Momentum-space analysis of multipartite entanglement at quantum phase transitions

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We investigate entanglement properties at quantum phase transitions (QPTs) of a one-dimensional integrable extended Hubbard model in the momentum-space representation. Two elementary subsystems are recognized: the single mode of an electron and the pair of modes (electrons coupled through the η-pairing mechanism). We first detect the two or multipartite nature of each quantum phase transition by a comparative study of the singularities of Von Neumann entropy and quantum mutual information. We establish the existing relations between the quantum correlations in the momentum representation and the relevant (superconducting) ones exhibited in the complementary picture: the direct-lattice representation. We then investigate the presence of multipartite entanglement in momentum space by means of a generalization of the Meyer-Wallach measure and we relate its behavior to the nature of the various QPTs.

I. INTRODUCTION

The idea of studying and characterizing quantum phase transitions (QPTs) by means of tools and concepts borrowed from the quantum information theory has provided in recent years a significant amount of interesting results.[1] In particular, the notion of entanglement and its measures is of central importance within this framework. Indeed, for several and different models in condensed-matter physics, it has been shown that partial derivatives of appropriate measures of entanglement with respect to the field driving the QPT keep track of the underlying critical phenomenon by developing a singularity.[2–13] Moreover, from an entanglement study of QPTs one can gain further information, such as the order or the scaling exponents, as well as a deeper insight on the structure of the correlations involved.[14]

For instance in Ref. 9 it has been argued how, for an extended Hubbard model, a comparison of the Von Neumann entropy of a single site—a measure of the quantum correlation existing between a site and the rest of the system—with the quantum mutual information—measuring the total correlations between pairs of sites—allows one to infer which kind of correlations plays the prominent role at a given transition. One is thus led to distinguish between the QPTs where the quantum correlations between pairs of sites are more relevant ("two-point QPTs") from those where the multipartite correlations play a more prominent role ("multipartite QPTs"). Such a scheme has been tested in Refs. 13 and 15. In particular in Ref. 13 the two-point QPTs have been investigated by means of punctual measures of two-point quantum correlations. As for the multipartite ones, the analysis becomes harder. In fact, the evaluation of the known direct measures of multipartite correlations[16] requires either some optimization process that often turns out to be in practice unfeasible or the knowledge of the reduced density matrix relative to arbitrarily large subsystems.[1]

Entanglement is, in general, a notion that depends on the choice of the subsystems whose correlations one is interested in analyzing. In particular, one can be interested in the quan-tum correlations existing between two definite subsystems (bipartite entanglement) or one can try to describe the quantum correlations shared by a finite subset of subsystems (multipartite entanglement). Furthermore, the same Hilbert space $\mathcal{H}$ can support different tensor product structures, and thus different choices of subsystems are possible.[17] In describing many-body condensed-matter systems, one is naturally led to consider at least two different structures: the one induced by the real-space topology of the system under consideration, i.e., the *direct-lattice picture*, and the one corresponding to the momentum space, i.e., the *reciprocal-lattice picture*. Although the literature on entanglement in condensed matter has privileged the first description, one expects that the information obtained by the analysis of entanglement properties of elementary subsystems of the direct lattice (subsets of single sites of the ambient lattice) can be fruitfully integrated with that obtained by considering as elementary subsystems the momenta modes of the reciprocal lattice.

In this paper we provide the momentum-space description of the ground-state entanglement properties of the one-dimensional (1D) extended Hubbard model discussed in Refs. 9, 13, and 18. The study in momentum space allows for a different and rich picture of the structure of correlations and of their relations with QPTs. Indeed, the relevance itself of multipartite (multimode) and two-point (two-mode) correlations at a given QPT can significantly vary when the above change of perspective is performed. Furthermore, the comparison of the (quantum) correlations in the momentum and direct-lattice picture turns out to be a fruitful method of analysis. Indeed, this procedure allows one to enlighten the origin of the off-diagonal long-range order (ODLRO) displayed by the ground state for appropriate values of the parameters: This is directly related to the value of negativity between modes k and $-k$.[19]

Moreover, the possibility of determining the reduced density matrices of arbitrary subsystems composed by sets of momentum modes allows one to overcome the above-mentioned difficulties in measuring directly multipartite correlations. We exploit such possibility to compute the gener-

alization of the Meyer-Wallach measure of multipartite entanglement.[20,21] We thus show that by increasing the subsystem size, the partial derivative of Q develops a singularity in correspondence with precisely those QPTs at which the dominant correlations were conjectured to be of multipartite nature.[22]

The paper is organized as follows. In Sec. II we describe the phase diagram of the model under investigation and we introduce the momentum-space description: its ground state in the various phases. In Sec. III we first discuss the general structure of the correlations in the ground state in the whole phase diagram; we related the picture emerging in the momentum space with the one previously obtained in the direct-lattice picture; we discuss the role of the correlations at QPTs; and we evaluate and discuss the Meyer-Wallach measure of multipartite entanglement. In Sec. IV we summarize our conclusions.

II. BOND-CHARGE EXTENDED HUBBARD MODEL

The model we investigate is the one-dimensional bond-charge extended Hubbard model for a particular value of the bond-charge interaction at which the model becomes integrable.[18] In units of the nearest-neighbors hopping amplitude, its Hamiltonian reads

$$H = -\sum_{\langle i,j\rangle\sigma}[1-(n_{i\bar{\sigma}}+n_{j\bar{\sigma}})]c_{i\sigma}^{\dagger}c_{j\sigma}+u\sum_{i}n_{i\uparrow}n_{i\downarrow}, \quad (1)$$

where $c_{i\sigma}^{\dagger}$ and $c_{i\sigma}$ are fermionic creation and annihilation operators on a one-dimensional periodic chain of length L, $\sigma=\{\uparrow,\downarrow\}$ is the spin label, $\bar{\sigma}$ denotes its opposite, $n_{j\sigma}=c_{j\sigma}^{\dagger}c_{j\sigma}$ is the spin-σ electron charge, and $\langle i,j\rangle$ stands for neighboring sites on the chain. u is a dimensionless on-site Coulomb repulsion.

