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We consider the von Neumann and Rényi entropies of the one dimensional quarter-filled Hubbard model. We observe that for periodic boundary conditions the entropies exhibit an unexpected dependence on system size: for $L = 4 \bmod 8$ the results are in agreement with expectations based on conformal field theory, while for $L = 0 \bmod 8$ additional contributions arise. We explain this observation in terms of a shell-filling effect, and develop a conformal field theory approach to calculate the extra term in the entropies. Similar shell filling effects in entanglement entropies are expected to be present in higher dimensions and for other multicomponent systems.

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Over the course of the last decade, entanglement measures have developed into a powerful tool for analyzing many-particle quantum systems, in particular in relation to quantum criticality and topological order [1]. Within the realm of one dimensional (1D) systems, arguably the most important result concerns the universal behaviour in critical theories, which is characterized by the central charge of the underlying conformal field theory (CFT) [2–4]. Let consider the ground state $|\mathrm{GS}\rangle$ of a finite, periodic 1D system of length L and partition the latter into a finite block A of length ℓ and its complement $\bar{A}$. The density matrix of the entire system is then $\rho = |\mathrm{GS}\rangle\langle\mathrm{GS}|$, and we will denote the reduced density matrix of block A by ρ_A. Widely used measures of entanglement are the Rényi entropies

$$S_n = \frac{1}{1-n} \ln[\mathrm{Tr}\rho_A^n] \, . \tag{1}$$

They encode the full information on the spectrum of ρ_A [5], and in the limit $n \to 1$ reduce to the von Neumann entropy $S_1 = -\mathrm{Tr}\rho_A \ln \rho_A$. When the subsystem size ℓ is large compared to the lattice spacing, S_n are given by

$$S_n = \frac{c}{6}\left(1 + \frac{1}{n}\right) \ln\left(\frac{L}{\pi} \sin\frac{\pi\ell}{L}\right) + c'_n + o(1) \, , \tag{2}$$

where c is the central charge, c'_n are non-universal additive constants, and $o(1)$ denotes terms that vanish for $\ell \to \infty$. The result (2) has been confirmed for many spin-chains and itinerant lattice models, see [1] for recent reviews. The knowledge of the entanglement entropies has led to a deeper understanding of numerical algorithms based on matrix product states [6] and has aided the development of novel computational methods [7].

The Hubbard model is a central paradigm of strongly correlated electron systems. Its 1D version has attracted much attention for decades, because it is exactly solvable and exhibits a Mott metal to insulator transition [8]. The Hamiltonian for periodic boundary conditions is

$$H_{\mathrm{Hubb}} = -t \sum_{j=1}^{L} \sum_{\sigma} c^\dagger_{j,\sigma} c_{j+1,\sigma} + \mathrm{h.c.} + U \sum_j n_{j,\uparrow}\, n_{j,\downarrow}, \tag{3}$$

where $c^\dagger_{j,\sigma}$ are fermionic spin-$\frac{1}{2}$ creation operators at site j with spin $\sigma = \uparrow, \downarrow$, $n_{j,\sigma} = c^\dagger_{j,\sigma} c_{j,\sigma}$, and we will assume repulsive interactions $U \geq 0$. In the following we will for the sake of definiteness fix the band filling to be one electron per two sites, i.e. $N_\uparrow = N_\downarrow = \frac{L}{4}$, but we stress that our findings generalize to other fillings and, in fact, to other models. It is known from the exact solution that the ground state of (3) below half filling (less than one fermion per site) is metallic and the low energy physics of the model is described by a spin and charge separated Luttinger liquid [8] equivalent to the semi-direct product of two $c = 1$ CFTs [9].

Given this state of affairs, it is quite surprising that the entanglement entropies do not always follow (2). This is shown in Fig. 1, which shows numerical results for S_1 obtained by density matrix renormalization group (DMRG) for a quarter-filled Hubbard model at $U = t$ for a number of different lattice lengths L. Interestingly, both the $L = 4 \bmod 8$ and the $L = 0 \bmod 8$ data exhibit scaling collapse, but to different functions. As we will show, the entropy for large lattice lengths $L = 4 \bmod 8$ is well-described by the CFT result (2)

