Entanglement of indistinguishable particles as a probe for quantum phase transitions in the extended Hubbard model

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We study the entanglement of indistinguishable particles in the extended Hubbard model at half-filling, with focus on its behaviour when crossing the quantum phase transitions. Our results show that the entanglement either has discontinuities, or presents local minima, at the critical points, where the phase transitions occur. We identify the discontinuities as related to first order transitions, and the minima as second order transitions. Thus we show that the entanglement of particles can be used to derive the phase diagram, except for the subtle transitions between the superconductor phases TS-SS, and SDW-BOW.

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I. INTRODUCTION

A subject that has attracted much interest in the literature concerns the connection between two important disciplines of physics, namely, quantum information theory and condensed matter physics, generating great activity at the border of these disciplines, with numerous interesting questions have been addressed so far [1]. An important part of this field is related to the properties of entanglement in many-body systems, and in particular the analysis of its behaviour when the quantum system undergoes a quantum phase transition.

In this work we deal with the entanglement of indistinguishable fermionic particles in the one-dimensional extended Hubbard model (EHM). It is a generalisation of the Hubbard model [2], which encompasses more general interactions between the fermionic particles, such as an inter-site interaction, thus describing more general phenomena and a richer phase diagram. Precisely, it is given by,

\[ H_{\text{EHM}} = -t \sum_{j=1}^{L} \sum_{\sigma=\uparrow,\downarrow} (a_{j,\sigma}^{\dagger} a_{j+1,\sigma} + a_{j+1,\sigma}^{\dagger} a_{j,\sigma}) + U \sum_{j=1}^{L} \hat{n}_{j,\uparrow} \hat{n}_{j,\downarrow} + V \sum_{j=1}^{L} \hat{n}_{j} \hat{n}_{j+1}, \]

where \( L \) is the lattice size, \( a_{j,\sigma}^{\dagger} \) and \( a_{j,\sigma} \) are creation and annihilation operators, respectively, of a fermion with spin \( \sigma \) at the site \( j \), \( \hat{n}_{j,\sigma} = a_{j,\sigma}^{\dagger} a_{j,\sigma} \), \( \hat{n}_{j} = \hat{n}_{j,\uparrow} + \hat{n}_{j,\downarrow} \), and we consider periodic boundary conditions (PBC), \( L + 1 = 1 \). The hopping (tunnelling) between neighbour sites is parametrized by \( t \), while the on-site and inter-site interactions are given by \( U \) and \( V \), respectively.

Despite the apparent simplicity of the model, it exhibits a very rich phase diagram which includes several distinct phases: charge-density wave (CDW), spin-density wave (SDW), phase separation (PS), singlet (SS) and triplet (TS) superconductors, and a controversial bond-order wave (BOW). A more detailed description of the model and its phases will be given in the next section.

Our numerical analysis is performed employing entanglement measures for indistinguishable particles introduced recently [3–5], in conjunction with the density-matrix renormalisation group approach (DMRG) [6, 7], which has established itself as a leading method for the simulation of one-dimensional strongly correlated quantum lattice systems. DMRG is a numerical algorithm for the efficient truncation of the Hilbert space of strongly correlated quantum systems based on a rather general decimation prescription. The algorithm has achieved unprecedented precision in the description of static, dynamic and thermodynamic properties of one-dimensional quantum systems, quickly becoming the method of choice for numerical studies.

The article is organised as follows. In Sec. II we review the model and its phase diagram. In Sec. III we present the distinct definitions of entanglement in systems of indistinguishable particles, focusing on the notion of “entanglement of particles”, employed in this work, as well as its quantification. In Sec. IV we present our results for the behaviour of entanglement in the model. We conclude in Sec. V.

II. EXTENDED HUBBARD MODEL

In this section we give a detailed description of the extended Hubbard model, and its distinct phases. The reader familiar to the subject can skip to the next section.