The two following features make Hamiltonian (1) integrable:[18] (i) the number of doubly occupied sites is a conserved quantity and (ii) the role of spin orientation is irrelevant. For an open chain, any sequence of spins in the chain cannot be altered by H_{BC}, while for periodic boundary conditions, only the sequences of spins related by a cyclic permutation can be obtained.

A. Eigenstates, eigenvalues, and ground-state phase diagram

The physics of the system described by H is basically that of $N_s=\langle\hat{N}_s\rangle$ spinless fermions moving in a background of $L-N_s$ bosons of which $N_d=\langle\hat{N}_d\rangle$ are pairs of particles and the remaining are empty sites. Both N_s and N_d are conserved quantities (and determine the total number of electrons $N=N_s+2N_d$) and the following ansätz for the form of the eigenstates can be formulated in momentum space:

$$|\psi(N_s,N_d)\rangle = \mathcal{N}(\widetilde{\eta}^{\dagger})^{N_d}a_{k_1\sigma_{k_1}}^{\dagger}\cdots a_{k_{N_s}\sigma_{k_{N_s}}}^{\dagger}|\mathrm{vac}\rangle. \quad (2)$$

Here $\mathcal{N}=[(L-N_s-N_d)!/(L-N_s)!N_d!]^{1/2}$ is the normalization factor and $a_{k_j\sigma}^{\dagger}\doteq\frac{1}{\sqrt{L}}\sum_{l}e^{i\frac{2\pi}{L}lj}c_{l\sigma}^{\dagger}$. The operator $\eta^{\dagger}=\sum_{j}a_{-k_j\uparrow}^{\dagger}a_{k_j\downarrow}^{\dagger}$ is the so-called eta operator; its action being to create a zero-momentum couple of fermions delocalized over the recipro-
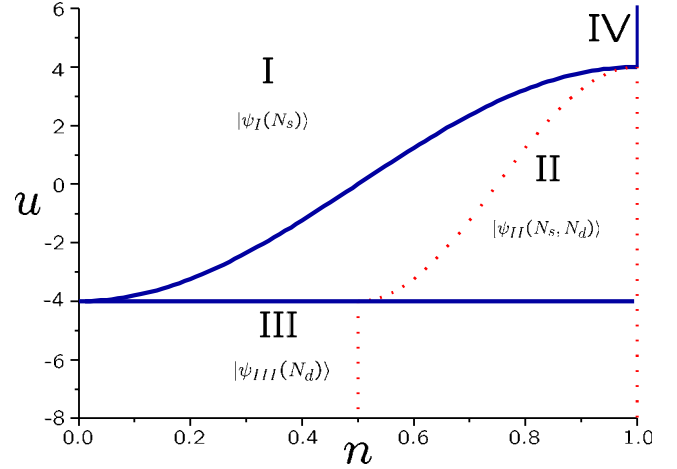

FIG. 1. (Color online) k-space representation of the ground-state phase diagram of H in the n-u plane. Dotted lines represent some cases of *isocorrelation* curves (see Sec. III B).

cal lattice. The above-mentioned irrelevance of the spin orientation implies the degeneracy of the ground-state manifold and, for our calculations; we thus decide to choose a definite sequence $\{\sigma_{k_1},\ldots,\sigma_{k_{N_s}}\}$ of spin orientations.

The actual ground state $|\psi_{\mathrm{gs}}(N_s,N_d)\rangle$ is chosen among the eigenstates (2) by requiring that N_s and N_d minimize the corresponding eigenvalue, which in the thermodynamic limit reads ($n_s=N_s/L$, $n_d=N_d/L$),

$$e(n_s,n_d) = -\frac{2}{\pi}\sin(\pi n_s) + u n_d. \quad (3)$$

The minimization equations can be solved, thus obtaining the ground-state phase diagram shown in Fig. 1 in the n-u plane (with $n=N/L$ average per site-occupation number). Three distinct regimes are recognized depending on n_s and n_d. For sufficiently high u, $n_d=0$ characterizes the conducting region I, which for $n=1$ becomes insulating (phase IV). In this case $n_s=n$. Keeping n fixed and decreasing $u<u_c(n)=-4\cos(\pi n)$, we pass to region II where the pairing mechanism becomes convenient and the energy minimum is realized for $n_d\neq0$. By further decreasing u we enter in region III, where pairs are energetically favored with respect to single fermions; the energy minimum is thus obtained imposing the condition $n_s=0$ (i.e., $n_d=n/2$). Although both phases I and II are characterized by a conducting behavior, they are qualitatively different since only in phase II the occurrence of ODLRO—which also survives in phase III—shows up.[13]

The standard approach to the study of (quantum) phase transitions consists of investigating the behavior of the (ground-state) energy density at critical points. Within this framework, all QPTs studied here are second-order ones: They are signaled by nonanalyticities of the second-order partial derivatives of the ground-state density energy. When $u=\pm4$ two transitions take place: II→IV and II→III. Here the significant derivative is the one with respect to the field u. Indeed, it is the second derivative that diverges at the critical points $u_c=\pm4$,

$$\partial_u^2 E_{gs}(u,0) = \frac{-1}{2\pi\sqrt{16-u^2}}. \qquad (4)$$

At the transition II→I the QPTs are again signaled by the nonanalyticities of the second-order partial derivatives, but—at variance with the previous case—these simply exhibit a discontinuity and do not diverge at the transition points $u_c = -4\cos(\pi n)$,

$$\lim_{u \to u_c^+} \partial_u^2 E_{gs}(u,n) = 0 \neq \frac{-1}{8\pi\sqrt{1-\cos^2(n\pi)}} = \lim_{u \to u_c^-} \partial_u^2 E_{gs}(u,n),$$

$$\lim_{n \to n_c^+} \partial_n^2 E_{gs}(u,n) = 0 \neq 2\pi\cos(n\pi) = \lim_{u \to n_c^-} \partial_n^2 E_{gs}(u,n). \qquad (5)$$