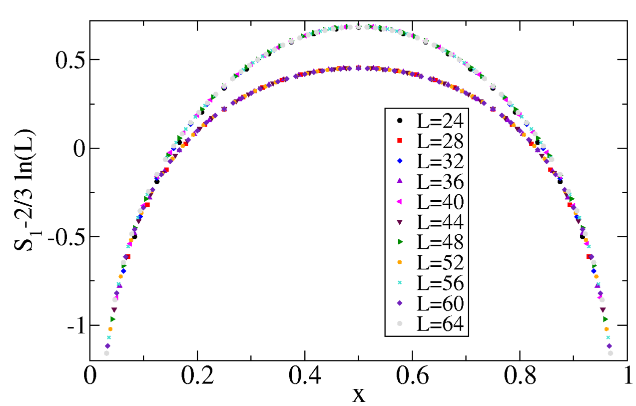

FIG. 1: DMRG data for $S_1 - 2/3 \ln L$ as a function of $x = \ell/L$ for $U = t$ and $L = 24, 28, 32, 36, 40, 44, 48, 52, 56, 60, 64$. The lower and upper branches corresponds to lattice lengths $L = 4 \bmod 8$ and $L = 0 \bmod 8$ respectively.

with $n = 1$, while for $L = 0 \bmod 8$ there is an additional positive contribution $-F_1'(\ell/L)$, where

$$F_1'(x) = \ln\left|2\sin(\pi x)\right| + \psi\left(\frac{1}{2\sin(\pi x)}\right) + \sin(\pi x). \quad (4)$$

Here $\psi(x)$ is the digamma function. We stress that this behaviour is very different from the lattice "parity effects" for Luttinger liquids [10, 11], which refer to $o(1)$ corrections in $S_{n\geq 2}$ only.

The shell-filling effect. In order to understand the origin of the difference in entanglement entropies between $L = 4 \bmod 8$ and $L = 0 \bmod 8$, we consider the ground state in the limit $U \to 0$. Here we are dealing with with non-interacting, spinful fermions, for which the boundary conditions on a ring fix the momenta to be $p_m = 2\pi m/L$ with integer $m \in [-L/2, L/2)$. For a chain of length $L = 8n+4$, quarter filling corresponds to an odd number $N_\sigma = L/4 = 2n+1$ of spin-σ fermion, and the unique ground state is the *symmetric* Fermi sea

$$|2n+1\rangle_{\rm FS} = \prod_{m=-n}^{n} c^\dagger_\uparrow(p_m) c^\dagger_\downarrow(p_m)|0\rangle\ , \quad (5)$$

where $c^\dagger_\sigma(k) = L^{-1/2}\sum_{j=1}^{L} e^{-ikj} c^\dagger_{j,\sigma}$ are creation operators in momentum space and $|0\rangle$ is the fermionic vacuum state. On the other hand, when $L = 8n$, $N_\sigma = L/4 = 2n$ is even and it is impossible for a given spin species to form a symmetric Fermi sea. As a result the ground state is degenerate. In particular, there are two degenerate ground states with $N_\sigma = L/4 = 2n$, that have zero momentum and are parity eigenstates (parity is a good quantum number)

$$|\sigma\rangle = \frac{c^\dagger_\uparrow(k_{\rm F})c^\dagger_\downarrow(-k_{\rm F}) + \sigma c^\dagger_\downarrow(k_{\rm F})c^\dagger_\uparrow(-k_{\rm F})}{\sqrt{2}}|2n-1\rangle_{\rm FS}. \quad (6)$$

Here $k_F = \pi/4$ is the Fermi momentum. As is shown below, the $U \to 0$ limit of the Hubbard model ground state gives the state $|+\rangle$. The shell-filling effect is now clear: for $L = 4 \bmod 8$ the ground state is a symmetrically filled Fermi sea, while for $L = 0 \bmod 8$ it is given by the linear superposition of two asymmetric Fermi seas. In terms of spin symmetries this state corresponds to the $S^z = 0$ component of a $S = 1$ multiplet. We note that the entropy for the superpositions $|\sigma\rangle$ are higher. Intuitively this derives from the fact that the states $|\sigma\rangle$ are less constrained, as the momentum difference between up spin and down spin fermions can take two values.

