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Two-Point Versus Multipartite Entanglement in Quantum Phase Transitions

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We analyze correlations between subsystems for an extended Hubbard model exactly solvable in one dimension, which exhibits a rich structure of quantum phase transitions (QPTs). The $T = 0$ phase diagram is exactly reproduced by studying singularities of single-site entanglement. It is shown how comparison of the latter quantity and quantum mutual information allows one to recognize whether two-point or shared quantum correlations are responsible for each of the occurring QPTs. The method works in principle for any number D of degrees of freedom per site. As a by-product, we are providing a benchmark for direct measures of bipartite entanglement; in particular, here we discuss the role of negativity at the transition.

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In the past years, the characterization of complex quantum phenomena has received a strong impulse from the recent developments in quantum-information theory. Within such framework, a crucial notion is that of entanglement. Besides being recognized as a fundamental resource for quantum computation and communication tasks [1], it has also been used to better characterize the critical behavior of different many-body quantum systems when some characteristic parameter of the related Hamiltonian is varied; the latter phenomenon being known as quantum phase transition (QPT) [2].

In fact, a deep comprehension of universal properties of QPTs has not been fully reached yet. The peculiarity of using entanglement in this context is that, being a single direct measure of quantum correlations, it should allow for a unified treatment of QPTs; at least, whenever the occurring QPT is to ascribe to the quantum nature of the system, which is always the case at $T = 0$ since thermal fluctuations are absent.

A first description of the relations between entanglement of one or two spins and QPTs in spin-$1/2$ chains was given in [3], where it was noticed how derivatives of concurrence show divergences in correspondence of QPT, with appropriate scaling exponents. The entanglement of blocks of L spins and its scaling behavior in spin models showing critical behavior was then investigated in [4]. The problem of characterizing the ground-state phase diagram of fermionic systems by means of entanglement has been addressed more recently in [5], where it was shown how the study of *single-site entanglement* allows one to reproduce the relevant features of the known (numerical) phase diagram. While this is a promising starting point, it remains to be clarified which quantum correlations are responsible for the occurring QPT: if two points or shared (multipartite), if short or long ranged. The answer to the above issue would, in fact, require exhaustive investigation of the entanglement between any two subsystems. In case the subsystems have just 2 degrees of freedom, concurrence properly quantifies the quantum correlations [6]. A generalization of such quantity to (sub)systems with a higher number of degrees of freedom D has been proposed, and is known as *negativity* [7]. Also, the total amount of correlations between any two subsystems is captured by *quantum mutual information* [8].

In the following we describe a method based on the comparison of the latter quantities for arguing whether the occurring transition is to ascribe to two-point or multipartite quantum correlations; the method works for arbitrary D. Our strategy is tested on a one-dimensional extended Hubbard model that was solved [9,10], exhibiting a rich structure of phase diagram at $T = 0$. We show that the phase diagram is exactly reproduced by the singularities of single-site entanglement. We then infer which of the QPTs is originated from a singular behavior of two-point or multipartite entanglement; our results are confirmed by the exact solution.

Correlations and subsystems.—We are interested in the existing correlations between (a) the single site i and the rest of the system; (b) the generic site i and a generic site $j \neq i$; (c) the generic pair of site (i, j) (dimer) and the rest of the system.

In order to measure the *total correlations* between two generic subsystems A and B, we use the quantum mutual information [1,8,11]. The latter is defined as

$$\mathcal{I}_{AB} = S(\rho_A) + S(\rho_B) - S(\rho_{AB}), \tag{1}$$

where ρ_{AB}, ρ_A, and ρ_B are the total system's and subsystems' density matrices, respectively, and $S(\rho) = -\Sigma_i \lambda_i \log_2 \lambda_i$ (λ_i being the eigenvalues of ρ) is the von Neumann entropy. In [8,11] it was shown how $\mathcal{I}_{AB}$ is a proper measure of all (quantum and classical) correlations between A and B. In case A and B are single sites, we refer to the latter as two-point quantum (Q2) and classical (C2) correlations.

