Shell-Filling Effect in the Entanglement Entropies of Spinful Fermions

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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 $L = 4 \text{ mod } 8$ the results are in agreement with expectations based on conformal field theory, while for $L = 0 \text{ mod } 8$ 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 $|\text{GS}\rangle$ of a finite, periodic 1D system of length $L$ and partition the latter into a finite block $A$ of length $\ell$ and its complement $\bar{A}$. The density matrix of the entire system is then $\rho = |\text{GS}\rangle \langle \text{GS}|$, and we will denote the reduced density matrix of block $A$ by $\rho_A$. Widely used measures of entanglement are the Rényi entropies

$$S_n = \frac{1}{1-n} \ln \text{Tr} \rho^n_A .$$

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

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

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

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

where $c_{j,\sigma}^\dagger$ are fermionic spin-$\frac{1}{2}$ creation operators at site $j$ with spin $\sigma = \uparrow, \downarrow$, $n_{j,\sigma} = c_{j,\sigma}^\dagger c_{j,\sigma}$, 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 $L$. The data is seen to collapse on two curves, with only the lower one following the CFT result (2). Interestingly, both the $L = 4 \text{ mod } 8$ and the $L = 0 \text{ mod } 8$ data exhibit scaling collapse, but to different functions. We stress that this

![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 $L = 4 \text{ mod } 8$ and $L = 0 \text{ mod } 8$ respectively.](image-url)
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 \(L = 4 \mod 8\) and \(L = 0 \mod 8\), 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-\(\sigma\) fermion, and the unique ground state is the symmetric Fermi sea

\[
|2n + 1\rangle_{FS} = \prod_{m=-n}^{n} c^\dagger_m(p_m)c^\dagger_{-m}(p_m)|0\rangle ,
\]

where \(c^\dagger_m(k) = L^{-1/2} \sum_{j=1}^{L} e^{-i k j} c^\dagger_{j,m}\) 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)

\[
|\sigma\rangle = \frac{1}{\sqrt{2}} (c^\dagger_{k_F}(k_F)c^\dagger_{-k_F}(k_F) + \sigma c^\dagger_{k_F}(k_F)c^\dagger_{-k_F}(k_F))|2n - 1\rangle_{FS} .
\]

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 \(L = 4 \mod 8\) the ground state is a symmetrically filled Fermi sea, while for \(L = 0 \mod 8\) 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.

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 \[8\] \[16\]

\[
k_jL = 2\pi I_j - \sum_{\alpha=1}^{N_\uparrow} \theta \left( \frac{\sin k_j - \Lambda_\alpha}{u} \right), \quad j = 1, \ldots, N, \]

\[
\sum_{j=1}^{N} \theta \left( \frac{\Lambda_\alpha - \sin k_j}{u} \right) = 2\pi J_\alpha + \sum_{\beta=1}^{N_\downarrow} \theta \left( \frac{\Lambda_\alpha - \Lambda_\beta}{2u} \right), \quad \alpha = 1, \ldots, N_\downarrow .
\]

Here \(u = U / (4t)\), \(\theta(x) = 2 \arctan(x)\) and \(N = N_\uparrow + N_\downarrow\). For real solutions of the BA equations \[6\], the “quantum numbers” \(I_j\) (\(J_\alpha\)) are integers if \(N_\uparrow\) (\(N_\downarrow\)) 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

\[
P = \sum_{j=1}^{N} k_j, \quad \text{while the energy (in units of } t\text{) is given by}
\]

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

where \(\mu\) is the chemical potential. Following Ref. \[17\], we define regular BA states as eigenstates of Eq. \[5\] arising from solutions of \[6\] with \(2N_\uparrow \leq N\), where all \(k_j\) and \(\Lambda_\alpha\) are finite. We denote these states by \(|\{I_j\}; \{J_\alpha\}\rangle_{\text{reg}}\). 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 \[13\], and a complete set of energy eigenstates is obtained by acting on them with the SO(4) raising operators. For \(L = 4 \mod 8\) it is known \[8\] \[16\] that the quarter filled ground state is a regular BA state characterized by the choice \(I_j = -2n - \frac{3}{2} + j\). For \(L = 8n (n \text{ a positive integer})\), we find that there are two degenerate lowest energy regular, real solutions of \[6\] with \(N_\uparrow = N\downarrow = 2n\) fermions. They are obtained by the two choices \(J_\alpha^{(1,2)} = -n - \frac{1}{2} + \alpha\) and \(J_\alpha^{(3)} = -2n + j\). For \(L = 8n\), 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 \(\Lambda_\alpha\)’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 \(J_\alpha^{(0)} = -2n - \frac{1}{2} + j\). Crucially, the state

\[
S^- |\{J_\alpha^{(0)}\}; \{J_\alpha^{(0)}\}\rangle_{\text{reg}},
\]

is a (non-regular) eigenstate of the Hubbard Hamiltonian with \(N_\uparrow = N\downarrow = L / 8\) fermions. Here \(S^- = \sum_{j=1}^{L} c^\dagger_{j,\uparrow} c^\dagger_{j,\downarrow}\) is the spin lowering operator. As \([S^-, H] = 0\) its energy is the same as that of the regular BA state \(|\{J_\alpha^{(0)}\}; \{J_\alpha^{(0)}\}\rangle_{\text{reg}}\). The energy difference between \[8\] 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 \[8\] 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 \[12\]

