How hidden orders generate gaps in one-dimensional fermionic systems

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We demonstrate that hidden long-range order is always present in the gapped phases of interacting fermionic systems on one dimensional lattices. It is captured by correlation functions of appropriate nonlocal charge and/or spin operators, which remain asymptotically finite. The corresponding microscopic orders are classified. The results are confirmed by DMRG numerical simulation of the phase diagram of the extended Hubbard model, and of a Haldane insulator phase.

The behavior of strongly correlated electron systems has been widely investigated to understand the physics of several phenomena in condensed matter, ranging from the insulating regime to high-T_c superconductivity. Due to the many degrees of freedom involved, many aspects of the micro- and macroscopic behavior of these systems remain unclear. Recently their simulation by means of ultracold gases of two-component fermionic atoms trapped onto optical lattices has opened new possibilities, leading for instance to the direct observation of the predicted magnetic[1] and Mott insulating (MI) phases.[2] The latter is efficiently modeled by the Hubbard Hamiltonian. In this case, it has been noticed quite recently[3] that in one dimension (1D) it is possible to identify a nonlocal order parameter in the MI phase, which displays long-range order (LRO); a result that is in agreement with Coleman-Hohenberg-Mermin-Wagner theorem[4] since no continuous symmetry of the system has been broken. The discovery envisaged a description of the underlying parity charge order, whose microscopic configurations are depicted below in the second cartoon of Fig. 1: The Mott phase consists of a chain of single fermions with up and down spin, where fluctuations of pairs of empty and doubly occupied sites (holons and doublons) are bounded. The behavior is reminiscent of that observed in the insulating regime of a degenerate gas of bosonic atoms.[5]

In general, the observation of gapped phases in 1D systems is not believed to be necessarily related to the presence of some type of LRO, since the strong quantum fluctuations are expected to destroy any such order. In this paper we show that LRO is instead hidden in *every* gapped phase of one-dimensional correlated fermionic systems. The result is achieved by means of a general analysis of the bosonization treatment applied on a prototype lattice model Hamiltonian for these systems. We identify in the lattice the nonlocal parity and string operators responsible for the different types of LRO. As a byproduct, both charge and spin excitations turn out to be independently ordered, while local operators intrinsically generate both. It is tempting to conclude that nonlocal operators are "more fundamental" with respect to the usual local ones, at least for the description of the possible orders in the ground state phase diagram of these systems. To test our results we perform a density matrix renormalization group (DMRG) analysis at half filling and zero temperature of the standard extended Hubbard case, focusing on the insulating phases.

We start from the general class of lattice model Hamiltonians introduced in Ref. 6 to describe the effects of Coulomb repulsion among electrons on their behavior, the standard Hubbard model being the most familiar example. The low energy behavior of these models is described by an effective Hamiltonian $\mathcal{H}$ obtained by bosonization treatment (see Ref. 7 and references therein). Upon neglecting terms of higher scaling dimension (see also Ref. 8), $\mathcal{H}$ turns out to be the sum of two decoupled sine-Gordon models. Explicitly, we have

$$\mathcal{H} = \sum_{\nu=c,s} \left(H_0^{(\nu)} + \frac{2g_\nu}{(2\pi\alpha)^2} \int dx \, \cos[q_\nu \sqrt{8}\, \Phi_\nu(x)] \right), \quad (1)$$

with $H_0^{(\nu)} = \frac{v_\nu}{2\pi} \int dx [K_\nu(\pi \Pi_\nu)^2 + K_\nu^{-1}(\partial_x \Phi_\nu)^2]$. Here Φ_ν is the compactified boson describing the charge ($\nu = c$) and spin ($\nu = s$) excitations, with velocity v_ν, Gaussian coupling K_ν, and conjugate momentum $\Pi_\nu = \partial_x \Theta_\nu/\pi$; α is a cutoff. Moreover, in terms of the standard notation $g_c \equiv g_{3\perp}\delta_{n,q_c^{-1}}$, the corresponding term generated from Umklapp processes being nonvanishing only at commensurate fillings $n = p/q$ (p,q integer; we assume $p = 1$); $g_s \equiv g_{1\perp}$, and $q_c = q$, $q_s = 1$.

