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Convexity of the entanglement entropy of $SU(2N)$ -symmetric fermions with attractive interactions

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The positivity of the probability measure of attractively interacting systems of $2N$ -component fermions enables the derivation of an exact convexity property for the ground-state energy of such systems. Using analogous arguments, applied to path-integral expressions for the entanglement entropy derived recently, we prove non-perturbative analytic relations for the Rényi entropies of those systems. These relations are valid for all sub-system sizes, particle numbers and dimensions, and in arbitrary external trapping potentials.

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Introduction. – In recent years, research in many-body and condensed matter physics in general has developed a growing intersection with the areas of quantum information and quantum computation [1]. Considerable attention has been given to the notion of entanglement, in particular to the entanglement entropies as a means to identify and characterize quantum phase transitions (especially topological ones) [2, 3]. The conformal field theories governing the low-energy behavior at those critical points are also of relevance for high-energy physics, black-hole physics and string theory [4], where some exact results have been available for many years.

In spite of much progress, the calculation of the entanglement properties has been a difficult challenge for many-body theories. Indeed, even the calculation of the asymptotic form of the entanglement entropy for large (sub-)systems of non-interacting fermions was the subject of much discussion (see e.g. [5]); and for interacting systems it was until recently challenging to even formulate a way amenable to quantum Monte Carlo calculations. However, there are currently a few alternatives (see e.g. [6]), and in this work we will use the formalism of Ref. [7], in which Grover proposes a way to calculate fully interacting reduced density matrices using auxiliary-field quantum Monte Carlo (AFQMC) (see also Ref. [8]). The resulting path-integral expression for the entanglement entropy will be central to our arguments.

Such AFQMC calculations, in particular those on the lattice, rely on the positivity of the fermion determinant as the natural probability measure arising from the field integration of the fermion degrees of freedom. While this property is essential from a computational standpoint, it has also enabled the non-perturbative analytic proof of a variety of exact inequalities among the hadron masses arising from Quantum Chromodynamics (QCD); the most recent contribution in this direction (as of this writing) is due to Detmold [9], but earlier versions have been around for many years [10] (see Ref. [11] for a review on QCD inequalities).

In this work, we use measure-positivity arguments to

derive an exact inequality that expresses the convexity of the entanglement entropy with respect to particle number in a system of $SU(2N)$ fermions, i.e. a system of $2N$ species of otherwise identical fermions, with attractive interactions (depicted in Fig. 1). The inequality holds for all Rényi entropies, all sub-system sizes, particle numbers and dimensions, as well as arbitrary external trapping potentials.

To carry out the proof, we combine a path-integral expression for the Rényi entanglement entropy of interacting Fermi systems, derived recently in Ref. [7], with (the proof of) a theorem that establishes the spectral convexity of $SU(2N)$ -symmetric fermions with attractive interactions, first proven by D. Lee in Ref. [12]. Interestingly, this theorem was originally motivated by the properties of nuclear structure [13] and the importance of Wigner $SU(4)$ symmetry in that context [14]. To facilitate contact with the original derivation, we follow closely the main steps, and use similar notation. However, some modification is needed due to the presence of “replicas” of the auxiliary field, as explained below, among other details. The main result is depicted in Fig. 3, and it indicates that the entanglement entropy of N_{part} fermions, for $2NK \leq N_{\text{part}} \leq 2N(K+1)$, with K a positive integer, is always greater or equal than the average of the entanglement entropies of $2NK$ and $2N(K+1)$ fermions. Here, the $2NK$ fermions are to be understood as K particles per component, and the $2N(K+1)$ fermions appear as $K+1$ particles per component. The states between these have $K+1$ particles for some species and K particles for the rest. It is well-known that other inequalities exist that relate the entanglement entropy of disjoint subregions of a system (see e.g. [15]). The inequality established here, however, is unrelated to the property of sub-additivity, and is therefore of a different kind, as explained below.

Derivation of the inequality. – The n -th Rényi entanglement entropy S_n of a sub-system A of a given quantum

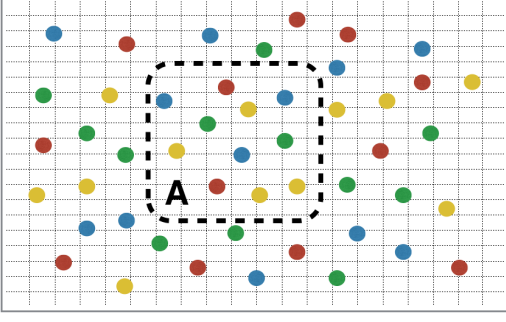


FIG. 1: (color online) The system considered here is made out of $2N$ species of otherwise identical fermions, on a space-time lattice. All of the species live in the whole volume, but the entanglement entropy is computed for a subregion A .

system is defined by

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

where $\hat{\rho}_A$ is the reduced density matrix of sub-system A (i.e. the degrees of freedom of the rest of the system are traced over).

