Entanglement enhancement in spatially inhomogeneous many-body systems

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We investigate the effects of spatial inhomogeneities on the entanglement of modes of strongly correlated systems in the framework of small Fermi-Hubbard chains. We find regimes where entanglement is strongly enhanced by the presence of inhomogeneities. This contrasts recent reports of entanglement destruction due to inhomogeneities. We further study this phenomenon using concepts of Density Functional Theory and, thus, provide a general recipe for the prediction of entanglement enhancement in nanostructures. We find enhancement of up to ∼27%, as compared to impurity-free chains.

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I. INTRODUCTION

Nanoscale spatial inhomogeneities are ubiquitous in strongly correlated systems. Either naturally occurring, as in disordered media, or artificially prepared in nanostructures and ultracold atoms, spatial inhomogeneity can influence optical, electrical, magnetic, transport and entanglement properties [1–17]. Therefore, it is of great fundamental and technological interest.

The impact of spatial inhomogeneities on entanglement, which is a key ingredient in quantum information theory, has been investigated in spin chains, Kondo and Hubbard models [12–19]. The main goal is the development of solid-state devices for quantum information processing [13 20], for which accessing high degrees of entanglement, despite the inhomogeneities, is essential. For the important case of the inhomogeneous 1D fermionic Hubbard model, the entanglement of modes [21 22] or occupation-number entanglement has been studied. In this case, the ground-state entanglement between two sections (or subsystems) of the chain is quantified by the von Neumann entropy (see Eq. (2) below). The influence of several types of inhomogeneities was analyzed: localized impurities and superlattice structures [17], harmonic traps [17–19] and disorder [12]. Although entanglement depends on the specific inhomogeneous component of the potential, the effect of inhomogeneities was, remarkably, found to be qualitatively the same in all cases: entanglement decreases.

All those studies focused, however, on the entanglement between a single site – the smallest possible subsystem – and the remaining lattice sites. The scaling relations from the single-site entanglement to the entanglement of larger subsystems, called block entanglement, have been extensively explored from the statistical point of view [23 29]. Nevertheless, it is still a fundamental open question whether the block entanglement is also destroyed by spatial inhomogeneities. Furthermore, from the viewpoint of realistic applications, it is crucial to build a detailed characterization of the regimes, at which entanglement is strong regardless of unavoidable inhomogeneities.

In this paper, we address this issue by investigating the block entanglement of small 1D Fermi-Hubbard chains, where the inhomogeneity is induced by an external potential, simulating either localized impurities or superlattice structures. We find that entanglement is not always destroyed: there are regimes where it can be even enhanced by the presence of inhomogeneities. We explore the physics behind this phenomenon from the perspective of Density Functional Theory, and estimate the optimally achievable entanglement enhancement under rather general conditions. Applying our approach to several superlattices, we predict entanglement enhancement of up to ∼27% as compared to the homogeneous case.

The 1D inhomogeneous Hubbard model is given by [30]

$$\hat{H} = -t \sum_{<ij>,\sigma} \hat{c}^\dagger_{i\sigma} \hat{c}_{j\sigma} + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow} + \sum_i V_i \hat{n}_{i\uparrow}, \quad (1)$$

with on-site repulsion \(U\) and repulsive impurities of strength \(V_i\), which will both measure in units of the tunneling strength \(t\) between adjacent sites. We adopt balanced populations (\(N_\uparrow = N_\downarrow\)), where \(N = N_\uparrow + N_\downarrow\) is the total number of particles, \(L\) the lattice size, and \(n = N/L\) the filling factor. The ground-state entanglement between a block of \(x\) lattice sites and the remaining \(L - x\) sites is quantified by the von Neumann entropy

$$S_x = -\text{Tr}[\rho_x \log_2 \rho_x], \quad (2)$$

where \(\rho_x = \text{Tr}_{(L-x)}[\rho]\) is the reduced density matrix, and \(\rho\), which is calculated by exact Lanczos diagonalization, is the ground state’s total density matrix.

To set the stage, let us recall the general properties of the entanglement as defined by \(S_x\): The latter depends on the degree of purity of the reduced density matrix, when it is pure (\(\rho_x = |\psi_x\rangle \langle \psi_x|\)), \(S_x = 0\); and the more mixed \(\rho_x\), the greater \(S_x\). That means entanglement vanishes whenever one of the possible states (in the reduced sys-
The block entanglement is addressed from three distinct perspectives. We consider the entanglement \( i \) between impurities and the remaining sites, the so-called impurity entanglement \([15, 16]\), and \( ii \) between bipartitions containing both impurity and non-impurity sites. We also study \( iii \) the average over all possible bipartitions, which quantifies the overall impact of inhomogeneities (incorporating \( i \) and \( ii \)), particularly important for the treatment of disorder.