The cosine terms in Eq. (1) become irrelevant in the renormalization group (RG) flow equations unless the fields Φ_ν are pinned to fixed values;[9] in this case, the energy is minimized by the choices

$$\sqrt{2}\Phi_\nu = \frac{\pi}{2q_\nu}(2l + 1), \quad g_\nu > 0 \qquad (2)$$

$$\sqrt{2}\Phi_\nu = \frac{\pi}{2q_\nu}2l, \quad g_\nu < 0 \qquad (3)$$

with $l \in \mathbb{N} \cup \{0\}$. Inspection of the RG equations shows that both choices of locked values for Φ_c amount to the opening of a charge gap Δ_c, whereas a spin gap Δ_s can open only for $g_s < 0$, due to the SU(2) spin symmetry of the Hubbard class of Hamiltonians. To resume, in all systems described by $\mathcal{H}$ it is possible to observe up to six phases (shown in Table I). In most phases the known dominant correlations of two-point local operators decay to zero with distance following a power law, in agreement with bosonization predictions. Only in charge-density and bond-ordered wave (CDW and BOW, respectively) phases—appearing when just onsite and nearest neighbors diagonal Coulomb interactions are present—LRO was identified with the nonvanishing in the asymptotic limit of appropriate two-point correlators of

TABLE I. Correspondence between ground state quantum phases and nonlocal operators that manifest LRO. We indicate with u when fields are unlocked.

	$q\sqrt{2}\Phi_c$	$\sqrt{2}\Phi_s$	Δ_c	Δ_s	LRO
LL	u	u	0	0	none
LE	u	0	0	open	$O_P^{(s)}$
MI	0	u	open	0	$O_P^{(c)}$
HI	$\pi/2$	u	open	0	$O_S^{(c)}$
BOW	0	0	open	open	$O_P^{(c)}, O_P^{(s)}$
CDW	$\pi/2$	0	open	open	$O_S^{(c)}, O_P^{(s)}$

local operators.[7] Quite recently it was noticed that for the standard Hubbard model LRO in MI and Luther Emery (LE) liquid phases is described instead by two-points correlators of suitable nonlocal operators.[3] In the present work we extend the idea of nonlocal order to all possible gapped phases of Table I for the general Hamiltonian $\mathcal{H}$.

First of all, we define for the lattice model the parity and string operators at a given site j as

$$O_P^{(v)}(j) = \prod_{l=1}^{j} e^{i\pi S_l^{(v)}}, \quad O_S^{(v)}(j) = S_j^{(v)} \prod_{l=1}^{j-1} e^{i\pi S_l^{(v)}}, \quad (4)$$

respectively, with $v = c, s$, and $S_j^{(c)} = (n_j - 1)$, $S_j^{(s)} = (n_{j\uparrow} - n_{j\downarrow})$. Here $n_{j\sigma}$ is the number operator counting the electrons with spin σ ($\sigma = \uparrow, \downarrow$) at site j, namely $n_{j\sigma} \equiv c_{j\sigma}^{\dagger} c_{j\sigma}$, $c_{j\sigma}$ being the operator which annihilates one electron of this type and $c_{j\sigma}^{\dagger}$ its Hermitian conjugate; moreover $n_j \equiv n_{j\uparrow} + n_{j\downarrow}$. The related two-point correlators $C_P^{(v)}(r) \equiv \langle O_P^{(v)}(j) O_P^{(v)\dagger}(j + r) \rangle$ (parity correlator), and $C_S^{(v)}(r) \equiv \langle O_S^{(v)}(j) O_S^{(v)\dagger}(j + r) \rangle$ (string correlator) can be approximated in the continuum limit according to the analysis outlined in Refs. 3 and 9, exploiting symmetry or antisymmetry under a particle-hole transformation. This gives

$$C_P^{(v)}(x) = \langle \cos\sqrt{2}\Phi_v(0) \cos\sqrt{2}\Phi_v(x) \rangle \quad (5)$$

$$C_S^{(v)}(x) = \langle \sin\sqrt{2}\Phi_v(0) \sin\sqrt{2}\Phi_v(x) \rangle, \quad (6)$$

where $\langle \rangle$ stands for the average evaluated in the ground state. From the above result one can realize that at least one of the parity or string correlators is nonvanishing for $x \to \infty$ in every gapped phase. Indeed these take place when some Φ_v is pinned to a fixed value, as shown in Table I. In that case we observe

$$\lim_{x \to \infty} C_\alpha^{(v)}(x) = \langle O_\alpha^{(v)} \rangle^2 \equiv C_\alpha^{(v)}, \quad \alpha = P, S,$$

and an order parameter $\langle O_\alpha^{(v)} \rangle$ emerges.