\[
H = \sum_{\alpha=c,s} \frac{\nu_\alpha}{2} \int dx \left[ (\partial_x \Phi_\alpha)^2 + (\partial_x \Theta_\alpha)^2 \right],
\]

where \(\nu_{c,s}\) are the velocities of the collective charge and spin degrees of freedom. For \(L = 0 \mod 8\) the mode expansions
of the canonical Bose fields $\Phi_a = \varphi_a + \bar{\varphi}_a$, and their dual fields $\Theta_a = \varphi_a - \bar{\varphi}_a$ follow from

$$
\varphi_a(x, t) = \tilde{P}_a + \frac{x}{L a_0} \tilde{Q}_a + \sum_{n=1}^\infty e^{\frac{i2\pi n}{4\pi} x} a_{a,n} + \text{h.c.},
$$

$$
\bar{\varphi}_a(x, t) = \tilde{P}_a + \frac{x}{L a_0} \tilde{Q}_a + \sum_{n=1}^\infty e^{\frac{i2\pi n}{4\pi} x} a_{\bar{a},n} + \text{h.c.},
$$

where $x = x + vt$ and $a_0$ is the lattice spacing. The structure of the ground state for $L = 0 \mod 8$ is encoded in the zero modes, which have commutations relations $[\tilde{P}_{a}, \tilde{Q}_{a}] = -\tilde{P}_a = -\tilde{Q}_a$. The eigenvalues of $Q_a$ are

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

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

$$
H = \sum_{a = c, s} \tilde{P}_{a} + \sum_{\sigma = \uparrow, \downarrow} (K_c + 1)m_\sigma + (1 - K_c)\bar{m}_\sigma, \\
\sum_{n=1}^\infty 2\pi n (a_{a,n}a_{a,n} + \bar{a}_{a,n}\bar{a}_{a,n}).
$$

There are two degenerate ground states

$$
|\pm\rangle = \frac{1}{\sqrt{2}} \left[ |1, 0; 0, 1\rangle \pm |0, 1; 1, 0\rangle \right],
$$

where we have introduced a notation $|m_\uparrow, m_\downarrow; \bar{m}_\uparrow, \bar{m}_\downarrow\rangle$ for states that are annihilated by all $a_{a,n}, \bar{a}_{a,n}$ and have eigenvalues $q_a(m_\uparrow, m_\downarrow)$ and $q_{\bar{a}}(\bar{m}_\uparrow, \bar{m}_\downarrow)$ of the zero mode operators $Q_a$ and $\bar{Q}_a$ 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 $|+\rangle$. Carrying out the usual conformal map from the cylinder to the plane, we can express this state in radial quantization as

$$
|+\rangle \propto \lim_{\tilde{z} \rightarrow 0} \cos \left( \sqrt{2\pi}\Phi_a(z, \tilde{z}) \right) |0\rangle,
$$

where $|0\rangle$ is the vacuum state of the free boson theory on the plane and $z = \exp(\frac{2\pi}{L a_0}(vt - ix))$, $\tilde{z} = \exp(\frac{2\pi}{L a_0}(vt + ix))$. The key result of the above considerations is that in the Luttinger liquid approximation to the Hubbard model, the ground state for $L = 0 \mod 8$ is given by the excited state of the form $O(0, 0)|0\rangle$ is given by

$$
S_n = \frac{c}{6} \left(1 + \frac{1}{n}\right) \ln \left[ \frac{L}{\pi \sin \left( \frac{\pi L}{2} \right)} \right] + c_n',
$$

where $c'$ is an $O$-independent constant, and the scaling functions $F_n(x)$ are given by

$$
\lim_{n \rightarrow \infty} \frac{\ln \left[ \frac{F_{n}(x)}{\langle O(x) \rangle} \right]}{n} = \frac{2\sin(\pi x)}{\pi n} \langle O(x) \rangle.
$$

Using that for the Hubbard model $c = 2$ we then obtain a CFT prediction for the shell filling effect by combining equations [14] and [15]. In order to obtain an expression for the von Neumann entropy we need to take the limit $n \rightarrow 1$, which gives

$$
S_1 = \frac{c}{3} \ln \left( \frac{L}{\pi \sin \left( \frac{\pi L}{2} \right)} \right) + c_1' - F_1(x) + o(L),
$$

where

$$
F_1(x) = \ln \left[ 2\sin(\pi x) \right] + \psi \left( \frac{1}{2\sin(\pi x)} \right) + \sin(\pi x).
$$

Here $\psi(x)$ is the digamma function. We note that both [18] and [19] apply also to certain excited states in spin chains. For small $x$, we have $(F_1(x))^2 = \pi x^2/3 + O(x^4)$ 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 [19] and
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 $\ell$, when lattice effects become important. In this region $S_2$ furthermore exhibits strong oscillatory behaviour as expected. For larger values of $U > 0$ (and fixed $S^z = 0$) and is thus not based on a degeneracy. Finally, we expect shell-filling effects to exist for interacting bosons as well as for fermions in one dimension, as well as in higher dimensional critical systems. They can for example play a role in numerical studies of two-dimensional gapless spin liquids, which display a spinon Fermi surface.

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