To establish our main result, we put the system on a d -dimensional spatial lattice of side N_x and consider implementing the projection AFQMC method, with some trial state $|\Psi\rangle$, which we assume has a non-vanishing overlap with the true ground state.

In Ref. [7], Grover derived an auxiliary-field path-integral form for $\hat{\rho}_A$, from which he showed that S_n can be accessed via AFQMC calculations. Indeed, for a system of $2N$ -component fermions, S_n can be written in that formalism as

$$\exp((1-n)S_n) = \int \mathcal{D}\{\sigma\} P[\{\sigma\}] Q[\{\sigma\}] \quad (2)$$

where

$$\mathcal{D}\{\sigma\} = \prod_{k=1}^n \frac{\mathcal{D}\sigma_k}{\mathcal{Z}}, \quad (3)$$

$$\mathcal{Z} = \int \mathcal{D}\sigma \prod_{m=1}^{2N} \det U_m[\sigma], \quad (4)$$

$$P[\{\sigma\}] = \prod_{k=1}^n \prod_{m=1}^{2N} \det U_m[\sigma_k], \quad (5)$$

$$Q[\{\sigma\}] = \prod_{m=1}^{2N} \det M_m[\{\sigma\}] \quad (6)$$

$$M_m[\{\sigma\}] = \prod_{k=1}^n (\mathbb{1} - G_{A,m}[\sigma_k]) \times \left[\mathbb{1} + \prod_{k=1}^n \frac{G_{A,m}[\sigma_k]}{\mathbb{1} - G_{A,m}[\sigma_k]} \right], \quad (7)$$

and the path integral $\int \mathcal{D}\{\sigma\}$ is over the n “replicas” σ_k of the Hubbard-Stratonovich auxiliary field. Here, $U_m[\sigma]$ is a matrix which encodes the dynamics of the m -th component in the system, namely the kinetic energy and the form of the interaction after a Hubbard-Stratonovich transformation; it also encodes the form of the trial state $|\Psi\rangle$ (see e.g. Ref. [16]), which we take to be a Slater determinant. $G_{A,m}[\sigma_k]$ is the restricted non-interacting single-particle Green’s function of the m -th component in the background field σ_k , as explained in Ref. [7] (see also Ref. [17]). The size of $U_m[\sigma]$ is given by the number of particles of the m -th species present in the system. The size of $G_{A,m}[\sigma_k]$, on the other hand, is given by the number of lattice sites enclosed by the region A . Note that, separating a factor of \mathcal{Z}^n in the denominator of Eq. 2, an explicit form can be identified in the numerator as the result of the so-called “replica trick” (namely a partition function for n copies of the system, “glued” together in the region A).

Because we are considering a finite lattice, the single-particle space is of finite size N_x^d . As in Ref. [12], we may define our trial state $|\Psi\rangle$ as a Slater determinant, letting j components fill some N_B single-particle orbitals in a subset \mathcal{B} (the same set of orbitals for all those j components), and letting the remaining $2N - j$ components fill some other set \mathcal{C} of, say, N_C orbitals (see Fig. 2). The total number of fermions is therefore $N_{\text{part}} = jN_B + (2N - j)N_C$.

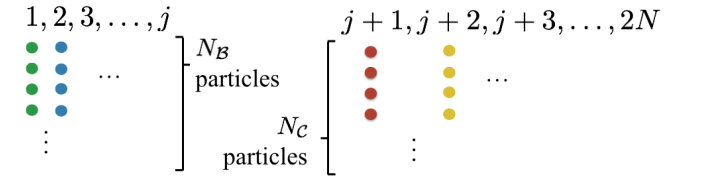


FIG. 2: (color online) Distribution of particles among $2N$ fermion species for the proof of the inequality.

