Entanglement in spatially inhomogeneous many-fermion systems

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We investigate entanglement of strongly interacting fermions in spatially inhomogeneous environments. To quantify entanglement in the presence of spatial inhomogeneity, we propose a local-density approximation (LDA) to the entanglement entropy, and a nested LDA scheme to evaluate the entanglement entropy on inhomogeneous density profiles. These ideas are applied to models of electrons in superlattice structures with different modulation patterns, electrons in a metallic wire in the presence of impurities, and phase-separated states in harmonically confined many-fermion systems, such as electrons in quantum dots and atoms in optical traps. We find that the entanglement entropy of inhomogeneous systems is strikingly different from that of homogeneous systems.

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An intense interdisciplinary research effort is currently directed at analyzing entanglement in a wide variety of physical systems. Apart from the intrinsic interest in entanglement as one of the most counterintuitive predictions of quantum mechanics, this research effort is largely motivated by the prospect of simulating or exploiting entanglements of quantum mechanics, this research effort is largely motivated by the prospect of simulating or exploiting entanglement in physical systems. Apart from the intrinsic interest in 

\[ \rho = \int dx \rho(x) \]

In the following, we make the realistic assumption that \( \rho \) or \( \mathcal{E} \) can be calculated, at least approximately, for a spatially uniform system, such as a lattice in which all sites are equivalent, or a uniform continuum system without boundaries. In such spatially homogeneous systems, the density \( n \) reduces to a constant, and the functional \( \mathcal{E}[n(x)] \) becomes the function \( \mathcal{E}_{\text{hom}}(n) \). Our aim is to develop a simple, yet reliable, approximation scheme for obtaining the ground-state entanglement entropy of inhomogeneous systems, \( \mathcal{E}[n(x)] \).

To this end we propose the local-density approximation

\[ \mathcal{E}[n(x)] \approx \mathcal{E}_{\text{LDA}}[n(x)] = \int dx \mathcal{E}_{\text{hom}}(n_{n-1:n}(x)), \]

in which the functional \( \mathcal{E}[n(x)] \) is approximated by evaluating the per-site entropy of the homogeneous system, \( \mathcal{E}_{\text{hom}}(n) \) at the density distribution of the inhomogeneous system. This local-density approximation (LDA) for the entanglement entropy is inspired by the LDA made in density-functional theory (DFT) for the exchange-correlation energy \( \mathcal{E}^0 \). There is also a conceptual relation to the LDA for the thermodynamic entropy made in classical DFT of inhomogeneous liquids \( \mathcal{E}^0 \) and in DFT for thermal ensembles \( \mathcal{E}^0 \).

Clearly, the LDA for the entanglement entropy is a general concept, applicable to a wide variety of systems, but to be specific, and to compare to previous work, we here consider interacting fermions on a lattice, described by the Hubbard model,

\[ \hat{H} = -t \sum_{i,\sigma} (c_{i\sigma}^\dagger c_{i+1,\sigma} + H.c.) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_{i,\sigma} v_i \hat{n}_{i\sigma} \]

where \( \hat{n}_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma} \), with \( \sigma = \uparrow, \downarrow \), is the local density operator expressed in terms of fermionic creation and annihilation operators, \( U \) is the on-site interaction, \( t \) the inter-site hopping (below taken to be the unit of energy), and \( v_i \) represents external electric and magnetic fields. Inclusion of this last term makes the model inhomogeneous. The HK theorem guarantees that the global density distribution \( n = n_1, \ldots, n_L \) determines the ground-state wave function of the inhomogeneous \( L \)-site model.

The homogeneous Hubbard model \( (v_i = 0) \) accounts, approximately, for spin and charge degrees of freedom,
for the itinerancy of the charge carriers, and for their interactions. Its rich phase diagram and nontrivial physics, together with the available exact solution in one dimension, has attracted much interest also in the quantum information community. In particular, several groups investigated entanglement measures for the Hubbard model (see, e.g., Refs. [7, 8, 13] and references therein). As a result, the single-site entanglement entropy (in which subsystem $A$ is one site) of the homogeneous Hubbard model in one dimension is known analytically [7, 8, 13]:

$$\mathcal{E}^{\text{hom}}(n, U) = -2 \left( \frac{n}{2} - \frac{\partial e}{\partial U} \right) \log_2 \left[ \frac{n}{2} - \frac{\partial e}{\partial U} \right] - \left( 1 - n + \frac{\partial e}{\partial U} \right) \log_2 \left[ 1 - n + \frac{\partial e}{\partial U} \right] - \frac{\partial e}{\partial U} \log_2 \left[ \frac{\partial e}{\partial U} \right]. \quad (3)$$