As already mentioned in Sec. I, the behavior of the ground-state entanglement properties in correspondence to the QPTs described above were studied in Ref. 13 in terms of (quantum) correlations between different subsystems in the direct-lattice picture. There the natural subsystems were the single (pairs) of *sites* in the lattice. In this picture, the principal measures of correlations taken into account were: (i) the Von Neumann entropy $\mathcal{S}_l$ that measures the total quantum correlations of the generic single site l with the rest of the chain; (ii) the mutual information $\mathcal{I}_{l,m}$ that measures the total (quantum and classical) correlations between the sites l,m; and (iii) the negativity[23] $\mathcal{N}_{l,m}$ (and concurrence[24]) that measures only the quantum contribute to the correlations between the two sites l,m. Remarkably, the study of the derivatives of these measures of correlations allowed to distinguish the various QPTs in terms of relative relevance of the two-point (i.e., two-site) and multipartite correlations. In particular, the divergence (4) exhibited by the energy density is the same shown by the first derivative of both quantum mutual information and Von Neumann entropy at both transitions. This is to understand as a signature of the relevance of two-point entanglement at the transitions that originates from the spreading of the two-point quantum correlations along the whole chain. This spreading can be quantified by the range of entanglement.[25]

In correspondence with transition II→I, signaled by the discontinuities of the energy density (5), while the partial derivative of the Von Neumann entropy still exhibits a logarithmic divergence, the partial derivative of the quantum mutual information is simply discontinuous. This is to be understood as a manifestation of the relevance of multipartite entanglement at such transition. Indeed, the absence of a divergence in the variation of the two-point correlations (measured by the derivative of the quantum mutual information) suggests that the quantum correlations pertaining to a single site and measured by the Von Neumann entropy must have a multipartite nature.

B. *k*-space representation

The main aim of this paper is to extend the study of how the QPTs introduced in Sec. II A can be described in terms of correlations in the k-space picture. The k-space representa-

tion of the eta-paring states with N_d fixed and $N_s = 0$ has been thoroughly analyzed in Ref. 19. Here first we give a brief description of the main ingredients needed for the analysis; second we see how the picture can be extended to region II in which $N_s \neq 0$; i.e., the ground state is filled at the same time by single fermions and pairs of particles.

As previously mentioned, each single eta operator in the k-space representation can be written as

$$\eta^\dagger = \sum_j \hat{\eta}_{k_j}^\dagger = \sum_j a_{-k_j\uparrow}^\dagger a_{k_j\downarrow}^\dagger, \qquad (6)$$

where $\hat{\eta}_{k_j}^\dagger = a_{-k_j\uparrow}^\dagger a_{k_j\downarrow}^\dagger$ and $a_{k_j\sigma}^\dagger, a_{k_j\sigma}$ are fermionic operators that create (annihilate) a particle with given spin σ_{k_j} in one of the L momentum modes $k_j = 2\pi j/L$ whose local basis is $\mathcal{B}_{k_j} = \{|0\rangle_{k_j}, |\uparrow\rangle_{k_j}, |\downarrow\rangle_{k_j}, |\uparrow\downarrow\rangle_{k_j}\}$. First, let us notice that the different regions in Fig. 1 correspond through Eq. (2) to different realizations of the ground states in k space. In particular, in region I at variance with the direct-lattice picture, the ground state—being constituted by N_s electron with definite momentum—is completely factorized,

$$|\psi_I(N)\rangle = \otimes_{j=1}^N |\sigma_{k_j}\rangle. \qquad (7)$$

In region II the ground state (2) is built by occupying with N_s fermionic particles (with fixed spin σ_{k_j}) the following modes of the reciprocal lattice

$$k_j \in K_{k \le k_{N_s}} = \{K_{\min} = -\pi(N_s-1)/L, \dots,$$
$$K_{\max} = \pi(N_s-1)/L\}. \qquad (8)$$

Since in region II part of the momentum space is occupied by N_s single particles, the delocalization implemented by the eta operators can only take place over a subset of momenta,

$$K_{k > k_{N_s}} = \{\pi N_s/L, \dots, \pi\} \cup \{-\pi + 2\pi/L, \dots,$$
$$-2\pi(N_s/2+1)/L\}.$$

The number of distinct values of momenta available for the creation of pairs of particles, i.e., the order of $K_{k>k_{N_s}}$, is $L - N_s$. This fact can be represented by observing that the partition of the set of possible k modes in $K_{k \le k_{N_s}} \cup K_{k>k_{N_s}}$ corresponds to a bipartition of the k-state space: $\mathcal{H} = \mathcal{H}_{k \le k_{N_s}} \otimes \mathcal{H}_{k>k_{N_s}}$. Considering the vacuum

$$|vac\rangle_{\mathcal{H}} = |vac\rangle_{\mathcal{H}_{k \le k_{N_s}}} \otimes |vac\rangle_{\mathcal{H}_{k>k_{N_s}}} \qquad (9)$$

the ground state in Eq. (2) can be written as

$$|\psi_{II}(N_s,N_d)\rangle \doteq \mathcal{N}(\eta^\dagger)^{N_d} a_{k_1\sigma}^\dagger \dots a_{k_{N_s}\sigma}^\dagger |vac\rangle_{\mathcal{H}}$$
$$= (\eta^\dagger)^{N_d} |vac\rangle_{\mathcal{H}_{k>k_{N_s}}} |\psi_I(N_s)\rangle.$$