Bethe Ansatz (BA) solution. We now turn to the case $U > 0$. Eigenstates of the Hubbard chain are parametrized in terms of the solutions $\{\Lambda_\alpha, k_j\}$ of the following set of coupled BA equations [8, 16]

$$\begin{aligned} k_j L &= 2\pi I_j - \sum_{\alpha=1}^{N_\downarrow}\theta\Big(\frac{\sin k_j - \Lambda_\alpha}{u}\Big), \quad j = 1,\ldots,N\ ,\\ \sum_{j=1}^{N}\theta\Big(\frac{\Lambda_\alpha - \sin k_j}{u}\Big) &= 2\pi J_\alpha + \sum_{\beta=1}^{N_\downarrow}\theta\Big(\frac{\Lambda_\alpha-\Lambda_\beta}{2u}\Big),\\ &\qquad \alpha = 1,\ldots,N_\downarrow. \end{aligned} \quad (7)$$

Here $u = U/(4t)$, $\theta(x) = 2\arctan(x)$ and $N = N_\uparrow + N_\downarrow$. For real solutions of the BA equations (7), the "quantum numbers" I_j (J_α) are integers if $N_\downarrow$ is even (if $N_\uparrow$ is odd) and half-odd integers if $N_\downarrow$ is odd (if $N_\uparrow$ is even). The momentum is expressed in terms of the parameters $\{\Lambda_\alpha, k_j\}$ by $P = \sum_{j=1}^{N} k_j$, while the energy (in units of t) is given by

$$E = uL - \sum_{j=1}^{N}\left[2\cos(k_j) + \mu + 2u\right]\ , \quad (8)$$

where μ is the chemical potential. Following Ref. [17], we define *regular* BA states as eigenstates of Eq. (3) arising from solutions of (7) with $2N_\downarrow \leq N$, where all k_j and Λ_α are finite. We denote these states by $|\{I_j\};\{J_\alpha\}\rangle_{\rm reg}$. As was shown in Ref. [17], all regular BA states are lowest-weight states with respect to the SO(4) symmetry of the Hubbard model [18], and a complete set of energy eigenstates is obtained by acting on them with the SO(4) raising operators. For $L = 4 \bmod 8$ it is known [8, 16] that the quarter filled ground state is a regular BA state characterized by the choice $I_j = -2n - \frac{3}{2} + j\ ,\ j = 1,\ldots,4n+2$ and $J_\alpha = -n-1+\alpha\ ,\ \alpha = 1,\ldots,2n+1$.

For $L = 8n$ (n a positive integer), we find that there are two degenerate lowest energy regular, real solutions of (7) with $N_\uparrow = N_\downarrow = 2n$ fermions. They are obtained by the two choices $J^{(1,2)}_\alpha = -n - \frac{1}{2} + \alpha\ ,\ \alpha = 1,\ldots,2n$ and $I^{(1)}_j = -2n + j\ ,\ j = 1,\ldots,4n$ or $I^{(2)}_j = -2n-1+j\ ,\ j = 1,\ldots,4n$. We stress that the distribution of the I_j is asymmetric around zero in both cases. Interestingly, these are not ground states. The regular solution with the lowest energy involves one pair of complex conjugate Λ_α's known as a 2-string, but it is not the ground state either.

Let us now consider regular BA states with total spin quantum number $S^z = 1$, i.e. $N_\uparrow = 2n+1$, $N_\downarrow = 2n-1$. These are by construction lowest weight states of the spin-SU(2) symmetry algebra. The lowest energy regular BA state in this sector corresponds to the (symmetric) choice $I^{(0)}_j = -2n - \frac{1}{2} + j\ ,\ j = 1,\ldots,4n$, and $J^{(0)}_\alpha = -n+\alpha\ ,\ \alpha = 1,\ldots,2n-1$. Crucially, the state

$$S^-|\{I^{(0)}_j\};\{J^{(0)}_\alpha\}\rangle_{\rm reg}, \quad (9)$$

is a (non-regular) eigenstate of the Hubbard Hamiltonian with $N_\uparrow = N_\downarrow = L/8$ fermions. Here $S^- = \sum_{j=1}^{L} c^\dagger_{j,\downarrow}c_{j,\uparrow}$ is the spin lowering operator. As $[S^-, H] = 0$ its energy is the same as that of the regular BA state $|\{I^{(0)}_j\};\{J^{(0)}_\alpha\}\rangle_{\rm reg}$. The energy difference between (9) and the regular solutions discussed above can be calculated for large L using standard methods [9] and is found to be negative. Considering other non-regular Bethe Ansatz states in an analogous way, we find that (9) is in fact the ground state.