In Table I, LL stands for the gapless Luttinger Liquid phase, which is the only case without LRO, as both the bosonic fields Φ_v are unlocked. LE is the conducting phase with open spin gap which takes place for $\Phi_s = 0$, and is characterized by a nonzero $\langle O_P^{(s)} \rangle$. Charge-gapped phase with $\Delta_s = 0$ can open for (i) $\Phi_c = 0$ (MI), in which case $\langle O_P^{(c)} \rangle \neq 0$[3]; (ii) for $\Phi_c = \pi/\sqrt{8}$, which case we indicate as Haldane insulator (HI) since the Haldane-like string order $\langle O_S^{(c)} \rangle$ is nonvanishing. Finally, BOW and CDW phases are fully gapped phases with two
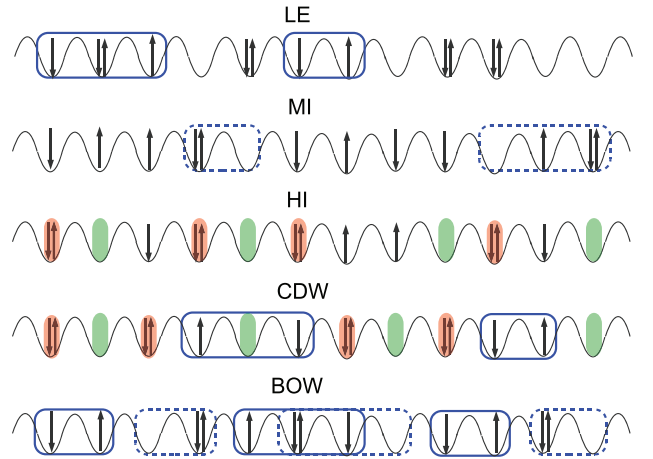

FIG. 1. (Color online) Cartoon illustrating the possible orders in presence of fluctuations. The blue continuous (dashed) lines show the correlated pairs of up-down spin (holon-doublon) allowing $\langle O_P^{(s)} \rangle$ ($\langle O_P^{(c)} \rangle$) to remain nonvanishing. The green and red circles show the alternation of sites occupied by doublons and holons in the chain of single fermions preserving $\langle O_S^{(c)} \rangle \neq 0$.

finite $\langle O_\alpha^{(v)} \rangle$'s. Only in these latter cases, the two nonlocal order parameters combine to form a local LRO, namely the BOW and CDW orders mentioned above.[7,9]

The nonvanishing of the parity and/or string correlators gives further physical insight about the kind of microscopic orders underlying the phases. These are illustrated schematically in Fig. 1. At half filling a nonzero value of the charge (spin) parity correlator implies the formation of bound pairs of holons and doublons (up and down spins) in a background of single electrons (holons and doublons) as it occurs in the MI (LE) phase.[3] Whereas a finite value of the charge (spin) string correlator amounts to a holon (spin up) always followed by a doublon (spin down) site on the holon-doublon (single electrons) sublattice created in a background of up and down electrons (holons and doublons). The microscopic configurations in the different phases unveil the mechanisms at the basis of the formation of charge and spin gaps. With respect to the perfect MI of singly occupied sites, the Mott charge gap at half filling is maintained by adding localized pairs formed by a doublon and a holon, whereas a HI charge gap takes place when the added doublons and holons do alternate into the sublattice they occupy. The LE case illustrates how an open spin gap, ideally amounting to a configuration with holons and doublons only, is preserved when single electrons are arranged in localized pairs with up and down spins; the observation giving a microscopic interpretation to the fact that superconducting correlations are dominant in such phase. Finally, combinations of the above possibilities determine the structures of the two fully gapped phases (CDW and BOW).