From the point of view of the delocalization implemented by the eta operators, region III represents the limiting case where the N_d pairs can be created over the full momentum space,

$$|\psi_{III}(N_d)\rangle \doteq \mathcal{N}(\eta^\dagger)^{N_d} |vac\rangle_{\mathcal{H}}. \qquad (10)$$

The above discussion about region II implies that the only modes that are nontrivially correlated are those belonging to $\mathcal{H}_{k>k_{N_s}}$, while the modes in $\mathcal{H}_{k\leq k_{N_s}}$ are simply in a tensor product state where each mode is singly occupied by a spin-σ particle. The characterization of region II and of the transitions II→III,I can thus be done in terms of the correlations between the modes over which the pairs of particles created by the eta operators are delocalized. The influence of the single particles in this picture is the reduction of the space available for the delocalization and this reduction has an important role in determining many properties of the state correlations.

III. RESULTS IN MOMENTUM REPRESENTATION

We now generalize the results obtained in Ref. 19 for the eta-pairing states with $N_s=0$ to the generic states (2) where the eta operators act on a reference state characterized by the presence of single particles with a given momentum. The extension allows one to investigate, in k space, the behavior of the correlations at the QPTs exhibited by the model (1).

A. Local structure of correlations in k space

A first significant result in the analysis of the structure of correlations is the acknowledgment that both the generic single mode k_j and the *paired modes* $(-k_j, k_j)$ are fundamental building blocks. The basic objects that one has to evaluate in order to derive the appropriate measures of correlations are the reduced density matrices of the given subsystems: (i) ρ_{k_j} for the single mode; (ii) ρ_{k_i,k_j} for two generic modes; and (iii) $\rho_{(-k_i,k_i),(-k_j,k_j)}$ for two pairs of modes. The general considerations that allow one to determine the structure of these density matrices are the following. Since the state $(\eta^\dagger)^{N_d}|\mathrm{vac}\rangle_{\mathcal{H}_{k>k_{N_s}}}$ is built by the repeated application of operators $\eta^\dagger_{k_j}$, each time the $-k_j$ mode is occupied the k_j one must be occupied correspondingly. Therefore, for example, the only nonvanishing elements of ρ_{k_j} are the diagonal ones. As far as ρ_{k_i,k_j} [$\rho_{(-k_i,k_i),(-k_j,k_j)}$] is concerned, the only d-modes ($d=2$ and 4, respectively) projectors $P^d_{\nu_d}$ that have nonvanishing expectation values are those preserving the number $\nu_d=0,\ldots,d$ of pairs of particles $(\sigma_{k_j}, \bar\sigma_{-k_j})$. For a given ν_d the expectation values are all equal and in the thermodynamical limit (TDL), they read

$$\langle P^d_\alpha \rangle = a^{\nu_d}(1-a)^{d-\nu_d}, \quad \text{where} \quad a = \frac{n_d}{1-n_s}. \quad (11)$$

It turns out that these calculations can be generalized to an arbitrary number of both single and paired modes; one can thus explicitly find the diagonal form of the reduced density matrix of any subsystem. In the TDL, *the latter and consequently all measures of correlations depend exclusively on the parameter a.*

Some basic considerations are here in order. As previously observed, the presence of the N_s single particles with fixed spin σ_{k_j} ($k_j < k_{N_s}$) in region II has the effect of reducing the available modes over which the eta operators can delo-

calize the pairs of particles they create. This effect can be substantiated by considering the average number of particles with a given momentum k_j: $\langle n_{k_j} \rangle = \langle n_{k_j\uparrow} + n_{k_j\downarrow} \rangle$. The latter is simply constant and equal to one for all $k_j \in K_{k\leq k_{N_s}}$. For $K_{k>k_{N_s}}$ we have that $\langle n_{k_j} \rangle = 2\langle n_{k_j\sigma} \rangle = 2N_d/(L-N_s) = 2n_d/(1-n_s) = (n-n_s)/(1-n_s) = 2a$. This means that, in general, the effect on correlations of the delocalization implemented by the eta operators depends only on the density of particles; i.e., it is related to the filling $N = N_s + 2N_d$ and the number of available modes $|K_{k>k_{N_s}}| = L - N_s$.

We can now turn to the detailed description of the structure of correlations at a local level. In particular, the generic mode k_j is quantum correlated with the rest of the system and, in the TDL, the Von Neumann entropy reads $\mathcal{S}_{k_j} = -2[a \log a + (1-a)\log(1-a)]$; furthermore, k_j has two-mode correlations only with the mode $-k_j$,

$$\mathcal{I}_{k_i,k_j} = \begin{cases} \mathcal{S}_{k_i} + 2a(1-a) & k_i = -k_j \\ 0 & k_i \neq -k_j \end{cases}, \quad (12)$$

$$\mathcal{N}_{k_i,k_j} = \begin{cases} a(1-a)/3 & k_i = -k_j \\ 0 & k_i \neq -k_j \end{cases}, \quad (13)$$

where $\mathcal{I}_{k_i,k_j}$ ($\mathcal{N}_{k_i,k_j}$) is the mutual information (negativity) between two generic modes (k_i, k_j).