Bosonization. The low-energy physics of the Hubbard model is described by a spin-charge separated two-component Luttinger liquid Hamiltonian [12]

$$H = \sum_{\mathtt{a}=c,s}\frac{v_{\mathtt{a}}}{2}\int dx\left[(\partial_x\Phi_{\mathtt{a}})^2 + (\partial_x\Theta_{\mathtt{a}})^2\right], \quad (10)$$

where $v_{c,s}$ are the velocities of the collective charge and spin degrees of freedom. For $L = 0 \bmod 8$ the mode expansions of the canonical Bose fields $\Phi_{\mathsf{a}} = \varphi_{\mathsf{a}} + \bar{\varphi}_{\mathsf{a}}$, and their dual fields $\Theta_{\mathsf{a}} = \varphi_{\mathsf{a}} - \bar{\varphi}_{\mathsf{a}}$ follow from

$$\begin{aligned}\bar{\varphi}_{\mathsf{a}}(x,t) &= \bar{P}_{\mathsf{a}} + \frac{x_+}{La_0}\bar{Q}_{\mathsf{a}} + \sum_{n=1}^{\infty} \frac{e^{-i\frac{2\pi n}{La_0}x_+}\bar{a}_{\mathsf{a},n} + \text{h.c.}}{\sqrt{4\pi n}},\\ \varphi_{\mathsf{a}}(x,t) &= P_{\mathsf{a}} + \frac{x_-}{La_0}Q_{\mathsf{a}} + \sum_{n=1}^{\infty} \frac{e^{i\frac{2\pi n}{La_0}x_-}a_{\mathsf{a},n} + \text{h.c.}}{\sqrt{4\pi n}}, \quad (11)\end{aligned}$$

where $x_\pm = x \pm vt$ and a_0 is the lattice spacing. The structure of the ground state for $L = 0 \bmod 8$ is encoded in the zero modes, which have commutations relations $[P_{\mathsf{a}}, Q_{\mathsf{a}}] = -\frac{i}{2} = -[\bar{P}_{\mathsf{a}}, \bar{Q}_{\mathsf{a}}]$. The eigenvalues of Q_{a} are

$$\begin{aligned}q_c &= \sqrt{\frac{\pi}{8K_c}} \sum_{\sigma=\uparrow,\downarrow} (K_c+1)m_\sigma + (1-K_c)\bar{m}_\sigma \ ,\\ q_s &= \sqrt{\frac{\pi}{2}}(m_\uparrow - m_\downarrow) \ , \quad (12)\end{aligned}$$

where K_c is the Luttinger parameter in the charge sector, m_σ are half odd-integer numbers, and the eigenvalues of $\bar{Q}_{\mathsf{a}}$ are obtained by interchanging $m_\sigma \leftrightarrow \bar{m}_\sigma$. The Hamiltonian then has the mode expansion

$$H = \sum_{\mathsf{a}=c,s} \frac{v_{\mathsf{a}}}{La_0}\Big[Q_{\mathsf{a}}^2 + \bar{Q}_{\mathsf{a}}^2 + \sum_{n=1}^{\infty} 2\pi n (a_{\mathsf{a},n}^\dagger a_{\mathsf{a},n} + \bar{a}_{\mathsf{a},n}^\dagger \bar{a}_{\mathsf{a},n})\Big]. \quad (13)$$

There are two degenerate ground states

$$|\pm\rangle = \frac{1}{\sqrt{2}}\left[\Big|\frac{1}{2},0;0,\frac{1}{2}\Big\rangle \pm \Big|0,\frac{1}{2};\frac{1}{2},0\Big\rangle\right], \quad (14)$$

where we have introduced a notation $|m_\uparrow, m_\downarrow; \bar{m}_\uparrow, \bar{m}_\downarrow\rangle$ for states that are annihilated by all $a_{\mathsf{a},n}$, $\bar{a}_{\mathsf{a},n}$ and have eigenvalues $q_{\mathsf{a}}(m_\sigma, \bar{m}_\sigma)$ and $\bar{q}_{\mathsf{a}}(m_\sigma, \bar{m}_\sigma)$ of the zero mode operators Q_{a} and $\bar{Q}_{\mathsf{a}}$ respectively. In the Hubbard model the degeneracy between $|+\rangle$ and $|-\rangle$ is removed by the presence of a marginally irrelevant interaction of spin currents and the ground state in fact corresponds to $|+\rangle$. In principle one could now generalize the CFT calculation of entanglement entropies of Ref. [3] to the case at hand. Rather than doing so, we pursue the following shortcut. Let us carry out the conformal map from the cylinder to the plane [13], i.e. $z = \exp\big(\frac{2\pi}{La_0}(vt - ix)\big)$, $\bar{z} = \exp(\frac{2\pi}{La_0}(vt + ix))$. Then expectation values in the state $|+\rangle$ of operators in the bosonic theory (13) with zero-mode quantization conditions (12) are formally the same as the expectation values of the corresponding operators in the "usual" compactified boson theory in the state

$$\lim_{z,\bar{z}\to 0} \cos\big(\sqrt{2\pi}\Phi_s(z,\bar{z})\big)|0\rangle \ . \quad (15)$$