Many efforts have been devoted to the investigation of the EHM’s phase diagram at half-filling, using both analytical and numerical methods [8–15]. Despite the apparent simplicity of the model, it exhibits a very rich phase diagram which includes several distinct phases: charge-
Considering a strong repulsive inter-site interaction, \( V \gg U \), leading to a charge-density wave (CDW). Its order parameter is

\[
\sigma = \langle \hat{n}_j \rangle = \frac{1}{2} \langle \hat{c}_j \hat{c}^\dagger_j \rangle.
\]

In the limit \( V \rightarrow \infty \), the ground state is dominated by the following configurations,

\[
|\psi\rangle_{cdw} \approx \frac{1}{\sqrt{2}} \left( \left| \uparrow \downarrow, 0, \uparrow \downarrow, 0, \ldots, \uparrow \downarrow_{L-1}, 0 \right> + \left| 0, \uparrow \downarrow, 0, \uparrow \downarrow, 0, \ldots, \uparrow \downarrow_L \right> \right) .
\]

In the range of strong attractive interactions, \( U/V < 0 \) or \( U > 0, V < 0 \) with \( |V| \gg |U| \), the fermions cluster together, and the ground state becomes inhomogeneous, with different average charge densities in its distinct spatial regions. Such a phase is called phase separated state. In the limit \( V \rightarrow -\infty \), the ground state is dominated by the following configurations,

\[
|\psi\rangle_{ps} \approx \frac{1}{\sqrt{L}} \sum_{\{\bar{n}\}} \hat{\Pi} \left| \downarrow, \uparrow, \ldots, \uparrow_{(\bar{z}), 0, \ldots, 0} \right> ,
\]

where \( \{\hat{\Pi}\} \) is the set of translational operators.

In the weak coupling limit, different phases appear. For small attractive inter-site interactions \( V < 0 \), superconducting phases are raised, characterized by the pairing correlations,

\[
\Delta_x = \frac{1}{\sqrt{L}} \sum_j a_j \uparrow a_{j+x} \downarrow ,
\]

and its respective order parameter \( O_s = \sum_{x,x'} \langle \Delta_x \Delta_{x'} \rangle \).

If the on-site interactions are lower than the inter-site interactions, \( U < -2V \), the fermions will pair as a singlet superconductor, characterized by a nearest-neighbor \( \Delta_{ss_{nn}} \) or on-site \( \Delta_{ss_s} \) singlet pairing correlations, given by,

\[
\Delta_{ss_{nn}} = \Delta_x - \Delta_{-x} = \frac{1}{\sqrt{V}} \sum_j (a_j \uparrow a_{j+x} \downarrow - a_j \downarrow a_{j+x} \uparrow),
\]

\[
\Delta_{ss_s} = \Delta_0 = \frac{1}{\sqrt{L}} \sum_j a_j \uparrow a_{j+1} \downarrow ,
\]

where \( x = 1 \). On the other hand, if the on-site interactions are higher than the inter-site interactions, \( U > 2V \), we have a triplet superconductor, characterized by a nearest-neighbor triplet pairing correlations \( \Delta_{ts_{nn}} \), given by,

\[
\Delta_{ts_{nn}} = \Delta_x + \Delta_{-x} = \frac{1}{\sqrt{V}} \sum_j (a_j \uparrow a_{j+x} \downarrow + a_j \downarrow a_{j+x} \uparrow),
\]

where \( x = 1 \).

Note that the difference between the singlet and triplet pairing correlations are simply a plus or minus sign, respectively. It can be clarified if we consider, for example, the case of two fermions in a singlet or triplet spin state, given respectively by \( \langle i| j \rangle \pm \langle j|i \rangle \) \( (|\uparrow\rangle \mp |\downarrow\rangle) \). Expand-
ing this state we have,
\[ |ij\rangle (|↑↓⟩ \mp |↓↑⟩) \mp |ji\rangle (|↑↓⟩ \mp |↓↑⟩), \]
\[ = |i\uparrow,j\downarrow⟩ \mp |i\downarrow,j\uparrow⟩ \pm |j\uparrow,i\downarrow⟩ - |j\downarrow,i\uparrow⟩, \]
\[ = (i\uparrow,j\downarrow) - (i\downarrow,j\uparrow) \mp (i\downarrow,j\uparrow)\mp (j\uparrow,i\downarrow), \]
\[ = \left(a_{m}^{\dagger}a_{n}^{\dagger} - a_{m}^{\dagger}a_{n}^{\dagger}\right) |\text{vac}\rangle, \quad (11) \]
identifying the $\mp$ ($\pm$) sign with the singlet (triplet) pairing correlation.