With this trial state, the matrix U_m will be the same for species $1, \dots, j$ and we shall denote it U_B ; similarly, U_m will be the same for species $j+1, \dots, 2N$ and we shall denote it U_C . Therefore,

$$P[\{\sigma\}] = \prod_{k=1}^n (\det U_B[\sigma_k])^j \prod_{k=1}^n (\det U_C[\sigma_k])^{2N-j}, \quad (8)$$

and

$$Q[\{\sigma\}] = (\det M_B[\{\sigma\}])^j (\det M_C[\{\sigma\}])^{2N-j}. \quad (9)$$

In order to prove the advertised convexity property, we use Hölder's inequality, which states that

$$\int dx |f(x)g(x)| \leq \left[\int dx |f(x)|^p \right]^{1/p} \left[\int dx |g(x)|^q \right]^{1/q}, \quad (10)$$

for any functions $f(x)$, $g(x)$ for which the integral exists, and where $1/p + 1/q = 1$. We apply this identity to our path integral expression for $\exp((1-n)S_n)$ in Eq. 2. Before doing that, the following should be noted. This separation of components into j and $2N-j$ implies that the integrand on the right-hand-side of Eq. 2 is not in general positive definite (unless j is even and only if the determinants are real). However, the integral of Eq. 2 is naturally bounded from above by the integral over the *absolute value* of the integrand, which is what we will identify as the left-hand side of Eq. 10.

For this purpose, we choose integers n_1, n_2 such that $0 \leq 2n_1 \leq j \leq 2n_2 \leq 2N$, and take the integration measure dx to be $\mathcal{D}\{\sigma\}\tilde{P}[\{\sigma\}]$, where

$$\tilde{P}[\{\sigma\}] = (\det M_B[\{\sigma\}])^{2n_1} (\det M_C[\{\sigma\}])^{2N-2n_2} \times \prod_{k=1}^n (\det U_B[\sigma_k])^{2n_1} (\det U_C[\sigma_k])^{2N-2n_2}, \quad (11)$$

which is positive definite as long as the determinants are real. This can be guaranteed for attractive interactions. We take, furthermore,

$$|f(x)| \rightarrow |\det M_B[\{\sigma\}]|^{j-2n_1} \prod_{k=1}^n |\det U_B[\sigma_k]|^{j-2n_1}, \quad (12)$$

$$|g(x)| \rightarrow |\det M_C[\{\sigma\}]|^{2n_2-j} \prod_{k=1}^n |\det U_C[\sigma_k]|^{2n_2-j}, \quad (13)$$

and

$$p = (2n_2 - 2n_1)/(j - 2n_1), \quad (14)$$

$$q = (2n_2 - 2n_1)/(2n_2 - j). \quad (15)$$

Putting everything together, it is a matter of simple algebra to see that

$$S_n[\mathcal{B}^j, \mathcal{C}^{2N-j}] \geq \frac{j-2n_1}{2n_2-2n_1} S_n[\mathcal{B}^{2n_2}, \mathcal{C}^{2N-2n_2}] + \frac{2n_2-j}{2n_2-2n_1} S_n[\mathcal{B}^{2n_1}, \mathcal{C}^{2N-2n_1}] \quad (16)$$

for all $n > 1$, where $S_n[\mathcal{B}^j, \mathcal{C}^{2N-j}]$ is the estimate of the entanglement entropy obtained with the trial state described above. If the trial state has a non-vanishing overlap with the ground state of the system, as commonly assumed in AFQMC calculations, then $S_n[\mathcal{B}^j, \mathcal{C}^{2N-j}]$ will converge to the true entanglement entropy of the system S_n in the limit of large imaginary times.

This is, in essence, the final result. It indicates that S_n is a convex function, in the sense that its values for

any j between $2n_1$ and $2n_2$ are larger than the average of the values at those two points. We note also that the inequality is trivially saturated in the absence of interactions, as no path integral is present in Eq. 10 in that case.

Discussion.— Taking $N_B = K$ and $N_C = K+1$, we see that the total number of fermions is $N_{\text{part}} = jN_B + (2N-j)N_C = 2NK+j$. Since $0 \leq j \leq 2N$, we see that S_n must be convex between $2NK$ and $2N(K+1)$, for any K . The inequality holds in particular for $K=0$, which shows that S_n is convex for all particle numbers $0 \leq N_{\text{part}} \leq 2N$ as well. These statements are depicted in Fig. 3. We stress that these results are valid for arbitrary sub-region A , Rényi entropy n , and spatial dimension. Furthermore, the system may be in an arbitrary external potential, in particular a harmonic trap such as those routinely used in ultracold atom experiments.