In order to support our predictions, we present below a numerical analysis of LRO parameters given by Eqs. (5) and (6) for the insulating phases of the extended Hubbard model at half filling in case of repulsive interactions. In this case the

lattice Hamiltonian reads

$$H = -t \sum_{j\sigma} (c_{j\sigma}^\dagger c_{j+1,\sigma} + \text{H.c.})$$
$$+ U \sum_j n_{j\uparrow} n_{j\downarrow} + V \sum_j n_j n_{j+1}, \qquad (7)$$

where U and V represent the diagonal on-site and neighboring sites contribution of the interaction potential; we fix the energy scale $t = 1$. Such a model is of fundamental relevance in condensed matter (see Refs. 7, 10, and 11, and references therein) and in the younger field of ultracold systems. Indeed, recent experiments with Fermi gas of magnetic atoms[12] or polar molecules[13] allow us to quantitatively simulate the Hamiltonian (7); both the interaction parameters can be tuned independently, by changing the direction of the dipoles with external fields, or by means of the transverse frequency of the laser used to create the lattice. In particular, we explore at half filling the regime of positive values of U and V, for which the phase diagram amounts to three insulating phases.

The analysis is performed using a DMRG algorithm on finite size chains with periodic boundary conditions. We have chosen to consider small system sizes, from $L = 12$ to 48, with up to 1600 DMRG states and six sweeps in order to have a good precision on our quantities.

The parity and string operators introduced above are expected to behave as order parameters for the three insulating phases. In details (see Table I), the asymptotic value of $\langle O_P^{(c)} \rangle$ should be the only nonvanishing parameter for the MI phase, whereas in the BOW phase also $\langle O_P^{(s)} \rangle$ should become different from zero at the MI-BOW transition. Finally, at the BOW-CDW transition $\langle O_s^{(c)} \rangle$ should become finite, while $\langle O_P^{(c)} \rangle$ becomes vanishing.

We have calculated $C_P^{(v)}(r) = \langle \exp(i\pi \sum_{l=j}^{j+r} S_l^{(v)}) \rangle$ and $C_S^{(v)}(r) = \langle S_j^{(v)} \exp(i\pi \sum_{l=j+1}^{j+r-1} S_l^{(v)}) S_{j+r}^{(v)} \rangle$; their asymptotic values have been evaluated at the midpoint $r = L/2$, upon an extrapolation in the thermodynamic limit (TDL) $L \to \infty$. Special care must be payed in separating the uniform and staggered parts of the parity operator, since the relation $C_P^{(c)}(r) = (-1)^r C_P^{(s)}(r)$ holds. Figure 2 collects our numerical results, showing a clear evidence of the expected behavior. Our findings can be compared with those obtained in Ref. 14 by considering the expectation value of a different nonlocal operator, namely the exponential position operator z_L. Since in bosonization analysis such value takes the form $\langle \cos \sqrt{8} \Phi_c \rangle$, it is different from zero for both pinned values of Φ_c allowed in an insulating phase, hence vanishing only at the conducting point where the BOW-CDW transition takes place.[15]