The last phase in the diagram is the controversial bond-order-wave (BOW). By studying the EHM groundstate broken symmetries using level crossings in excitation spectra, obtained by exact diagonalization, Nakamura [9] has argued for the existence of a novel bond-order-wave (BOW) phase for small to intermediate values of positive $U$ and $V$ in a narrow strip between the CDW and the SDW phases. This phase is characterized by alternating strengths of the expectation value of the CDW and the SDW phases. This phase is characterized by alternating strengths of the expectation value of the kinetic-energy operator on the bonds, characterized by the following order parameter,
\[ O_{\text{BOW}}(k) = \frac{1}{L} \sum_{m,n} e^{ik(m-n)} \left\{ \langle B_{m,m+1}B_{n,n+1} \rangle - \langle B_{m,m+1} \rangle \langle B_{n,n+1} \rangle \right\}, \quad (12) \]
where $B_{m,m+1} = (a_{m}^{\dagger}a_{m+1} + h.c.)$ is the kinetic-energy operator associated with the $n$th bond. Nakamura argued that the CDW-SDW transition is replaced by two separate transitions: (i) a continuous CDW-BOW transition; and (ii) a Berezinskii-Kosterlitz-Thouless (BKT) spin-gap transition from BOW to SDW. Such a remarkable proposal was later confirmed by several works [10–15], using different numerical methods for its study, such as density matrix renormalisation group (DMRG) method, Monte Carlo method, or exact diagonalization. Nevertheless, while the BOW-CDW phase boundary can be quite well resolved, since it involves a standard second-order (continuous) phase transition, the SDW-BOW boundary is more difficult to locate, for it involves a BKT transition in which the spin gap opens exponentially slowly as one enters the BOW phase. The precise location of the BOW phase is then still a subject of debate. The best estimates for the transitions, considering e.g. $U/t = 4$, corresponds to a CDW-BOW transition at $V/t \approx 2, 16$, and to a BOW-SDW transition at $V \approx 1.88 - 2.00$.

### III. Entanglement of Indistinguishable Particles

Despite being widely studied in systems of distinguishable particles, less attention has been given to the study of entanglement, or even a more general notion of quantum correlations, in the case of indistinguishable particles. In this case, the space of quantum states is restricted to symmetric $S$ or antisymmetric $A$ subspaces, depending on the bosonic or fermionic nature of the system, and the particles are no longer accessible individually, thus eliminating the usual notions of separability and local measurements, and making the analysis of correlations much subtler. In fact, there are a multitude of distinct approaches and an ongoing debate around the entanglement in these systems [3 16 27]. Nevertheless, despite the variety, the approaches consist essentially in the analysis of correlations under two different aspects: the correlations genuinely arising from the entanglement between the particles (“entanglement of particles”) [3 16 21], and the correlations arising from the entanglement between the modes of the system (“entanglement of modes”) [22–25]. These two notions of entanglement are complementary, and the use of one or the other depends on the particular situation under scrutiny. For example, the correlations in eigenstates of a many-body Hamiltonian could be more naturally described by particle entanglement, whereas certain quantum information protocols could prompt a description in terms of entanglement of modes. The modes notion associates a Fock space to the several distinguishable modes of a system of indistinguishable particles, which allows one to employ all the tools commonly used in distinguishable quantum systems. The entanglement of particles on the other hand has different definitions which may differ in its characteristics; but once one has opted for a certain definition, there are several proposed methods for its computation [3 5 25–31].

In this work we focus, as aforementioned, on the entanglement of indistinguishable particles (fermions) and its behaviour when crossing quantum phase transitions. The different definitions for the entanglement of particles agree with each other in the fermionic case, in the sense that the set of unentangled pure states is defined as the set of states than can described by a single-Slater determinant; more precisely, for a system with $N$ fermions, the set of pure states given by,
\[ |ψ⟩_{\text{un}} = a_{k_{1}}^{\dagger}a_{k_{2}}^{\dagger}...a_{k_{N}}^{\dagger} |\text{vac}\rangle, \quad (13) \]
where $\{a_{k_{i}}^{\dagger}\}$ is a general set of fermionic operators, i.e., $\{a_{k_{i}}^{\dagger}, a_{k_{j}}^{\dagger}\} = \{a_{k_{i}}, a_{k_{j}}\} = 0$, and $\{a_{k_{i}}^{\dagger}, a_{k_{j}}\} = δ_{k_{i}k_{j}}$.