As for the paired modes $(-k_j, k_j)$, each of them exhibits quantum correlations only with the rest of the system as a whole; indeed, while their Von Neumann entropy reads

$$\mathcal{S}_{k_i,k_j} = -2[a \log a + (1-a)\log(1-a)] + a(1-a), \quad (14)$$

the *two-pairs* correlations $\mathcal{I}_{(-k_j,k_j),(-k_i,k_i)} = 2a(1-a)[2+a(1-a)(3\log_2 3-5)]$ are just of classical nature since $\mathcal{N}_{(-k_j,k_j),(-k_i,k_i)} = 0$.

The above picture naturally suggests to investigate at QPTs the behavior of the correlations concerning the single and the paired modes. As already anticipated the expression of $\langle n_{k_j} \rangle$ is at the basis of the definition and the behavior of Eqs. (11)–(14) and, in general, of the correlations between any pair of subsystems (in the limit of large L). Therefore, the derivative of the measures of correlations at the various phase transitions can be expressed in terms of the derivatives of $\langle n_{k_j} \rangle$ and this turns out to have important consequences for the discrimination of the various QPTs.

The above description of the network of correlations in k space can be fruitfully completed by analyzing the relations between such kind of correlations and some meaningful quantities that are defined in the direct-lattice picture. In particular one can see how ODLRO, which is defined in the direct lattice, is in fact directly related to negativity between paired modes generalizing the relation established in Ref. 19. Indeed, in this model the ODLRO is defined as

$$\lim_{|i-j|\to\infty} \langle \eta^\dagger_i \eta_j \rangle = n_d(1-n_d) \propto \mathcal{I}^{III}_{i,j}, \quad (15)$$

where $\eta^\dagger_i = c^\dagger_{i,\uparrow} c^\dagger_{i,\downarrow}$ is the operator that creates a pair of particles at the lattice site i; the proportionality to the quantum mutual information between two sites i,j evaluated in region

III, i.e., $\mathcal{I}_{i,j}^{III}$, was found in Ref. 13. Here we find that

$$\lim_{|i-j|\to\infty} \langle \eta_i^\dagger \eta_j \rangle = n_d(1 - n_s - n_d) \propto \mathcal{N}_{k_i,-k_i}(1-n_s)^2, \quad (16)$$

which means that even in region II, i.e., where $n_s \neq 0$, the negativity and the ODRLO are directly related and the latter relation reduces to the one found in Ref. 19 when evaluated in region III ($n_s=0$).

The relation between quantities defined in the different pictures can be further extended by considering the full expression of $\mathcal{I}_{i,j}^{II}$, i.e., the quantum mutual information between two sites i,j in region II. We recall that in Ref. 13 we derived the following expression:

$$\mathcal{I}_{|i-j|}^{II} = \mathcal{I}_{|i-j|}^{I} + \mathcal{I}_\infty^{II}, \quad (17)$$

where $\mathcal{I}_{|i-j|}^{I}$ is the mutual information between the sites i,j evaluated in region I ($n_d=0, n=n_s$) and $\mathcal{I}_\infty^{II}=\lim_{|i-j|\to\infty} \mathcal{I}_{|i-j|}^{II}$ is the mutual information between two infinitely distant sites in region II. This equation suggests that in region II one can distinguish the part of the direct-lattice *two-sites* correlations, i.e., $\mathcal{I}_{|i-j|}^{I}$, which are determined by the fraction of n_s single particles, which are not correlated in k space by another contribution, $\mathcal{I}_\infty^{II}$, which takes into account—in direct lattice—the effect of the eta-paring mechanism, with which the rest of the fraction of particles n_d are created. Here we can now fully understand this peculiar behavior in terms of quantum correlations between paired modes. Indeed on one hand, by using the elements of the two-sites reduced density matrix, which were analytically evaluated in Refs. 9 and 13, one can show that the proportionality established in Eq. (15) can be in some sense extended in region II: we have that in this region the ODLRO coincides with $\mathcal{I}_\infty^{II}$. On the other hand, thanks to Eq. (16), this quantity can be directly linked to the $\mathcal{N}_{k_i,-k_i}$ and this roots the origin of this part of the *two-site* correlations in the existing correlations between *paired momentum modes*.

It turns out that the above-described important relation between the (quantum) correlations pertaining to the two complementary pictures will also be relevant in Sec. III B, when we discuss the behavior of the various correlation measures at the QPTs.

B. Entanglement and quantum phase transitions

In previous papers[9,13] we showed how, in the direct-lattice picture, the transition II→I (see Fig. 1) can be distinguished from transitions II→III and I→IV on the basis of the different kind of correlations (two site versus multipartite) among different subsystems. Such a distinction between these QPTs can be achieved in the k-space picture only in a different way. In fact, we first note that at variance with the direct-lattice picture, here the insulating state, which represents the ground-state at half filling for $u>4$ (insulating phase IV), as far as correlations are concerned is not qualitatively distinct from the conducting state (7), which occurs at arbitrary filling when $u \geq -4 \cos(\pi n)$. Indeed, in k space the conducting state (7) is fully factorized for any filling n so that entanglement is identically zero at any n and the transition I→IV cannot be detected from entanglement analysis.

TABLE I. Behavior of the evaluated partial derivatives at the various QPTs (left column). "FD" stands for finite discontinuity, "Multi" for multipair, while "Two" stands for two pair.

	$\partial_x \mathcal{S}_{k_j}, \partial_x \mathcal{S}_{k_j,-k_j}, \partial_x \mathcal{I}_{k_j,-k_j}$	$\partial_x \mathcal{N}_{k_j,-k_j}$	$\partial_x \mathcal{I}_{-k_j k_j, -k_i k_i}$
II→I($x=u$)	$\log(u_c-u)$	FD	Multi
II→I($x=n$)	$\log|n-n_c|$	FD	Multi
II→III($x=u$)	$-1/\sqrt{u-u_c}$	$-1/\sqrt{u-u_c}$	Two

In the ambient lattice the factorization property holds at half filling only.