To enforce our analysis we also computed the Luttinger constants K_ν defined as $K_\nu \sim \lim_{q \to 0} \pi \mathcal{S}_\nu(q)/q$, with $\mathcal{S}_\nu(q) = \frac{1}{L} \sum_{kl} e^{iq(k-l)} (\langle S_{k,z}^v S_{l,z}^v \rangle - \langle S_{k,z}^v \rangle \langle S_{l,z}^v \rangle)$ in the TDL. These give precise information regarding the presence of gaps.[9] In particular the SDW-BOW belongs to the Berezinskii-Kosterlitz-Thouless universality class since a spin gap takes place entering in the fully gapped BOW phase, while maintaining a full rotational spin symmetry. The Luttinger theory predicts $K_s = 1$ in the gapless and $K_s = 0$ in the gapped phase. Numerically it is a hard task to get exactly these values since in the gapless phase logarithmic corrections affect the
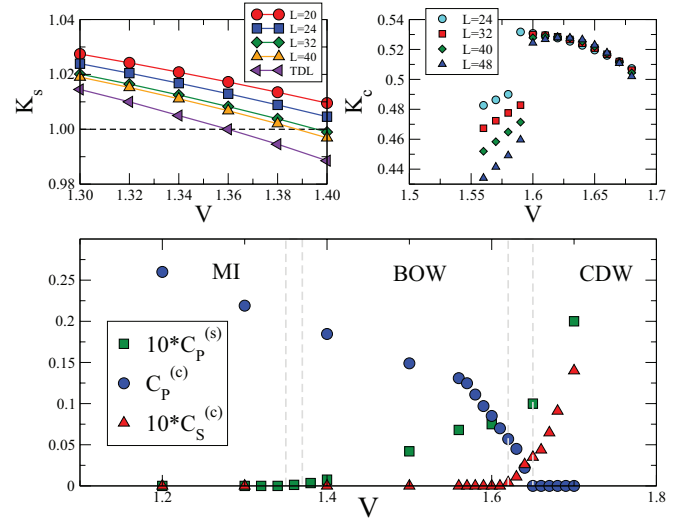

FIG. 2. (Color online) Lower panel: Nonlocal order parameters $C_\alpha^{(v)}(L/2)$ for $L \to \infty$ in the insulating phases of the extended Hubbard model (7) at $U = 3$. The dashed lines locate the critical points with uncertainty determined from the numerical analysis shown in the upper panels. Upper-left panel: K_s vs V at various L and in thermodynamic limit (TDL), the latter obtained by using a second order polynomial function. Continuous lines are guides for the eye. Upper-right panel: K_c vs V at various L. Numerical errors on the finite size data are of the order 10^{-6}, so the error magnitudes in the TDL turn out to be smaller than the symbol size.

results, while in the gapped region really large system sizes are necessary in order to get $K_s = 0$. It is customary to locate the transition point where K_s takes values smaller than 1 in the TDL. As shown in Fig. 2, the transition point obtained in this way is in good agreement with the one predicted by $O_P^{(s)}$. The BOW-CDW transition requires particular care since its nature can be either second or first order, depending on the value of U. Here we consider the region $U < 4$ where the transition is known to be second order. As shown in Ref. 11, while the two phases are fully gapped, due to the competition between the onsite and nearest-neighbor interactions the charge gap is minimal at the transition point, where it takes the value 0. Hence the theory predicts a Luttinger parameter $K_c \neq 0$ only at the gapless point and $K_c = 0$ elsewhere. In Fig. 2 we see that K_c develops a peak slightly dependent on the system size, where we locate the gapless point. Extrapolations in the TDL confirm the transition in the order parameters $\langle O_P^{(c)} \rangle$ and $\langle O_S^{(c)} \rangle$.

The scenario of Table I is completed by identifying the HI phase, where only $O_S^{(c)}$ is predicted to have finite LRO. The ground state phase diagram of the model (7) does not show such a phase.[16] Nevertheless, in Refs. 7 and 17 a charge gapped phase corresponding to the pinned value $\Phi_c = \pi/\sqrt{8}$ was identified by adding to the Hamiltonian (7) further correlated hopping terms of the form $X \sum_{\langle ij \rangle \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + \text{H.c.})(n_{i\bar\sigma} - n_{j\bar\sigma})^2$ for an appropriate range of values of U and V. Such a phase was denoted as bond-spin-density wave (BSDW), albeit the spin order cannot show LRO due to the unbroken SU(2) symmetry. On the basis of our analysis, since Φ_s is unpinned, we expect such a phase to exhibit the searched HI order. We
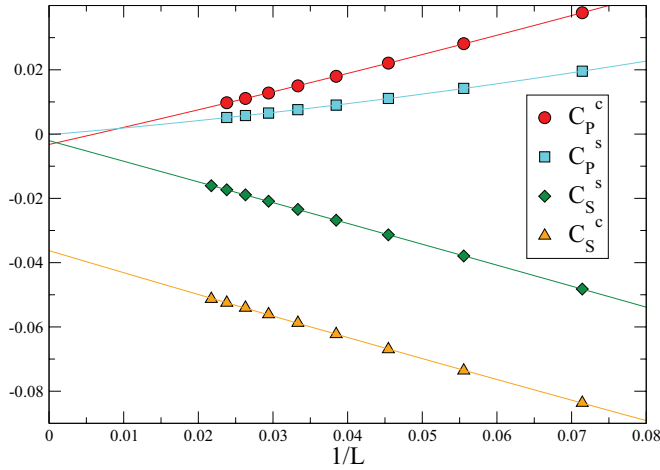
FIG. 3. (Color online) Nonlocal LRO in the Haldane insulator phase, at $U = 1$, $V = 0.5$ for the model (7) plus a correlated hopping term with $X = 0.25$ (see text). As predicted from Table I all correlation functions $C_\alpha^{(\nu)}(L)$ vanish asymptotically except for $C_S^{(c)}$. Continuous lines represent nonlinear fits for estimating the asymptotic limit.