Figure 2 shows the results for the single-site entanglement as a function of \( V \). We find that only the impurity entanglement (case \( i \)) vanishes for \( V >> t \), as the reduced density matrix of the impurity sites is pure in this limit (\( \rho = \rho_{imp} = |0\rangle \langle 0| \)). For the average over all possible bipartitions (case \( iii \)), we find that the entanglement decreases with \( V \), but saturates at a finite value, what is consistent with previous observations \([12, 17–19]\). Our results in Fig. 2 reveal that the main contribution to this decrease comes from the impurity entanglement. Surprising, though, is the behavior in the situation when blocks do not coincide with impurity sites (case \( ii \)), as can be seen in more detail in the inset of Fig. 2. In this case, the degree of entanglement is not reduced. On the contrary, it is even enhanced by \( V > 0 \). We study this interesting entanglement enhancement based on a Density...
FIG. 4. (Color online) Block entanglement as a function of the impurity strength \( V/t \) for (a) \( x = 2 \), (b) \( x = 3 \) and (c) \( x = 4 \), at different distances \( d \) and symmetrically (sym) or asymmetrically (asym) distributed impurities (also see Fig. 1). (d) Average over all possible bipartitions. \( L = 10, N = 6, U = 4t \) and periodic boundary conditions.

Functional Theory (DFT) \([32,34]\) point of view.

Within DFT, all observables are functionals of the single-particle density \( n(r) \) of the many-body interacting system. Unfortunately, the explicit form of the density functional of a given physical entity is, in general, unknown. However, for homogeneous Hubbard chains, where all the sites are equivalent (\( n(r) = n \)), the density functional for the single-site entanglement is exactly obtained from a Bethe-Ansatz solution \([31]\). One finds a broad regime of densities (\( n \lesssim 0.8 \) for \( U > 0 \)) where the entanglement monotonically grows with density. For inhomogeneous systems, which have by definition site-dependent densities (\( n(r) = \{n_i\} \)), it has been proven that the homogeneous functional is a good approximation for the single-site entanglement, within a local density approximation (LDA) replacing \( n \to n_i \) \([12,17,35]\). Consequently, the inhomogeneous single-site entanglement varies with density as in the homogeneous case \([31]\): monotonically increasing with density for \( n_i \lesssim 0.8 \).

This is precisely the mechanism behind the entanglement enhancement observed in Fig. 2: the particles are repelled from the impurities, inducing a larger effective density at the remaining \( L - 2 \) sites (\( n^{\text{eff}} = N/(L-2) > n \)), which thus leads to higher entanglement, by virtue of the above DFT argument \([36]\). This can be verified at strong impurity strengths, where the impurities represent physical boundaries and therefore mimic an effective system with open boundary conditions. In Figure 3a, we compare the density profiles of such effective chains to our original model with impurity strength \( V = 8t \): the very good agreement confirms our interpretation.

There are some additional features in Fig. 2 which necessitate some refinement of our above LDA argument. To start with, the entanglement of blocks \( d = 0 \) and \( d = 1 \) differs by \( \sim 6\% \) at \( V = 8t \) (inset of Fig. 2), while the difference between their densities is negligible (Fig. 3a). Furthermore, block \( d = 2 \) has the smallest density among the non-impurity blocks (Fig. 3a), but it does not exhibit the weakest entanglement (Fig. 2). The most curious feature occurs for the block at \( d = 0 \): its entanglement behaves as the other \( d > 0 \) blocks only for very small values of \( V \) and then decreases considerably (see inset of Fig. 2). All these features of the \( d \)-dependence of entanglement ought to be encoded, at least in principle, in the exact density functional for the entanglement, which is a highly nontrivial function of \( \{n_i\} \).

The simplest possible functional beyond LDA is to assume that the block entanglement is not only determined by the block density itself, but is also affected by the density at its border sites, i.e., at the outmost sites of the complementing block \( L - x \), in accord with the area law concept \([37]\). In our case, the boundary surface is fixed,
FIG. 5. (Color online) Entanglement for several superlattice structures for \(x = 3\) and \(x = 4\): SL\([a, \alpha, b, \beta]\) with period \([a, \alpha, b, \beta]\) where \(a, b\) are sequences of sites (layers) with \(V_i = V\), while \(\alpha, \beta\) are layers with \(V_i = 0\) (for instance, the unit cell for SL\([1, 1, 2, 2]\) and SL\([1, 2]\) are \([V0V0V0]\) and \([V00]\), respectively). In all cases the lattice parameters are \(U = 4t\), \(V = 8t\) and periodic boundary conditions. The entanglement enhancement is relative to the homogeneous chain \((V = 0\) for all sites) of same length \(L\). The upper data set ("SL\([1, 2]\)") is obtained from DMRG calculations for \(L = 36\), while all others from Lanczos diagonalization for \(L = 12\).

but weighted by the local particle density. Thus, incorporating the boundary density into our above relation between entanglement and local density, we conclude that the larger the interface density (up to \(\sim 0.8\)), the larger its contribution to block entanglement.