Here by usual we mean the boson theory (13) with zero-mode quantization conditions (12), where now $m_\sigma, \bar{m}_\sigma$ are integers, and $|0\rangle$ is the vacuum state $|0,0,0,0\rangle$ of this theory. While the state (15) is not an excited state, because $\cos\big(\sqrt{2\pi}\Phi_s\big)$ is not a local operator of the compactified boson theory, it has the same structure. This allows us to utilize results for entanglement entropies in low-lying excited states in CFTs.

CFT approach to the Rényi entropies. A general approach to the latter problem has been recently developed by Alcaraz et al. [14, 15] and their main result can be summarized as follows. The n'th Rényi entropy for an excited state of the form $\mathcal{O}(0,0)|0\rangle$ is given by

$$\begin{aligned}S_n &= \frac{c}{6}\big(1+\frac{1}{n}\big)\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] + c_n'\\ &+\frac{1}{1-n}\ln\left[F_n(\ell/L)\right] + o(L), \quad (16)\end{aligned}$$

where c_n' are $\mathcal{O}$-independent constants, and the scaling functions $F_n^{\mathcal{O}}(x)$ are given by

$$F_n(x) = \frac{\langle \prod_{k=0}^{n-1} \mathcal{O}\big(\frac{\pi}{n}(x+2k)\big)\mathcal{O}^\dagger\big(\frac{\pi}{n}(-x+2k)\big)\rangle}{n^{2n(h+\bar{h})}\langle \mathcal{O}\big(\pi x\big)\mathcal{O}^\dagger\big(-\pi x\big)\rangle^n} \ . \quad (17)$$

Here h and $\bar{h}$ are the conformal dimensions of the operator $\mathcal{O}$. In our case $\mathcal{O}(x) = 2\cos(\sqrt{2\pi}\Phi_s(x))$ and we need to evaluate ($\sigma = \sum_{l=1}^n \sigma_l$)

$$\langle \prod_{j=1}^{2n} \mathcal{O}(x_j)\rangle = \sum_{\sigma_1,\ldots,\sigma_n=\pm} \delta_{\sigma,0} \prod_{i<j} \Big|2\sin\big(\frac{x_i - x_j}{2}\big)\Big|^{-\sigma_i\sigma_j}, \quad (18)$$

where the x_j's are given by (17). We find that $F_n^s(x)$ can be expressed as the square root of a determinant, which, surprisingly, is identical to Eq. (56) of Ref. [15]. We have succeeded in expressing this determinant in a form amenable for analytic continuation in n

$$\begin{aligned}[F_n(x)]^2 &= \prod_{p=1}^{n}\Big[1 - \frac{(n-2p+1)^2}{n^2}\sin^2(\pi x)\Big]\\ &= \left[\Big[\frac{2\sin(\pi x)}{n}\Big]^n \frac{\Gamma\left(\frac{1+n+n\csc(\pi x)}{2}\right)}{\Gamma\left(\frac{1-n+n\csc(\pi x)}{2}\right)}\right]^2. \quad (19)\end{aligned}$$

Using that for the Hubbard model $c = 2$ we then obtain a CFT prediction for the shell filling effect by combining equations (19) and (16). In order to obtain an expression for the von Neumann entropy we need to take the limit $n \to 1$, which gives

$$S_1 = \frac{c}{3}\ln\left(\frac{L}{\pi}\sin\frac{\pi\ell}{L}\right) + c_1' - F_1'(\ell/L) + o(L) \ , \quad (20)$$

where $F_1'(x)$ is given by (4). We note that both (19) and (20) apply also to certain excited states in spin chains [15]. For small x, we have $(F_1(x))' = \pi^2x^2/3 + O(x^4)$ in agreement with the general result in [14].