As far as *quantum correlations* are concerned, we consider two different cases. When ρ_{AB} is a pure state, correlations between A and B are purely quantum and are

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measured by $S(\rho_A) = S(\rho_B)$. This happens when A corresponds to a single site i (or to the dimer i, j), and B corresponds to the remaining sites [12]; $S_i = S(\rho_i)$ (single-site entanglement) accounts for both the localized correlations (Q2) and the shared ones (QS in the following). When we deal instead with the correlations between two generic sites (i, j), the density matrix of the global system is the dimer's one: $\rho_{AB} = \rho_{ij}$. The latter generally corresponds to a mixed state. Thus, to evaluate the quantum correlations between two generic sites, we need a measure of entanglement for bipartite mixed states. In general, proposed measures are hard to compute whenever $D > 2$, since they require difficult optimization processes. However, there is at least one measure easy to compute [7], the negativity

$$\mathcal{N}(\rho_{AB}) = (\|\rho_{AB}^{T_A}\|_1 - 1)/2; \tag{2}$$

where $\rho_{AB}^{T_A}$ is the partial transposition with respect to the subsystem A applied on ρ_{AB}, and $\|O\|_1 \doteq \mathrm{Tr}\sqrt{O^\dagger O}$ is the trace norm of the operator O. $\rho_{AB}^{T_A}$ can have negative eigenvalues μ_i, and the negativity can also be expressed as $\mathcal{N}(\rho_{AB}) = |\Sigma_i \mu_i|$. Although negativity is not a perfect measure of entanglement [13], it gives important bounds for quantum-information protocols, i.e., teleportation capacity and asymptotic distillability. Its role in describing QPTs has not been fully investigated yet.

Entanglement and QPTs.—S_i has been proven to be a useful tool in describing QPTs [5]. As already pointed out, to give a better characterization of the latter, one could as well consider quantum correlations between different subsystems. The scheme we propose in this Letter is based on the idea of comparing S_i—not allowing one to distinguish Q2 from QS correlations—with different functionals quantifying instead just two-point correlations. We study $\mathcal{N}_{i,j}$, which is at least a lower bound for Q2 correlations, and $\mathcal{I}_{i,j}$, which properly captures total (Q2 and C2) correlations. As a first step, the exact phase diagram is obtained analyzing the singularities shown by S_i, $\mathcal{I}_{i,j}$, and $\mathcal{N}_{i,j}$. Successively, a comparison of the singular behavior of $\mathcal{I}_{i,j}$ with that of S_i allows one to discriminate whether a QPT is to ascribe to Q2 or QS correlations. In fact, whenever S_i exhibits a singular behavior due to Q2 correlations, the *same* type of singular behavior should be highlighted as well by $\mathcal{I}_{i,j}$ (since it also contains Q2 correlations), and possibly by $\mathcal{N}_{i,j}$, in case the latter would properly capture them for our model. On the contrary, when the singular behavior of S_i is to ascribe to QS correlations, the same singular behavior should not be displayed either by $\mathcal{I}_{i,j}$ or by $\mathcal{N}_{i,j}$, since both measures regard only two-point correlations.

The bond-charge extended Hubbard model.—The model we deal with is described by the following Hamiltonian:

$$H_{\mathrm{BC}} = u\sum_i n_{i\uparrow}n_{i\downarrow} - \sum_{\langle i,j\rangle\sigma}[1 - x(n_{i\bar{\sigma}} + n_{j\bar{\sigma}})]c_{i\sigma}^\dagger c_{j\sigma}, \tag{3}$$

where $c_{i\sigma}^\dagger$, $c_{i\sigma}$ are fermionic creation and annihilation operators on a one-dimensional 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; u and x $(0 \le x \le 1)$ are the (dimensionless) on-site Coulomb repulsion and bond-charge interaction parameters.

The model is considered here at $x = 1$, in which case the number of doubly occupied sites becomes a conserved quantity. The eigenstates of $H_{\mathrm{BC}}(x = 1)$ are obtained in [9,10,14]; the ground-state phase diagram is shown in the left part of Fig. 1. The latter presents various QPTs driven by parameters u and average number of electrons per site (filling) n. The charge-gapped phase IV is insulating and all sites are singly occupied; phases I, I′, and II fall in the Tomonaga-Luttinger class (neither spin nor charge gap); they are characterized by the presence of singly and empty sites (phase I), singly and doubly occupied sites (phase I′), both of which have dominant charge-charge correlations, and all types of sites (phase II) with superconducting correlations and off-diagonal long range order (ODLRO). The latter characterizes also phase III, where sites are empty or doubly occupied.