This simple, interface-density amended LDA approach is already enough to recover qualitatively all features of Fig. 2. In particular, it explains the special behavior at \(d = 0\): one of the border sites contribution is suppressed \((n_4 \sim 0\), see Fig. 3a\)), such that the entanglement saturates at a smaller value compared to all the other \(d > 0\) cases, in which both border sites (with non-vanishing densities) contribute to entanglement.

Extending this analysis to \(x > 1\), we can now infer which block exhibits the maximum entanglement enhancement for a given block size \(x\). Figure 3b indicates the blocks with optimal entanglement enhancement for our case with 2 impurities. Figure 4 confirms this expectation: The blocks with optimal entanglement enhancement are those with the highest interface density. Qualitatively all the features observed at \(x = 1\) are seen again for \(x > 1\) (except that, for \(x > 2\), as the block is larger than the number of impurities available, the impurity-entanglement scenario is not defined), but the precise scaling relation from \(x = 1\) to larger \(x\) remains non-trivial and unknown. The behavior of the average block entanglement (perspective iii), however, is similar for all \(x\), as Figure 4d shows. This average quantity contains less details, consequently, simpler scaling properties than each particular bipartition.

FIG. 6. (Color online) Entanglement enhancement in the superlattice structure SL\([1, 4, 3, 4]\) (with unit cell \([V000V0V000]\)) for block sizes \(x = 3\) and \(x = 4\) optimally located (as proposed in Fig.3): (a) as a function of the SL potential \(V/t\), for a fixed interaction \(U = 4t\); and (b) as a function of the interaction strength \(U/t\), for a fixed potential \(V = 8t\). In all cases the lattice size is \(L = 12\), with periodic boundary conditions, and the entanglement enhancement is relative to the homogeneous chain \((V = 0\) for all sites).

### III. SUPERLATTICE STRUCTURES

We now apply the general features of optimal entanglement enhancement to superlattices (SL) [1]. Here, we consider SL structures as defined by a periodic modulation of \(V_i\). From our previous analysis, one expects substantial entanglement enhancement in superlattices, whenever block and remainder are composed by border sites with \(V = 0\) and inner sites with \(V > 0\) (similar to the \(x = 4\) case, Fig. 3b).

Figure 5 shows the SL entanglement for blocks with this specific configuration in several distinct SL structures. We find entanglement enhancement for all cases in which the effective density \((n_{\text{eff}} = N/(L - I)\), \(I\) the total number of impurities) is larger than \(n\) (up to \(n_{\text{eff}} \sim 0.8\)), consistently with the localized impurities results. Remarkable though is the much higher relative enhancement: entanglement up to 27% larger than in the impurity-free system is observed.

The absolute entanglement values in SL are, in some cases, even higher than the maximum homogeneous en-

\[\frac{\text{Enhancement}}{\text{Homogeneous}}\]
tanglement one can achieve by properly adjusting the parameters, as predicted by Eq. (3) \( S_{\text{hom}}(x = 3) = 3.06 \) and \( S_{\text{hom}}(x = 4) = 3.33 \). This certainly encourages the manipulation of nanostructures towards progress in quantum information devices.

By using Density Matrix Renormalization Group (DMRG) techniques [35] we have also considered a few SL entanglement of larger periodic chains (up to \( L = 36 \)). We find that the impact of \( L \) on the entanglement enhancement is weak, as can be seen in Fig. 5, by comparing SL[1, 2] (for \( L = 12 \)) and *SL[1, 2] (for \( L = 36 \)).

We also analyze the enhancement as a function of \( U \) and \( V \), as shown in Figure 6. For \( V >> U \), the enhancement is guaranteed for any \( U \) and \( V \) whenever the densities \( n \) and \( n_{\text{eff}} \) are smaller than 0.8: the further from 0.8, the larger the entanglement enhancement.

In summary, our results demonstrate that spatial inhomogeneities can actually act in favor of entanglement and, accordingly, could be cleverly engineered in solid-state devices for optimal quantum information processes.