Here $\mathcal{E}^{\text{hom}}(n, U)$ is the single-site entanglement entropy (Shannon-von Neumann entropy of four probabilities) per site, and $e = E(n, U)/L$ is the ground-state energy per site, both as functions of interaction strength $U$ and particle density $n = N/L$, where $N$ and $L$ are the total number of particles and lattice sites, respectively. Since $e(n, U)$ can be obtained [14, 15] from the Bethe-Ansatz integral equations, Eq. (3) can be used to extract detailed quantitative information about entanglement in various phases and at the transitions between them [7, 8, 13]. However, this expression is valid only for the homogeneous Hubbard model, i.e., one in which all sites are equivalent. Such idealization is most useful for analytical and numerical work, but provides only a rather imperfect picture of the physical situation in real solids or devices.

To make use of expression (3) for the entanglement entropy of homogeneous Hubbard models also in inhomogeneous situations, we apply the local-density approximation [1] in the form

$$\mathcal{E}[n_i, U] \approx \mathcal{E}^{\text{LDA}}[n_i, U] = \sum_i \mathcal{E}^{\text{hom}}(n_i, U)[n_i \rightarrow n_i]. \quad (4)$$

For a given distribution $n_i$ of particles over sites, Eq. (4) can be evaluated immediately. If, on the other hand, this distribution is not known, it must be obtained in a separate calculation. This is the case, e.g., if the system is specified by giving the potential the particles move in, instead of the spatial distribution of particles. Experimentally, specifying the potential is more realistic, and we thus focus on this case.

To obtain the ground-state charge and spin densities for a given external potential, we again appeal to density-functional theory, this time employing the LDA in its standard formulation [8, 11], i.e., as an approximation to
the exchange-correlation energy that is to be added to the mean-field energy functional. Minimization with respect to $n(x)$ then yields the ground-state energy and ground-state density profile. Specifically for the Hubbard model, we use the Bethe-Ansatz LDA (BA-LDA) of Refs. [14, 15]. The combined calculation is thus a nested LDA, where BA-LDA is used to generate self-consistent density profiles, and the entropy LDA (1) is used to predict the entropy on the resulting inhomogeneous density distribution.

Both BA-LDA and entropy LDA by construction become exact for a spatially uniform system. BA-LDA has been shown by comparison to Monte Carlo, Bethe Ansatz, and density-matrix renormalization group data to provide density profiles that agree within a few percent with those of other many-body methods, even for systems far from the uniform limit [14, 15, 16]. To quantify the reliability of the entropy LDA, we turn to small finite chains, which are far from the uniform limit, but for which the exact density matrix $\rho$ can be obtained by full numerical diagonalization of the Hamiltonian, so that the exact entanglement entropy $\mathcal{E}$ is known. Since small systems are a worst-case scenario for LDAs (which derive from the thermodynamic limit), this is a particularly severe test for the entropy LDA and nested LDA concepts.

Panel (a) of Fig. 1 displays the site-resolved entanglement entropy of an open chain chain with an impurity at the central site. Exact data are obtained by numerically diagonalizing the many-body Hamiltonian (2) and constructing the density matrix and the entanglement entropy from the exact eigenfunctions. This process also yields the exact density profile, which we use to evaluate the function $\mathcal{E}^{\text{hom}}(n,U)$ entering the entropy LDA, Eq. (1). The deviation between both sets of data measures the quality of the entropy LDA. In a separate calculation, we also generate BA-LDA density profiles [14, 15, 16], and evaluate $\mathcal{E}^{\text{hom}}(n,U)$ on them. This results in the nested LDA procedure, which can also be applied where the exact solution is not available. As the figure shows, all three approaches agree closely, too within 1%, even far away from the limit in which LDAs become exact.

Having established the viability and reliability of the LDA for the entanglement entropy and of the nested LDA, we now turn to further experimentally relevant inhomogeneous systems. First, we investigate the effect a spatial modulation of system properties, in the form of a superlattice, has on the entanglement. Naturally occurring or man-made systems displaying spatial modulations of their properties on a nanoscale are important both as paradigms of simple nanotechnological devices, and as particular examples of emerging spatial inhomogeneity in strongly interacting many-electron systems. To model superlattice structures in the Hubbard model we follow Ref. [16], which, however, did consider only energies, not entropies.

Panel (b) of Fig. 1 displays the behaviour of $\mathcal{E}^{\text{LDA}}(n_i)$ for two representative superlattice structures. According to the nested LDA concept, the data were obtained by first running an ordinary BA-LDA calculation for a fixed distribution of on-site interaction and potentials, in order to generate the densities $n_i$. In a second step the resulting self-consistent density profile is substituted in Eq. (1), in order to obtain $\mathcal{E}^{\text{LDA}}(n_i)$, for the specified values of $U_i$ and $v_i$.