In Table I we report the behavior of the relevant partial derivatives of the studied quantities at QPTs: Von Neumann entropy, quantum mutual information, and negativity.

We start by taking as elementary subsystem the generic single mode k_j. At all the considered transitions we can recognize that the *two-mode* correlations play a prominent role. Indeed, the correspondence of the divergencies of $\partial_x \mathcal{S}_{k_j}$ and $\partial_x \mathcal{I}_{k_j,-k_j}$ allows one to acknowledge the two-mode *total* correlations between k_j and $-k_j$ as relevant for the transitions II→I and II→III. The distinction between the latter resides in the fact that only at transition II→III $\partial_u \mathcal{N}_{k_j,-k_j}$ is singular, suggesting that only in this case the two-mode *quantum* correlations between the modes $-k_j$ and k_j play a prominent role. We note, however, that the two-mode character of the transition II→III is of a different nature with respect to the one seen in the direct-lattice picture, where we observed a diverging entanglement range.[25]

This distinction is enforced by the relation between the negativity and the ODLRO and the fact that the derivatives of these two quantities display the same divergence at the transition II→III. The comparison between these quantities and the mutual information between two arbitrary sites of the direct lattice discussed at the end of Sec. III A allows once again to establish a link between the two-mode picture in k space and the two-site picture in direct lattice. Indeed, due to the relation (17) the divergence of $\partial_u \mathcal{I}_{|i-j|}^{II}$ at the transition II→III that allowed in Ref. 13 to describe this transition as a two-point one is in part determined by the divergence of the $\partial_u \mathcal{N}_{k_j,-k_j}$.[26]

We now consider the elementary subsystem formed by the paired modes $(-k_j, k_j)$. The vanishing negativity $\mathcal{N}_{(-k_j,k_i),(-k_j,k_j)}=0$ shows that the *two-pair* correlations measured by $\mathcal{I}_{(-k_i,k_i),(-k_j,k_j)}$ are always classical; this suggests the presence of just a *multipair* structure of quantum correlations. The divergencies of $\partial_{x=u,n} \mathcal{S}_{-k_j,k_j}$ show that these correlations play an important, though different, role in both kind of transitions. The different role can be described at the level of *two-pair* correlations allowing for a classification of the QPTs into two classes: two-pair (transition II→III) and multipair (transition II→I). Indeed, as shown in Table I and in Fig. 2, the singular behavior of $\partial_x \mathcal{I}_{(-k_i,k_i),(-k_j,k_j)}$ and $\partial_x \mathcal{S}_{k_j,-k_j}$ coincides only at transition II→III. As in the direct-lattice picture, we can then conclude that also in k space that the transition II→III is characterized by the fact that correlations of two-point (two-pair) nature are more sensible to the undergoing phase transition. On the contrary, the absence of a
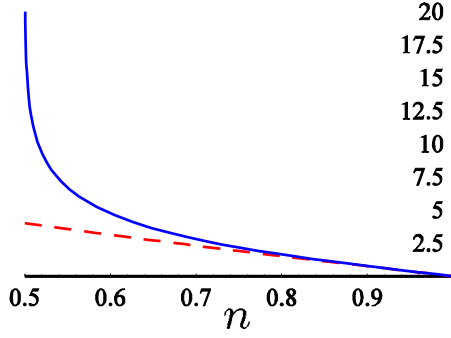
FIG. 2. (Color online) Plot of $\partial_n \mathcal{S}_{-k_j,k_j}$ (straight blue line) and $\partial_n \mathcal{I}_{(-k_i,k_i),(-k_j,k_j)}$ (dashed red line) in region II.

divergence of $\partial_x \mathcal{I}_{(-k_i,k_i),(-k_j,k_j)}$ suggests that correlations of multipartite (multipair) nature are more relevant at the transition II→I. In Sec. III C we will provide a further confirmation of such statement by directly evaluating a measure of multipartite correlations.

We now pass to the comparison of the singularities of the partial derivatives of the measures, as reported in Table I, with those shown by the second partial derivatives of ground-state energy (5) and (4). Interestingly, at transition II→III, all the computed quantities develop the same singularity of $\partial_n^2 E_{gs}(u,n)$. On the other hand, at transition II→I, $\partial_{x=u,n}^2 E_{gs}(u,n)$ exhibits a finite discontinuity and the same behavior is shown by both negativity and quantum mutual information while the Von Neumann entropy is logarithmically divergent (Fig. 3).

To summarize, it seems that when the transitions are signaled by divergencies the main role is played by "two-point" correlations. Instead, in the case of simple finite discontinuities the dominant role is played by the multipartite quantum correlations. In both cases, the appropriate derivatives of Von Neumann entropy diverges.

We conclude in this section by considering the half-filling case. The latter has to be treated separately since no divergencies in the derivative of any measure of correlation can be observed at the transitions. This feature is a particular case of a more general phenomenon. As previously highlighted, in the TDL all measures of correlation depend on the average occupation number of each of the modes belonging to the set $K_{k>k_{N_s}}$. Therefore the curves in the n,u plane defined by fixing $\langle n_{k_j} \rangle$ to a given constant value can be considered as *isocorrelation curves* (an example of them is given in Fig. 1).
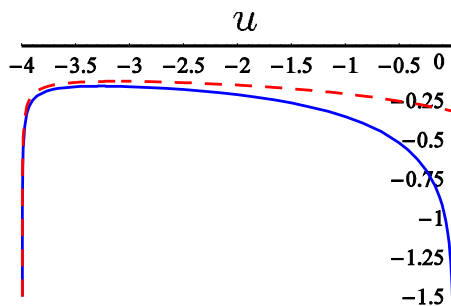

FIG. 3. (Color online) Plot of $\partial_u \mathcal{S}_{-k_j,k_j}$ (straight blue line) and $\partial_u \mathcal{I}_{(-k_i,k_i),(-k_j,k_j)}$ (dashed red line) in region II.