A good quantifier for the entanglement is the entropy
\[ E_{p}(|ψ⟩⟨ψ|) = S(ρ_{p}) = - \log_{2} N, \quad (14) \]
where $ρ_{p} = Tr_{1...N}(|ψ⟩⟨ψ|)$ is the single-particle reduced state, and $S(ρ) = Tr(−ρ \log_{2} ρ)$ is the von Neumann entropy. Such a quantifier is obtained simply noticing that single-Slater determinant fermionic states stand as extremal states in the single-particle reduced space, also called “$N$-representable” space [32], and this relation is unique (all extremal states in the reduced space are also respective to a single-Slater determinant state).

If the Hamiltonian has some symmetries, its ground state entanglement can be analytically calculated as a
simple function of its quadratures \[3\]. In our particular case, from \( \hat{S}_z \) and translational symmetry in the extended Hubbard model, formally given by,

\[
Tr(a_i^\dagger a_j \rho_g) = 0, \quad \forall i, j, \quad (15)
\]

\[
Tr(a_i \rho_g) = Tr(a_j^\dagger a_{(i+\delta)} \rho_g), \quad (16)
\]

where \( a_i \) is the annihilation (creation) fermionic operators of a particle in the \( j \)th site, with spin \( \sigma \), and \( \rho_g = \langle g \rangle \langle g \rangle \) is the ground state of the Hamiltonian, we have that its single-particle reduced state, \( \rho_r(i\sigma, j\sigma) = \frac{1}{N} Tr(a_{j\sigma} a_{i\sigma} \rho_g) \), is disjoint in the subspaces with distinct spin, \( \rho_r = \rho_r^{\sigma=\uparrow} \oplus \rho_r^{\sigma=\downarrow} \), and each of these terms is given by a circulant matrix,

\[
\rho_r^\sigma = \frac{1}{N} \begin{pmatrix}
 x_0 & x_1 & \cdots & x_{L-2} & x_{L-1} \\
 x_{L-1} & x_0 & x_1 & \cdots & x_{L-2} \\
 \vdots & \vdots & \ddots & \vdots & \vdots \\
 x_2 & \cdots & \cdots & x_1 \\
 x_1 & x_2 & \cdots & x_{L-1} & x_0
\end{pmatrix},
\]

\[
x_\delta = \langle a_i^\dagger a_j \rangle, \quad (18)
\]

where \( L \) is the lattice size. In this way the matrix is easily diagonalised, and its eigenvalues \( \{ \lambda_k^\sigma \} \) are given by a Fourier transformation of the quadratures,

\[
\lambda_k^\sigma = \frac{1}{L} \sum_{\delta=0}^{L-1} e^{ik\delta x_\delta}, \quad k = \left[ 0, \frac{2\pi}{L}, \ldots, (L-1) \frac{2\pi}{L} \right]. \quad (19)
\]

The entanglement is then directly obtained from Eq. (14).

**IV. ENTANGLEMENT AND QUANTUM PHASE TRANSITIONS**

Our results with the entanglement of particles in the extended Hubbard model at half-filling are shown in Fig. 2 to be dissected below. It is quite remarkable that such picture highlights the known phase diagram of the model. We first note that, as physically expected, we have a maximum of entanglement at the strong coupling limits (\( E_p \rightarrow 1 \)), and as we decrease the interactions between the particles, the entanglement tends also to decrease its value, until the unentangled case for the non-interacting Hamiltonian (\( U = V = 0 \)); the figure thus presents the shape of a valley around this point. Following the discontinuities and the local minimum points in the entanglement, we can easily identify the quantum phase transitions, except for both the subtle transitions between the superconductor phases TS-SS, and the transition SDW-BOW. In the former case, it is quite reasonable the apathy of the measure on distinguishing the two phases, since the correlations between the particles in the two superconductors phases share essentially the same characteristics. For the SDW-BOW transition, one needs to recall that the simple observation of the BOW phase is by itself a hard task, since its gap opens exponentially slowly, and also that there are evidences that such transition is of infinite-order \[33 \[34\]; in this way we believe that a possible detection of such transition by the entanglement of particles would require higher precision numerical analysis as well as the study of larger lattice sizes.