The model's energy spectrum is fully independent of spin orientation [9]: any sequence of spins in the chain cannot be altered by the Hamiltonian, which, in fact, acts on a Hilbert space that at each site i has $D_i = 3$, and is spanned by the states $|0\rangle_i$ (empty), $|\varnothing\rangle_i$ (singly occupied), and $|2\rangle_i$ (doubly occupied). The physics of the system is essentially that of $N_s = \Sigma_i c_i^\dagger c_i$ spinless fermions and N_d bosons, with eigenstates given by

$$|\psi(N_s, N_d)\rangle = \mathcal{N}(\eta^\dagger)^{N_d} a_0^\dagger \cdots a_{N_s-1}^\dagger |\mathrm{vac}\rangle. \tag{4}$$

Here $\mathcal{N} = [(L - N_s - N_d)!/(L - N_s)!\,N_d!]^{1/2}$ is a normalization factor; $a_j^\dagger$ is the Fourier transform of the spinless fermion operator $c_j^\dagger$, $a_j^\dagger = \Sigma_q \frac{1}{\sqrt{L}} \exp(i\frac{\pi}{L} jq) c_q^\dagger$, with $j = 0, N_s - 1$; moreover, $\eta^\dagger = \Sigma_{i=1}^L \eta_i^\dagger$ is also known as

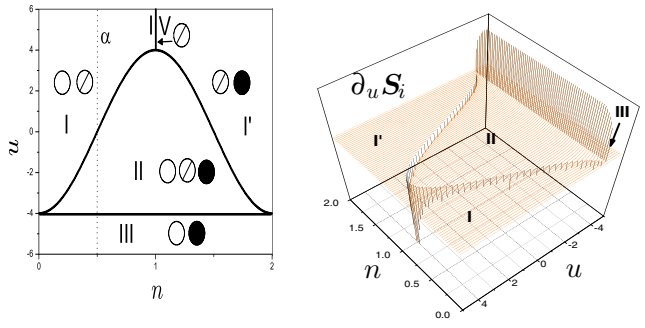

FIG. 1 (color online). Left: Ground-state phase diagram. Empty, slashed, and full dots stay for empty, singly, and doubly occupied sites. Right: $\partial_u S_i$.

the eta operator, and creates doubly occupied sites from empty ones ($\eta_i^\dagger|0\rangle_i = |2\rangle_i$); $|\mathrm{vac}\rangle$ is the electron vacuum. $(\eta^\dagger)^k|\mathrm{vac}\rangle$ is known to carry ODLRO and multipartite entanglement [15]. At fixed filling $n = (N_s + 2N_d)/L$, the actual value of N_s in (4) is chosen to minimize the corresponding eigenvalue $E(N_s, N_d) = -2\frac{L}{\pi}\sin(\pi\frac{N_s}{L}) + uN_d$.

The system density matrix in the ground state is defined by $\rho \doteq |\psi(N_s, N_d)\rangle\langle\psi(N_s, N_d)|$. Results of the calculation for the single-site ρ_i and the dimer ρ_{ij} reduced density matrices are reported below. With respect to the basis $|0\rangle$, $|\varnothing\rangle$, $|2\rangle$, $\rho_i = \mathrm{diag}\{1 - n_s - n_d, n_s, n_d\}$ with $n_\alpha \doteq \frac{N_\alpha}{L}$ ($\alpha = s, d$). Whereas with respect to the basis $|00\rangle$, $|0\varnothing\rangle$, $|\varnothing 0\rangle$, $|\varnothing\varnothing\rangle$, $|\varnothing 2\rangle$, $|2\varnothing\rangle$, $|02\rangle$, $|20\rangle$, $|22\rangle$,

$$\rho_{ij} = \begin{pmatrix} D_1 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & O_1 & O_2 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & O_2^* & O_1 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & D_2 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & P_1 & P_2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & P_2^* & P_1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & Q & Q & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & Q & Q & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 0 & D_3 \end{pmatrix}. \tag{5}$$

Here, assuming $\epsilon = 1/L$,

$$D_1 = P_{ij}\frac{(\delta_s - n_d)(\delta_s - n_d - \epsilon)}{\delta_s(\delta_s - \epsilon)}, \qquad O_2 = C_{ij}\frac{\delta_s - n_d}{\delta_s},$$

$$D_2 = P_{ij} + 1 - 2\delta_s, \qquad P_1 = \frac{n_d}{\delta_s}(\delta_s - P_{ij}),$$

$$D_3 = \frac{n_d(n_d - \epsilon)}{\delta_s(\delta_s - \epsilon)}P_{ij}, \qquad P_2 = \frac{n_d}{\delta_s}C_{ij},$$

$$O_1 = (\delta_s - P_{ij})\left(\frac{\delta_s - n_d}{\delta_s}\right), \qquad Q = \frac{n_d(\delta_s - n_d)}{\delta_s(\delta_s - \epsilon)}P_{ij}$$

with $P_{ij} = \delta_s^2 - |C_{ij}|^2$, $\delta_s = 1 - n_s$, and $|C_{ij}| = \epsilon\frac{\sin(n_s\pi|i-j|)}{\sin(\pi\epsilon|i-j|)}$. In the thermodynamic limit $\epsilon \to 0$, n_α finite, the above results may also be derived from [10].