Along such curves the correlations of any accessible subsystem do not change. Consequently by crossing the boundary separating regions II and III along these curves, no divergence in the derivative of the correlations measures would be observed.

In particular, the condition $n=1$, i.e., the half-filling case, defines a curve, which is simply parallel to the u axis. Thus, while N_s—that determines the number of available modes—and N_d can vary with u, $\langle n_{k_j} \rangle$ is constant along this curve and all measures of correlations in region II are constant and fixed to the maximal achievable value (e.g., $\mathcal{S}_{k_j}=2$). In other words, in the k-space picture the transition between regions II and III, while it is well described by all measures of correlations for $n \neq 1$ at half filling (at variance with respect to the direct-lattice case) and along the isocorrelation curves, it simply does not have any impact on the structure of the correlations of the state.

C. Multipartite entanglement

In order to evaluate directly the multipartite part of the correlations and their behavior at QPTs, we consider the generalization of the Meyer-Wallach measure of multipartite entanglement $Q(|\psi\rangle)$ (Ref. 20) to multiqudit states introduced by Scott in Ref. 21:

$$Q_{m,d} = \frac{d^m}{d^m-1}\left(1 - \frac{1}{C_m^n}\sum_{\vec{i}} \operatorname{tr}\rho_{\vec{i}}^2\right). \qquad (18)$$

Each multi-index $\vec{i}=\{i_1,\ldots,i_m\}$ identifies m elementary subsystems, e.g., momentum modes in our case, that compose a given principal subsystem $\mathcal{S}_m$, e.g., block of m modes. The latter is characterized by its reduced density matrix $\rho_{\vec{i}}$. The factor $d^m/(d^m-1)$ normalizes the measure to one; d is the dimension of the Hilbert space of each elementary subsystem, and in the case of momentum modes it is equal to four. The combinatorial coefficient $C_m^n=\binom{n}{m}$ takes into account the many ways in which one can choose a given principal subsystem $\mathcal{S}_m$. $Q_{m,d}$ can be expressed as the average linear entropy relative to $\mathcal{S}_m$ and thus quantifies the average entanglement between blocks of momentum modes and the rest of the system. The more the size of the blocks is increased, the more $Q_{m,d}$ can capture and measure the multipartite correlations present in the system.[21,27] In order to obtain a proper measure of the latter, it is thus necessary to be able to compute the reduced density matrix of blocks of modes of arbitrary dimension. While in the direct lattice this is possible only in region III,[28] in k space one can generalize the results obtained in Ref. 19 and extend them to region II. The extension is obtained again by recognizing that in k space the role of the single particle with given spin σ_{k_j} and momentum belonging to the set $K_{k_j \leq k_{N_s}}$ is to reduce the momentum spectrum available for the delocalization of the eta pairs to a subset of $L-N_s$ modes. One can thus derive the subsystems density-matrix spectrum and by implementing the definition of Eq. (18) one has for $m=D$,
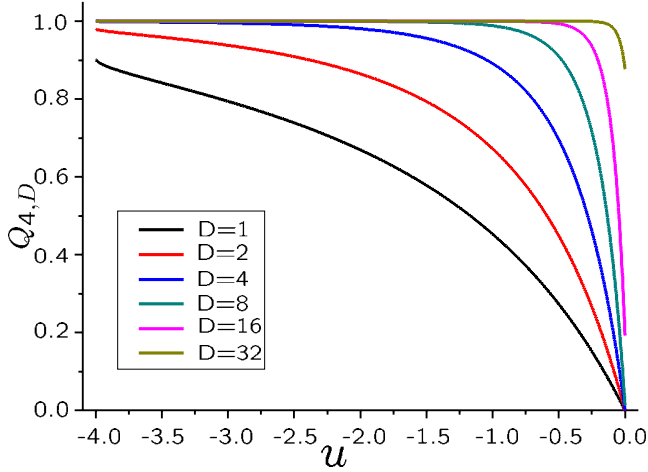
FIG. 4. (Color online) Plot of the Q measure for a chain of length $L=1000$ at quarter filling; $D=1,2,4,8,16,32$.

$$Q_{D,4} = \left[1 - \binom{L-N_s}{D}^{-1} \sum_{D_2=0}^{D} f(D_2) \text{Tr}(\rho_{D_1}^2) \text{Tr}(\rho_{D_2}^2) \right]$$
$$\times \frac{4^D}{4^D - 1}, \tag{19}$$

where

$$\text{Tr}(\rho_{D_1}^2) = \sum_{M=0}^{2D_1} \binom{2D_1}{M} \left[\frac{\binom{L-N_s-2D_1}{N_d-M}}{\binom{L-N_s}{N_d}} \right]^2, \tag{20}$$

$$\text{Tr}(\rho_{D_2}^2) = \sum_{\alpha=0}^{D_2} \left[\binom{D_2}{\alpha} \frac{\binom{L-N_s-D_2}{N_d-\alpha}}{\binom{L-N_s}{N_d}} \right]^2, \tag{21}$$

and

$$f(D_2) = \frac{\prod_{i=0}^{D_1-1}(L-N_s-2i)}{D_1!} \frac{\prod_{j=0}^{D_2/2-1}(L-N_s-2D_1-2j)}{D_2!} \tag{22}$$

is the number of equivalent partitions of D momentum modes into $D_1=D-D_2$ single modes k_j and $D_2/2$ paired of modes $(-k_j, k_j)$.