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[1] A. Wacker, Phys. Rep. 357, 1 (2002).
[2] V. I. Sankin, A. V. Andrianov, A. O. Zakhar’in, and A. G. Petrov, Appl. Phys. Lett. 100, 111109 (2012).
[3] R. Inoue, K. Muranaga, H. Takayanagi, E. Hanamura, M. Jo, T. Akazaki, and I. Suemune, Phys. Rev. Lett. 106, 157002 (2011).
[4] A. M. Kaiser et al., Phys. Rev. Lett. 107, 116402 (2011).
[5] M. Lubasch, V. Murg, U. Schneider, J. I. Cirac, and M. C. Banuls, Phys. Rev. Lett. 107, 165301 (2011).
[6] S. Trotzky, Yu-Ao Chen, U. Schnorrberger, P. Cheinet, and I. Bloch, Phys. Rev. Lett. 105, 265303 (2010).
[7] M. Valiente, M. Küster and A. Saenz, EPL 92, 100001 (2010).
[8] M. White, M. Pasienski, D. McKay, S. Q. Zhou, D. Ceperley, and B. DeMarco, Phys. Rev. Lett. 102, 055301 (2009).
[9] Oleg V. Yazyev, Phys. Rev. Lett. 101, 037203 (2008).
[10] André L. Malvezzi, Thereza Paiva, and Raimundo R. dos Santos, Phys. Rev. B 66, 064430 (2002).
[11] P. Avouris, Z. H. Chen, and V. Perebeinos, Nature Nanotechnology 2, 605 (2007).
[12] Vivian V. França and Irene D’Amico, Phys. Rev. A 83, 042311 (2011).
[13] A. Wagner, C. Bruder and E. Demler, Phys. Rev. A 84, 063636 (2011).
[14] L. Amico, R. Fazio, A. Osterloh, and V. Vedral, Rev. Mod. Phys. 80, 517 (2008).
[15] I. Affleck, N. Lafforgue, and E.S. Sørensen, J. Phys. A: Math. Theor. 42, 504009 (2009).
[16] E. S. Sørensen, M. S. Chang, N. Lafforgue, and J. Affleck, J. Stat. Mech. P08003 (2007).
[17] V. V. França and K. Capelle, Phys. Rev. Lett. 100, 070403 (2008).
[18] J. P. Coe, V. V. França, and I. D’Amico, EPL 93, 10001 (2011).
[19] J. P. Coe, V. V. França, and I. D’Amico, Phys. Rev. A 81, 052321 (2010).
[20] M. Stoneham, Physics NY 2, 34 (2009).
[21] Paolo Zanardi, Phys. Rev. A 65, 042101 (2002).
[22] Mark R. Dowling, Andrew C. Doherty, and Howard M. Wiseman, Phys. Rev. A 73, 052323 (2006).
[23] J. I. Latorre and A. Riera, J. Phys. A: Math. Theor. 42, 504002 (2009).
[24] P. Calabrese and J. Cardy, J. Phys. A: Math. Theor. 42, 504005 (2009).
[25] S. S. Deng, S. J. Gu, and H. Q. Lin, Phys. Rev. B 74, 045103 (2006).
[26] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. 90, 227902 (2003).
[27] V. E. Korepin, Phys. Rev. Lett. 92, 096402 (2004).
[28] P. Calabrese and J. Cardy, J. Stat. Mech. P06002 (2004).
[29] V. V. França and K. Capelle, Phys. Rev. A 77, 062324 (2008).
[30] J. Hubbard, Proc. Roy. Soc. (London) A 276, 238 (1963).
[31] V. V. França and K. Capelle, Phys. Rev. A 74, 042325 (2006).
[32] W. Kohn, Rev. Mod. Phys. 71, 1253 (1999).
[33] P. Hohenberg and W. Kohn, Phys. Rev. 136, B864 (1964).
[34] E. Runge and E. K. U. Gross, Phys. Rev. Lett. 52, 997 (1984).
[35] J. Silva-Valencia and A. M. C. Souza, Phys. Rev. A 85, 033612 (2012).
[36] For \( V < 0 \) there is no enhancement as the opposite occurs: particles (up to \( 4 \)) accumulate into the impurity sites, inducing a smaller effective density \( n_{\text{eff}} = (N - 4)/(L - 2) < n \).
[37] J. Eisert, M. Cramer, and M. B. Plenio, Rev. Mod. Phys. 82, 277 (2010).
[38] U. Schollwöck, Rev. Mod. Phys. 77, 259 (2005).