Results.—As a preliminary observation let us notice that in phases I, I′, and III (see Fig. 1, left side) the dimension of on-site vector space reduces to two, meaning that in these cases $\mathcal{N}_{i,j}$ should reproduce results evaluated through concurrence. This happens to be the case; in particular, in phase III $\mathcal{N}_{i,j}$ (and the concurrence) are vanishing $\forall\ |i - j|$, whereas $\mathcal{I}_{i,j}$ is equal to $n(2 - n)/2$, which is related to the value of the ODLRO parameter, in agreement with [15]. We also observe that whenever $C_{i,j}$ is zero (for instance, phases III and IV) the two-site density matrix is independent of the sites i and j. In the insulating phase IV this happens because the state is a tensor product of identical single-site states, and all correlations are identically zero. On the contrary, in phase III, since $Q \neq 0$, the surviving two-point quantum correlations are range independent. In such cases it may be useful to introduce global (i.e., sums over all sites) quantities instead of local ones, since it may happen that a correlation is locally vanishing but globally relevant; also finite size corrections (ϵ) have to be considered. For instance, it turns out that in so doing in phase III the total negativity becomes nonvanishing $\Sigma_{j\neq i}\mathcal{N}_{i,j} = n(2 - n)/[(2 - n)^2 + n^2]$.

We now turn to discuss what happens at QPTs by studying the behavior of S_i, $\mathcal{I}_{i,j}$, and $\mathcal{N}_{i,j}$. As mentioned, each of the observed measures of correlations keeps track of the undergoing transitions, exhibiting a singular behavior at the transition points. The latter can be characterized by the analysis of the partial derivatives of each measure. As an example, in the right part of Fig. 1 we plot $\partial_u S_i$. Noticeably, the divergences in the derivative are in perfect correspondence with the parameter's values at which the various QPTs occur, aside from transitions I, I′ → IV that must be revealed by $\partial_n S_i$. The systematic analysis of the behavior of the various derivatives at each QPT is carried on in Table I.

We first consider $\partial_x S_i$, $x = n, u$; it exhibits two different kinds of divergences: logarithmic for transitions I, I′ → IV and II → I, I′; algebraic for transitions II → III and II → IV, with exponent $\nu = 1/2$. The latter turns out to correspond to the shift exponent as extracted from finite size analysis [16].

In Table I we also report the behavior of $\partial_x\mathcal{I}_{i,j}$ and $\partial_x\mathcal{N}_{i,j}$ at QPTs. As described in the paragraph *Entanglement and QPTs,* the comparison of the three quantities can be used to understand whether bipartite or multipartite entanglement is relevant to the various transitions. In fact, all transitions corresponding to a (logarithmic) divergence in $\partial_x S_i$ are not seen as divergences either in $\partial_x\mathcal{I}_{i,j}$ or in $\partial_x\mathcal{N}_{i,j}$. In such cases, we infer that the transitions are to ascribe to QS correlations; this is also in agreement with the fact that in some of these transitions (II → I, I′) the component of the ground state given by the eta pairs (which carry multipartite entanglement and ODLRO) disappears. On the contrary, whenever the divergent behavior exhibited by $\partial_x S_i$ is also displayed by $\partial_x\mathcal{I}_{i,j}$, as seen for the two transitions II → III and II → IV, this is to be interpreted as a signal of the role of Q2 correlations in the QPT.

TABLE I. Behavior of the evaluated partial derivatives at critical points for the various QPTs (left column): FD is finite discontinuity, "Multi" refers to multipartite, and "Two" refers to two-point.