In Fig. 4 we plot the Q measure [Eq. (16)] at quarter filling ($L=1000$, $N=500$) as a function of the Coulomb interaction u and for increasing values of the subsystem size D. The data confirm that—despite the reduced portion of k space available for the construction of the eta pairs—the multipartite entanglement induced by their presence is of fundamental importance in the whole region II. Indeed, for all values of u, we observe an increasing saturation of $Q_{4,D}$ to its maximal value when increasing D (for $D \geq 4$). Furthermore, for any dimension D of the block of modes, $Q_{4,D}$ is a monotonic decreasing function of u and thus since n_d

$=1/2(n-n_s)=1/2[n-\arccos(-u/4)/\pi]$, it is a monotonic increasing function of the number N_d of eta pairs.

The multipartite entanglement contribution at the various QPTs can be inferred by analyzing the behavior of $Q_{4,D}$ at the critical points. Again, it is only for $D \geq 4$ that the correct qualitative behavior of $Q_{4,D}$ at large D is captured, while at the transition II→III the curves smoothly reach the (constant) value exhibited by the measure in region III. The plot clearly shows that $\partial_u Q_{4,D}$ is highly enhanced in proximity of the transition II→I. The result, confirmed by numerical analysis, thus indicates the presence of a divergent behavior at large D. This is a quantitative confirmation of the peculiar multipartite character of the transition II→I; at that transition, though all correlations vanish, the multipartite ones change in a much faster way. Hence, the direct measure of multipartite correlations fully confirms the predictions of their role at QPTs, as obtained in Sec. III B. We emphasize that a study at low values of D—such as the one that would be feasible in the direct-lattice picture—would have suggested the opposite conclusion regarding the relevance of multipartite correlations at the transitions.

We finally note that the determination of the reduced density matrices ρ_D for blocks of modes of arbitrary dimension D allows for the evaluation also of the block entropy, i.e., the Von Neumann entropy of ρ_D. This can be done by extending the results obtained in Ref. 19. This extension shows that even in the case analyzed in this paper the asymptotic behavior of the block entropy depends on the type of modes included in the block. In particular, the relevant result is that when the block is composed by $D/2$ paired modes only, the block entropy grows logarithmically with D. This typical growth shows on one hand the presence of multipartite entanglement and on the other hand the peculiar multipair nature of this kind of entanglement.

IV. CONCLUSIONS

We investigated in momentum representation the structure of correlations of the ground state of an extended 1D Hubbard model in relation to the undergoing QPTs. At variance with the standard real-space approach, the k-space representation allows in this case to explicitly derive the reduced density matrices of arbitrary subsystems and thus to evaluate rigorously all bipartite and multipartite correlations present in the system.

A first interesting result is directly related with the presence of single electrons with given spin and momentum; the consequence of the presence of these particles is the limitation of the portion of momentum space available for the implementation of the eta-paring mechanism. We show that this fact has various important implications in the structure and the behavior of the correlations present in the ground state. In particular, we show that the phase space of the model can be characterized by the presence of *isocorrelation* curves; i.e., curves in the phase space along which the value and the structure of the correlations do not change.

Due to the presence of the eta-pairing mechanism, at a local level the existing network of correlations can be described in terms of two elementary building blocks: the ge-

neric single mode k_j and the paired modes $(k_j, -k_j)$. The identification of such elementary subsystems and the comparison of their (quantum) correlations with the results obtained in the direct-lattice picture allows one to unveil the origin of the off-diagonal long-range order (ODLRO), whose value can be functionally expressed in terms of quantum correlations between two paired modes, i.e., negativity. As a consequence, we also show that the mutual information between two sites can be directly linked with the negativity between paired modes.

The identification of the above elementary subsystems has also allowed for the classification of the QPTs in terms of two-pair or multipair correlations depending on whether partial derivatives of quantum mutual information and Von Neumann entropy show the same singularity or not at a given QPT. These singularities can be related to those shown by second partial derivatives of the ground-state energy and, when possible, to the singularities of measures of correlations derived in the direct-lattice picture.

Finally, we have computed a proper direct measure of multipartite entanglement: the Q generalization of the Meyer-Wallach measure.[20,21] The latter requires the evaluation of the reduced density matrices relative to subsystems constituted by blocks of modes of arbitrary size D. We have shown that, besides the different behavior of the measure depending on the presence of paired (unpaired) modes in the blocks,[19] as D grows the partial derivative of Q develops a singularity in correspondence with those QPTs at which the dominant correlations were conjectured to be of a multipartite nature. On the other hand in correspondence with the QPTs classified as "two pair" by increasing D, the partial derivative of Q becomes smooth.

The comparison between the structure of correlations in momentum space and their direct-lattice counterpart turned out to be a useful method that allowed to unveil interesting relations between the correlations in the different pictures and to accurately characterize the ground-state phase space and the quantum phase transitions occurring in a strongly correlated electron system. We expect that such method can be fruitfully extended to other many-body complex systems.

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[25] The range of entanglement is defined as the maximum distance r between two subsystems $i, i+r$ (e.g. sites) at which a given measure of entanglement $E_{i,i+r}$ (e.g. concurrence or negativity) is different from zero. In Ref. 13 it was shown that in correspondence with QPTs classified as two point the range of entanglement is diverging ($r_{max} \to \infty$), while when approaching a multipartite QPT it remains finite.

[26] The two-mode character of the transition II$\to$III is however of a different nature with respect to the one seen in the direct-lattice picture where we observed a diverging entanglement range. In k space the only two-mode nonzero quantum correlations are those between the each paired modes k_j and $-k_j$. Thus we do not observe any kind of entanglement transition (Refs. 6 and 13).

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