consequently, the entropy is zero. The first elementary excitation has $N_A = N - 1$, which corresponds to pulling one fermion outside the Wigner sea (on either side). The probability of this event is given by [59]

$$p \sim e^{-2N\phi(\zeta)}, \tag{71}$$

where $\phi(\zeta)$ is also the (right) large deviation function [60] associated with the largest eigenvalue of the GUE random matrix given in Eq. (50). Note that as $\zeta \to \sqrt{2}$ from above, i.e., entering the small deviation (edge) regime, this function vanishes as $\phi(\zeta) = \frac{2^{7/4}}{3}(\zeta - \sqrt{2})^{3/2}$; hence, in this regime $p \sim e^{-\frac{4}{3}s^{3/2}}$, where s is given in Eq. (69).

Since $p \ll 1$ in the regime $\zeta > 2$, one has

$$\mathrm{Prob}(N_A) \approx p\delta_{N_A,N-1} + (1 - p)\delta_{N_A,N}, \tag{72}$$

which, using Eq. (23), leads to $D_A(\lambda) = (\lambda - 1)^{N-1}[\lambda - (1 - p)]$ and, hence,

$$\rho(a) \approx \left(1 - \frac{1}{N}\right)\delta(a - 1) + \frac{1}{N}\delta[a - (1 - p)]. \tag{73}$$

We thus obtain the entropy to leading order in small p,

$$S_q = \frac{N}{1-q}\int_0^1 da \ln[a^q + (1-a)^q]\rho(a)$$
$$\simeq \frac{1}{1-q}\ln[(1-p)^q + p^q] \approx \frac{1}{1-q}\ln(1-qp+p^q). \tag{74}$$

For fixed $q > 1$ this is

$$S_q \simeq \frac{q}{q-1}p, \tag{75}$$

but, on the other hand, for $q = 1$, this reduces to

$$S_1 \simeq -p\ln p. \tag{76}$$

There exists a scaling function interpolating between the two limits. Taking the limits $q-1\to 0$ and $p \to 0$, keeping the product $y = -(q-1)\ln p$ fixed, one has

$$S_q(p) = (-p\ln p)f(y), \quad f(y) = \frac{1-e^{-y}}{y}. \tag{77}$$

Therefore, for any $q \geqslant 1$ the entropy S_q is exponentially small in N when $\zeta > \sqrt{2}$.

We can arrive at the same conclusion also starting from Eq. (70), which describes the behavior of the entropy in the small deviation regime from the edge. In the region $\zeta > \sqrt{2}$ and N large, the edge-scaling variable $s = \sqrt{2}N^{2/3}(\zeta - \sqrt{2})$ becomes large. Hence, the operator

$$\tilde{K}(x,y) \equiv [P_s K_{\mathrm{Ai}} P_s](x,y)$$
$$= \theta(x)\theta(y)\int_0^{+\infty} dv \mathrm{Ai}(x+v+s)\,\mathrm{Ai}(y+v+s), \tag{78}$$

becomes uniformly small since $\mathrm{Ai}(x) \sim e^{-\frac{2}{3}x^{3/2}}$ for large positive x. Hence, we can expand Eq. (70) as

$$S_q \simeq \frac{2}{1-q}\mathrm{Tr}\ln(1-q\tilde{K}+\tilde{K}^q). \tag{79}$$

For fixed $q > 1$ and large s we obtain

$$S_q = \frac{2q}{1-q}\mathrm{Tr}\tilde{K} \sim \frac{q}{1-q}A(s)e^{-\frac{4}{3}s^{3/2}}, \tag{80}$$

where $A(s)$ is an unimportant prefactor which can easily be calculated from the Airy function asymptotics. Thus, it matches the result (75) obtained from the large deviation side. For $q = 1$ one instead obtains

$$S_1 \simeq -2\mathrm{Tr}\,\tilde{K}\ln\tilde{K}, \tag{81}$$

which corresponds to Eq. (76).

In conclusion, both in the large deviation regime ($\zeta > \sqrt{2}$), as well as in the tail of the small deviation regime ($s \ll 1$), the entropy is exponentially small for large N. Here we limited to compute the leading nonvanishing term, but a systematic large s expansion can, in principle, be performed from Eq. (70).