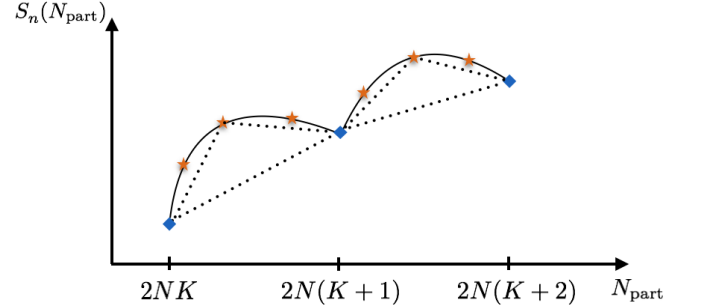


FIG. 3: (color online) Convexity of the entanglement entropy S_n as a function of particle number, for a system of $2N$ species. The convexity property is valid for systems with particle numbers between K and $K+1$ particles per component, with $K \in \mathbb{N}$, such that some components have K particles and the rest $K+1$. The property holds for arbitrary region A , Rényi entropy n , spatial dimension, and external potential.

Remarkably, our main result is also valid even if the region A is not a region of coordinate space. Indeed, the formalism of the proof presented here, itself based on the second-quantization derivations of Ref. [7], makes no explicit reference to the space in which the single-particle orbitals are defined. As a consequence, the inequality Eq. 16 is valid also when S_n is computed in momentum space, harmonic oscillator space, etc., as long as one can guarantee that $\det M_m[\{\sigma\}]$ is real.

The above proof can be generalized to finite temperature in the grand-canonical ensemble. The role of the matrix $U_m[\sigma_k]$ is now played by its full-sized $(N_x^d \times N_x^d)$ finite-temperature form $\mathcal{U}_m[\sigma_k]$, such that $U_m[\sigma_k] \rightarrow \mathbb{1} + z_m \mathcal{U}_m[\sigma_k]$, where z_m is the fugacity of the m -th species. The matrix M , on the other hand, retains its definition in terms of reduced Green's functions, but the latter are replaced by their finite-temperature counterparts. The proof then proceeds in the same fashion, but one assigns different chemical potentials μ_B to components $1 \dots j$, and μ_C to components $j+1, \dots, 2N$, rather

than specific particle numbers. The total average particle number is then $\langle N_{\text{part}} \rangle = j\langle N_B \rangle + (2N - j)\langle N_C \rangle$. Tuning the chemical potentials such that $\langle N_B \rangle = K$ and $\langle N_C \rangle = K + 1$, we see that S_n must be convex between $2NK$ and $2N(K + 1)$, for any K , also at finite temperature.

Throughout the proof we implicitly assumed to be considering non-relativistic systems, for which particle number is a good quantum number. The generalization of our result to relativistic systems, at least in the absence of gauge fields, can be expected to be straightforward, with states of fixed particle number replaced by states of fixed charge. Those systems will be considered elsewhere.

Summary and Conclusions.— In this work, we have connected a recently derived path-integral form of the Rényi entanglement entropy S_n with a theorem originally proven in the context of nuclear structure to show that S_n is a convex function when the particle number is varied. The inequality underlying the property of convexity is remarkably general, holding for all Rényi entropies, all sub-system sizes, particle numbers and dimensions, as well as arbitrary external trapping potentials. If an analytic continuation in n is possible then we expect convexity to be maintained for the von Neumann entropy. The fundamental constraint of the proof is the positivity of the probability measure, which in turn only depends on the $SU(2N)$ symmetry and the interaction being attractive. The inequality holds in particular for the attractive Hubbard model in arbitrary dimensions. These results can be further generalized to finite temperature and to relativistic systems.

While the experimental determination of the entanglement entropy is currently beyond reach, attempts are underway with ultracold atoms, in particular in optical lattices (see e.g. [18]). As is well known, these systems are remarkably malleable. Most relevant for this work is the study of few-atom systems of atomic species with a varying number of internal degrees of freedom, such as Yb and Sr isotopes [19]; these make it possible to realize $SU(6)$ and $SU(10)$ symmetries, thus going well beyond the usual $SU(2)$ case commonly realized with Li and K atoms. It is for these systems that the results of this work represent a prediction.

On the other hand, as pointed out in Ref. [12], it appears that real nuclei respect the inequalities that would strictly speaking only be valid in the attractive $SU(4)$ -symmetric limit of degenerate nucleons. It would therefore be of interest to determine whether the entanglement entropy of real nuclei also respects the convexity property. With recent advances in coupled-cluster and Green's function and lattice Monte Carlo calculations, this may be expected to be determined theoretically sooner than experimentally.

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