Comparison with numerical results. We performed extensive DMRG [19] computations of the periodic quarter-filled

Hubbard model by keeping $M = 3000$ states in order to achieve satisfactory convergence for periodic systems up to length $L = 64$. For small values of $U \lesssim t$ we find good agreement for both S_1 and S_2 with the predictions (20) and (16). A representative example is shown in Fig. 2. As expected the agreement with the CFT prediction is best for large block lengths $\ell \sim L/2$ and becomes poor for small ℓ, when lattice effects become important. In this region S_2 furthermore exhibits strong oscillatory behaviour as expected [10]. For larger values of $U \gtrsim t$ the agreement with the CFT predictions for both S_1 and S_2 becomes increasingly poor. We now turn to the origin of these discrepancies.

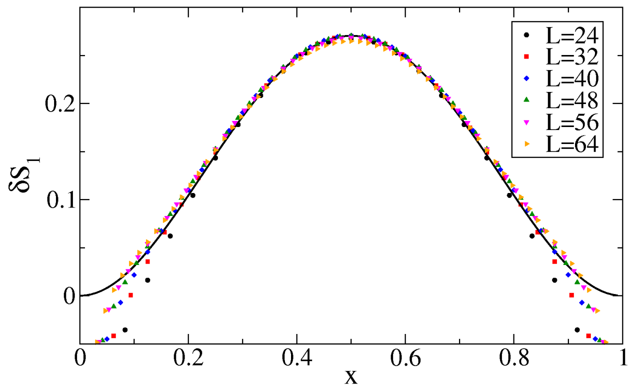

FIG. 2: $\delta S_1 \equiv S_1 - \frac{2}{3}\ln\left[\frac{L}{\pi}\sin\left(\frac{\pi\ell}{L}\right)\right] - c_1'$ as a function of $x = \ell/L$ for $U = 0.3t$ and $L = 24, 32, 40, 48, 56, 64$. The constant $c_1' = 1.205$ has been adjusted by hand. The solid curve is $-F_1'(x)$.

Effects of the marginal perturbation. It is well know that in the Hubbard model the low-energy Luttinger liquid Hamiltonian (10) is perturbed by a marginally irrelevant operator in the spin sector [12]. This leads to logarithmic corrections [20], which can be quite important for small system sizes. The effects of a marginal perturbation on the ground state entanglement in CFTs was studied in [21]. These corrections are small for the isotropic Heisenberg chain [22] as well as the Hubbard model for $L = 4 \bmod 8$. However, the effects of the marginal perturbation on the shell-filling effect are quite large already for moderate values of $U \gtrsim 2t$. In order to quantify them, we have considered an extended Hubbard model

$$H_{\rm ext} = H_{\rm Hubb} + V_2 \sum_{j,\sigma,\sigma'} n_{j,\sigma} n_{j+2,\sigma'} . \qquad (21)$$

At weak coupling the main effect of V_2 is to reduce the bare coupling constant of the marginal perturbation (see [23] for a similar application of this idea). We note that a nearest-neighbour density-density interaction would be ineffective at quarter filling and weak coupling [24]. We find that increasing V_2 from zero leads to a significant improvement in the agreement between the CFT prediction (20), (16) for the shell-filling effect for the available system sizes $L \leq 64$.

Conclusions. We have described a novel shell-filling effect in entanglement entropies of the 1D quarter-filled Hubbard model with periodic boundary conditions. We have verified that the effect occurs, as expected, also at other fillings and in extended Hubbard models. We have developed a CFT approach to calculate the additional contribution to the Rényi entropies, and found good agreement with numerical computations. The effect, while somewhat unexpected, has a simple origin: for certain ratios of lattice lengths to particle numbers in multi-component systems, the ground state cannot be thought of in terms of a product of Fermi seas (in general these will consist of appropriate elementary excitations), but is in fact a linear combination of different such seas. This suggests similarities with the results obtained [25, 26] for the entanglement of linear combinations of degenerate ground states. However, in our case the ground state is unique for $U > 0$ (and fixed $S^z = 0$) and is thus not based on a degeneracy. We expect shell-filling effects to exist for multi-component continuum or lattice models of interacting fermions or Fermi-Bose mixtures, as well as in higher dimensional critical systems. Examples of the former include multi-component gases with delta-function interactions [27], (extended) repulsive SU(N) Hubbard or tJ models [28]. Finally, we believe that shell-filling effects can play a role in numerical studies of two-dimensional gapless spin liquids, which display a spinon Fermi surface [29–31].

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