have numerically estimated the nonlocal correlators $C_\alpha^{(\nu)}(L/2)$ at various L in a single point inside the phase ($X = 0.25$, $U = 1$, $V = 0.5$). The results shown in Fig. 3 demonstrate that, within the numerical errors, in the asymptotic limit (and in the TDL) the only operator that supports LRO is $O_S^{(c)}$, as expected.

Further nonlocal orders may appear in fermionic systems as a consequence of reduced symmetries. For instance, relaxing the SU(2) spin symmetry to U(1) × $\mathbb{Z}_2$, may allow for the appearance of the value $\Phi_s = \pi/\sqrt{8}$ in Eq.(1), giving rise to Haldane-like correlations in the z component of the spin. Further breaking of the two U(1) symmetries related to particle number conservation and spin rotation in the xy plane open the way to a pinning of the dual fields Θ_c and Θ_s, respectively. As a consequence the correlators related to the operators $\cos(\sqrt{2}\Theta_\nu)$ and $\sin(\sqrt{2}\Theta_\nu)$ are also finite, thus generating a transverse Haldane-type order, similarly to what happens in spin-1 chains[18] or in the bosonic case.[19,20] This simple argument suggests that, in order to observe a Haldane order in all directions in fermionic systems, one must extend interacting models like Eq. (7) by including pair creation terms of the kind

$\sum_{j\sigma}(c_{j\sigma}^\dagger c_{j+1,-\sigma}^\dagger + \text{H.c.})$. In addition, the partial particle-hole transformation $c_{j\downarrow} \to (-1)^j c_{j\downarrow}^\dagger$ (that changes $U \to -U$ in the ordinary Hubbard model) establishes a link between spin and charge sectors.[3] Such analyses represents an intriguing topic that goes beyond the scope of the present work and will be addressed elsewhere.

In this paper, we have proven that nonlocal LRO underlies all the gapped phases of a large class of lattice model Hamiltonians, describing 1D correlated fermionic systems. Our results give precise indications for detecting LRO, outlining the appropriate two-points nonlocal correlators to seek for in experiments with trapped dipolar atoms.[21] These are directly accessible to experimental detection in optical lattices via single site resolution imaging.[5,22]

The generality of the analysis here described suggests the presence of a universal mechanism extendable to any system in 1D, stating the presence of appropriate LRO in every phase that shows a gap in the excitation spectrum. The property of nonlocality is instead restricted to fermions and is not readily extendable to spin models, where a LRO may become local, for instance, after a Jordan-Wigner transformation. A related interesting topic still under debate concerns the relationship of nonlocality with topological phases,[23] duality,[24] and long distance entanglement.[25]

The possible presence of the discussed types of nonlocal orders in higher dimension could be addressed with the help of the cartoons in Fig. 1. In principle, the parity LRO can be extended from strings to membranes in arbitrary dimension. At variance, $O_S^{(\nu)}$ seems more difficult to generalize to higher dimension. With this in mind, it is reasonable to expect that phases with parity order parameters (MI, LE, and BOW) could be present also in two dimensions. The conjecture is consistent with recent results on the relevance of parity correlator in the MI phase of the 2D Bose-Hubbard model,[26] as well as with findings on backflow correlations in the 2D Hubbard model,[27] which emphasize the role of holon-doublon attraction in the MI phase.

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