IV. CONCLUSIONS

In this paper we exploited and clarified the connection between entanglement entropy and random matrix theory for systems of free fermions. Such a connection has been already (more or less explicitly) pointed out in the literature [18–20], but in this paper we push to the level to have a complete analytic description of the entanglement entropy in the ground state of a free Fermi gas trapped by a harmonic potential. The main analytical results of this paper can be summarized by Eqs. (66), (70), and (77). Indeed, Eq. (66) provides the asymptotic behavior of the entropy in the scaling regime with $\ell/\sqrt{N}$ of order 1, but far enough from the edge (a problem which was numerically studied in Ref. [21]). Instead, Eq. (70) is the asymptotic behavior of the entropy in the edge - regime. Furthermore, an interesting by-product of this work is that the entanglement entropy for finite number of particles (in some circumstances like the case of a trapped gas) can be more effectively calculated by ingeniously discretizing the reduced correlation matrix (as described in Ref. [39]) than by using the overlap matrix.

We conclude by mentioning some possible extensions of this work which deserve further investigation. It would be interesting to understand whether random matrix theory could provide quantitative predictions not only for the ground state of a trapped Fermi gas, but also for excited states that in the homogeneous case present many interesting and universal features [61–63]. Whether the present approach can be generalized to the entanglement entropy of free bosonic systems, such as the harmonic chain (see, e.g., [64]), is also a relevant open question. Finally, generalizations to other entanglement estimators such as entanglement negativity [65], entanglement contour [66], or Shannon mutual information [67] are also waiting for an analytical description.

ACKNOWLEDGMENTS

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APPENDIX: THE DISTRIBUTION OF EIGENVALUES OF THE OVERLAP MATRIX

In this appendix, we report a technical by-product of this paper, which is the distribution of eigenvalues of the overlap matrix (which is the same as the one of the reduced correlation matrix) for a trapped Fermi gas in the intermediate regime [$\zeta \sim O(1)$, but far from the edge]. At the leading order in N, for the interval $A = [-\ell,\ell]$, assuming the distribution of N_A Gaussian, we have immediately

$$D_A(\lambda) = \lambda^N\left\langle\left(1-\frac{1}{\lambda}\right)^{N_A}\right\rangle$$
$$= \lambda^N e^{\langle N_A\rangle\ln(1-\frac{1}{\lambda}) + \frac{\ln[N\zeta(2-\zeta^2)^{3/2}]}{2\pi^2}\ln^2(1-\frac{1}{\lambda})}, \tag{A1}$$

so that the resolvent function (25) is

$$F(\lambda) = \frac{N}{\lambda} + \frac{\langle N_A \rangle}{\lambda(\lambda-1)} + \frac{\ln[N\zeta(2-\zeta^2)^{3/2}]}{\pi^2\lambda(\lambda-1)} \ln\left(1-\frac{1}{\lambda}\right). \tag{A2}$$

The resulting distribution of eigenvalues $\rho(a)$, at the leading order in N, can be extracted from Eq. (31), giving

$$\begin{aligned}\rho(a) &= -\frac{1}{\pi}\lim_{\epsilon\to 0^+} \mathrm{Im}F(a+i\epsilon)\\ &= \left(1-\frac{\langle N_A\rangle}{N}\right)\delta(a) + \frac{\langle N_A\rangle}{N}\delta(a-1)\\ &\quad + \frac{\ln[N\zeta(2-\zeta^2)^{3/2}]}{N\pi^2}\frac{1}{a(1-a)}.\end{aligned} \tag{A3}$$

This distribution reproduces the correct leading order of the entropy. Indeed, by using

$$\frac{1}{1-q}\int_0^1 \frac{da}{a(1-a)} \ln[a^q + (1-a)^q] = \frac{\pi^2}{6}\left(1+\frac{1}{q}\right), \tag{A4}$$

we obtain

$$\begin{aligned}S_q &= \frac{N}{1-q}\int da\, \rho(a) \ln[a^q + (1-a)^q]\\ &= \frac{\ln[N\zeta(2-\zeta^2)^{3/2}]}{\pi^2}\frac{\pi^2}{6}\left(1+\frac{1}{q}\right),\end{aligned} \tag{A5}$$

which coincides with the leading order of Eq. (66). Note that the third term in (A3) actually is nonintegrable near $a = 0$ and $a = 1$; however, when the entropy is evaluated in Eq. (A5), it gives a finite contribution.

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