	$\partial_x S_i$	$\partial_x\mathcal{I}_{i,j}$	$\partial_x\mathcal{N}_{i,j}$	Ent
I, I′ → IV ($x = n$)	$\log\lvert n_c - n\rvert$	FD	0	Multi
II → I, I′ ($x = u$)	$\log(u_c - u)$	FD	FD	Multi
II → I, I′ ($x = n$)	$\log\lvert n - n_c\rvert$	FD	FD	Multi
II → III ($x = u$)	$1/\sqrt{u - u_c}$	$1/\sqrt{u - u_c}$	FD	Two
II → IV ($x = u$)	$1/\sqrt{u_c - u}$	$1/\sqrt{u_c - u}$	FD	Two

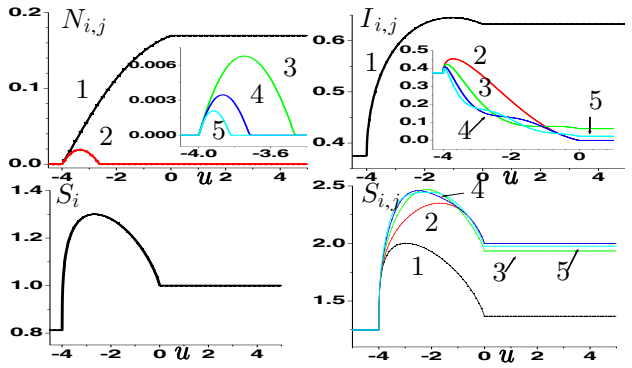

FIG. 2 (color online). Plots of $\mathcal{N}_{i,j}$, $\mathcal{I}_{i,j}$, S_i, and $S_{i,j}$ ($|i-j| = 1,\ldots,5$) for the section $n = 0.5$ (line α in Fig. 1).

Different from what happens for the first two quantities reported in Table I, we can check on the third column that $\partial_x \mathcal{N}_{i,j}$ never does display the same singular behavior as $\partial_x S_i$. In particular, this happens in correspondence of the transitions driven by two-point correlations, II $\rightarrow$ III and II $\rightarrow$ IV, suggesting that $\mathcal{N}_{i,j}$ is just a lower bound for Q2 correlations also for the present model. Apart from this fact, the behavior of $\mathcal{N}_{i,j}$ for various values of $|i-j|$ supports once more the idea that the transitions in question have to be ascribed to two-point correlations.

As an example, we report in the top left part of Fig. 2 $\mathcal{N}_{i,j}$ for the case $n = 0.5$; the transition II $\rightarrow$ III takes place at $u_c = -4$. As u gets close to u_c two-point quantum correlations begin to spread along the chain; this is shown by the nonzero value of $\mathcal{N}_{i,j}$ for an increasing number of pairs of sites whose distance $|i-j|$ grows up to ∞ as $u \rightarrow u_c$. This is a clear indication of a diverging correlation length originated from Q2 correlations at critical point. One could expect that again the total negativity is the right quantity to display a critical behavior, in agreement with similar conclusions about concurrence [17] in spin-1/2 systems. Moreover, the value at which $\mathcal{N}_{i,j}$ reaches its maximum gets closer to u_c by increasing $|i-j|$, indicating its possible scaling behavior. The same qualitative behavior of the maximum is observed for $\mathcal{I}_{i,j}$ (top right part of figure), even though such a quantity is, in general, different from zero also away from the critical point, suggesting once more that the quantum mutual information in the vicinity of the transition captures the divergent behavior of just the Q2 correlations. We finally analyze in Fig. 2 $S_{i,j} = S(\rho_{i,j})$, which describes all quantum correlations between the dimer i, j and the rest of the system. Interestingly, $S_{i,j}$ has for all i, j the same qualitative behavior of S_i at critical points. Such a feature is confirmed by our calculations in correspondence of all QPTs. This is expected within our scheme, since S_i and $S_{i,j}$ both describe the same correlations, Q2 and QS.

Conclusions.—We have studied the behavior of different measures of correlations in correspondence of QPTs for a solvable model of correlated electrons on a chain, displaying different kinds of metal-insulator-superconductor transitions. As a general output of our work, the role of quantum mutual information in the investigation of QPTs has been recognized. In particular, the comparison of singularities of the latter quantity with singularities of single-site entanglement allows one to distinguish at each QPT the contribution of bipartite from that of multipartite entanglement. At the same time, whenever a contribution from two-point quantum correlations is spotted, this can be used to test direct measures of bipartite entanglement. As an example, we tested the negativity, finding that in this case it does not capture all of the two-point quantum correlations, though it shows evidence of a diverging correlation length and interesting scaling behavior in the vicinity of the transitions ascribed to two-point correlations. The study of scaling properties of the proposed measures of entanglement and of total negativity [16] need to be further investigated.

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