Two things leap to the eye in Fig. 1(b): First, the larger the amplitude of the modulation, the less entangled the system becomes. Indeed, the spatial inhomogeneity of the superlattice is expected to disrupt the entanglement present between itinerant charge carriers in the homogeneous system. Second, modulations in the on-site potential have a much more drastic effect on the entanglement entropy than those of the on-site interaction. Clearly, local fluctuations in the potential disentangle the system much more efficiently than local fluctuations in the interaction. This is consistent with what was previously [16] observed for the ground-state energy, and again points to the importance of local electric fields in strongly correlated systems [14]. It also means that local electric fields are rather effective in reducing the degree of entanglement between itinerant charge carriers.

Next, we turn to impurity systems. Specifically, we inquire what effect a local impurity potential has on the entanglement between itinerant electrons. We model the impurity as $v_i = v_I \delta_{i,I} [\nu, \mathcal{E}]$, i.e., place a local electric potential on the central site of the L-site chain. Panel (c) of Fig. 1 shows that both for attractive ($v_I < 0$) and repulsive ($v_I > 0$) impurities, entanglement between the itinerant particles is diminished, but by a much smaller margin than in the superlattice case, where the potential is periodically repeated instead of acting on just one site. Stronger on-site interactions $U$ tend to freeze the density distribution and thus reduce the number of degrees of freedom, which lowers the entanglement entropy, as discussed for homogeneous systems in Ref. [14]. For small $U$, attractive impurities are more efficient in disrupting itinerant entanglement than repulsive ones, but this difference disappears for larger $U$. For attractive impurities, we observe a flat structure at small negative values of $v_I$. For these values, the average density of the impurity site remains fixed at $n_I = 1$, which means that the strenght of the impurity potential (which couples to the density) becomes irrelevant, until it increases enough to draw more than one particle to the impurity site, at which point the frozen site again becomes available as a degree of freedom and $\mathcal{E}$ is slightly increased. This freezing of the density distribution at $n = 1$ is a strong-interaction effect (it vanishes for $U = 0$), similar to the Mott insulator in solids, and to Coulomb blockade in quantum dots [18, 19], and to the density plateaus in our next example.

Finally, we consider harmonically confined fermions,
such as electrons in a quantum dot [13] or fermionic atoms in an optical trap [20]. Figure 2 displays the entanglement entropy and its derivative as a function of curvature of the trapping potential. Increasing confinement diminishes entanglement of the confined particles, but not in a uniform way. As the curvature becomes larger, the system passes through several states with distinct density profiles (see insets), whose nature has been clarified elsewhere [13, 21]. Interestingly, each transition corresponds to distinctive features in the entanglement entropy, many of which are more clearly visible in its derivative: the switching on of the confining potential leads to an initial drop in entanglement, a spike in the derivative signals the appearance of a Mott insulating region in the trap center, a smaller peak indicates ressurection of a metal-like region in the center, and another broad peak is associated with formation of a band-insulating state at the trap center. The entanglement entropy can thus be used as a tool for characterization of the various possible states, even though these are not phases in the thermodynamic sense.

On the other hand, it also becomes clear that the actual value of $\mathcal{E}$, and its variation with system parameters, depend in a highly nontrivial way on fine details of the system. This dependence is a severe obstacle for attempts to quantify and exploit entanglement in real-life environments. Note that this issue is conceptually distinct from the more commonly discussed problems due to decoherence, which also occurs in spatially homogeneous situations.

In summary, we find that for all types of inhomogeneity investigated here — superlattice structures with different modulation patterns, itinerant electrons in a metallic wire in the presence of impurities, and phase-separated states in harmonically confined many-fermion systems — the entanglement entropy of inhomogeneous systems is strikingly different from that of homogeneous systems. The influence of spatial inhomogeneity is an essential aspect of entanglement in real systems, which cannot be simulated or understood by approaches based exclusively on uniform systems. This influence must be understood and quantified if entanglement is to be used as a resource for performing quantum information processing in actual devices. The entropy LDA and the nested LDA concept, proposed here, may be useful tools for this investigation.

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and mean-field (i.e., Hartree) energies of an unpolarized system can be written as $\sum [v_{\text{ext},i} + (U_i/4)n_i]n_i$. Since $n_i \leq 1$, the term carrying the modulation in $U_i$ is suppressed relative to the modulated potential by a factor $\approx 4 - 12$.

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