The discontinuities in the entanglement are directly identified with the first order quantum phase transitions, whereas the minimum points are identified with the second order quantum phase transitions. The occurrence of such minima is due to the divergence of the correlation length when approaching the second order transitions, since, as noticed in the previous section, the eigenvalues \( \{ \lambda_k \} \) of the single-particle reduced state (Eq. (19)) are given in the momentum-space by the Fourier trans-
FIG. 3: (top) Single-particle quadratures $\langle a_L^j a_j \rangle$ along the lattice sites, and (bottom) momentum eigenvalues distribution $\lambda_k$ for the single particle reduced state in a fixed spin sector, as given in Eq. (19). We consider a fixed $U/t = 4$, and a system with $L = 128$ sites at half-filling. The vertical axis is in log-scale, in order to make clearer the visualisation. As we approach the BOW-CDW quantum phase transition point, at $V/t \simeq (2.16 \pm 0.03)$, we see that the quadratures tend to delocalise along the lattice, whereas the momentum eigenvalue distribution become more localised.

We present now the entanglement behaviour in some specific slices of the phase diagram, in order to clarify the above discussion and results. More specifically, we show the entanglement behavior in the PS-SS-CDW, PS-SS-SDW, and PS-SDW-CDW transitions.

A. PS-SS-CDW

In Fig. 4 we see the entanglement behavior across the PS-SS-CDW phases. We clearly see, for any fixed attractive on-site interaction ($U/t < 0$), a discontinuity in the entanglement followed by a local minimum point, as we increase the value of the inter-site interactions $V/t$. The discontinuity is related to the first order transition PS-SS, while the local minimum is related to the second order transition SS-CDW. We see, however, that the SS-CDW transition is not located exactly at $V/t = 0$, as expected from the phase diagram described in the literature, but at a value close to this one. We believe that this discrepancy is related to finite-size effects.

B. PS-TS-SDW

In Fig. 5 we see the entanglement behavior across the PS-TS-SDW phases. We see again the two kinds of behaviors for any fixed attractive inter-site interaction ($V/t < 0$): a first discontinuity, related to the first order transition PS-TS, followed by a local minimum point related to the second order transition TS-SDW. Note that, for large values of the attractive inter-site interaction, $V/t \simeq 1.5$, the discontinuity and minimum converge to the same point, and there is no $TS$ phase anymore.

C. PS-SDW-(BOW)-CDW

In Fig. 6 we see the entanglement behavior across the PS-SDW-(BOW)-CDW phases. We see that, as we increase the value of the inter-site interactions, for any fixed repulsive on-site interactions ($U/t > 0$), the entanglement identifies two transitions. Firstly we see a dis-
FIG. 5: Entanglement behavior across the PS-TS-SDW phases. The entanglement, for any fixed attractive inter-site interaction \((V/t)\), is characterized by a discontinuity (PS-TS transition), followed by a local minimum (TS-SDW transition). For large \(V/t\), the two transitions shrink at the same point, and there is no TS phase anymore. The red filled dots denote the local minimum points.

V. CONCLUSION

We have studied the entanglement of indistinguishable particles in the extended Hubbard model at half-filling, with focus on its behaviour when crossing the quantum phase transitions of the model. Our results showed that the entanglement either has discontinuities, or presents local minima, at the critical points. We identified the discontinuities as related to first order transitions PS-SDW, followed then by: (i) a discontinuity, when considering large \(U/t\), or (ii) a local minimum point, when considering small \(U/t\). Such discontinuity is related to the first order SDW-CDW transition, while the minimum points are related to the second order BOW-CDW transition (the SDW-BOW transition is not seen, as aforementioned in previous sections). We see that, the transitions to the CDW phase occur at \(U \approx 2V\), where for \(U/t = 4\), the BOW-CDW is located at \(V = (2.16 \pm 0.03)\), which agrees in good precision with the literature.

three main symmetry broken phases of the phase diagram, more specifically, the CDW, SDW and PS. Other phases were not identified due to the fact that they are associated to off-diagonal long-range order. Further investigation were performed analysing the block-block entanglement \([34, 36]\), i.e., the entanglement of a block with \(l\) sites with the rest of the lattice \((L - l\) sites), showing that this more general measure could in fact identify the superconducting phase, as well as the bond-order phase. The measure, however, could not identify the SS-TS transition, besides presenting some undesirable finite-size effects in the PS phase. On the other hand, the entanglement of particles studied in this work showed no undesirable finite-size effects in the PS phase, but could not also identify the superconductor SS-TS transition. Regarding the BOW phase, from the above discussion we see that it would be worth to analyse more general measures for the entanglement of particles, which encloses not only single-particle information. Some steps in the direction of a more general definition for the entanglement of par-
particles were made in [17], where it was defined a notion for the entanglement of “subgroups” of indistinguishable particles.

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