Quantum entanglement in fermionic lattices

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The Fock space of a system of indistinguishable particles is isomorphic (in a nonunique way) to the state space of a composite, i.e., many modes, quantum system. One can then discuss quantum entanglement for fermionic as well as bosonic systems. We exemplify the use of this notion—central in quantum information—by studying some, e.g., Hubbard, lattice fermionic models relevant to condensed matter physics.

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Much attention has been recently devoted to the notion of quantum entanglement [1]. As a matter of fact this fashion is mostly due to the vital role that such a notion is generally believed to play in quantum-information processing (QIP) protocols [2]. The definition of entanglement relies on the tensor-product structure of the state space of a composite quantum system [3].

On the other hand such a tensor-product structure is not present in a large class of systems of major physical interest: ensembles of *indistinguishable* particles. Indeed in this case it is known—basically since the birth of quantum theory—that the state space associated with N subsystems is constrained to be *subspace* of the N-fold tensor product. Depending on the bosonic or fermionic nature of the subsystems one has to select the totally symmetric or antisymmetric subspace. This is an instance of a *superselection* rule [5], i.e., a fundamental limitation on the possibility of preparing a given state.

We see therefore that the existence of quantum *statistics* [3] makes the notion of entanglement problematic for systems made of indistinguishable subsystems, e.g., particles. Notice that, even if one allows for general *parastatistics* [3], most of the product states $\otimes_{i=1}^N|i\rangle$ do *not* belong to the physical state space at all in that they do not have a proper transformation under permutations of $\mathcal{S}_N$, i.e., they do not belong to an $\mathcal{S}_N$ irrep [4].

Very recently some authors addressed the issue of entanglement (or more generally quantum correlations) in system of two fermions [6] and bosons [7]. Their approach appears to be the natural generalization of the one used for distinguishable particles.

In this paper we shall tackle the problem of the relation between entanglement and quantum statistics from a rather different perspective based on entanglement relativity as discussed in Ref. [8]. We shall mostly focus on the fermionic case [9]. In particular, we shall analyze the local, i.e., on-site entanglement associated with simple fermionic models on a lattice.

FERMIONS AND QUBITS

Let us start be recalling basic kinematical facts about many-fermion systems. Let $h_L:=\mathrm{span}\{|\psi_l\rangle\}_{l\in\mathbf{N}_L}$ ($\mathbf{N}_L:=\{1,\ldots,L\}$) be an L-dimensional *single-particle* state space. The labels in $\mathbf{N}_L$ will be referred to as *sites* and the associated single-particle wave functions will be thought of as describing a (spatially) localized state. Accordingly the set of l's will be referred to as a *lattice*.

Let $\mathcal{P}_L$ ($\mathcal{P}_L^N$) denote the whole family of subsets (with N elements) of $\mathbf{N}_L$. For any $A:=\{j_1,\ldots,j_N\}\in\mathcal{P}_L^N$ we define the antisymmetrized state vector

$$|A\rangle:=\frac{1}{\sqrt{N!}}\sum_{P\in\mathcal{S}_N}(-1)^{|P|}\otimes_{l=1}^N|\psi_{j_{P(l)}}\rangle. \tag{1}$$

The $|A\rangle$'s are an orthonormal set. The state space $\mathcal{H}_L(N)$ associated with N (*spinless*) fermions with single-particle wave functions belonging to h_L is given by the totally antisymmetric subspace of $h_L^{\otimes N}$, i.e., $H_L(N):=\mathrm{span}\{|A\rangle/A\in\mathcal{P}_L^N\}$. The fermion number ranges from 0 to L, the total *Fock* space is obtained as a direct sum of the fixed number of subspaces, i.e., $\mathcal{H}_L=\oplus_{N=0}^L H_L(N)=\mathrm{span}\{|A\rangle/A\in\mathcal{P}_L\}$. From the well-known relation $\dim\mathcal{H}_L=\Sigma_{N=0}^L\dim H_L(N)=\Sigma_{N=0}^L\binom{L}{N}=2^L$, it follows that the fermionic Fock space is isomorphic to an L-qubit space, each qubit being associated with a site [10]. The latter isomorphism is realized by the the mapping

$$\Lambda:\mathcal{H}_L\to(\mathbb{C}^2)^{\otimes L}:|A\rangle\to\otimes_{l=1}^L|\chi_A(l)\rangle, \tag{2}$$

where $\chi_A:\mathbf{N}_L\to\{0,1\}$ is the *characteristic* function of A. Clearly $\Lambda(|A\rangle)$ is nothing but a N-qubit basis state having in the jth site a 1 (0) if $j\in A$ ($j\notin A$). The zero-particle state $|\emptyset\rangle$ is mapped by Λ onto $|0\rangle:=|0\rangle^{\otimes L}$; thus the latter vector is referred to as *vacuum*.

In our considerations, once $\mathcal{H}_L$ is endowed by Λ with a multipartite structure, tensor products of individual single-particle spaces are not relevant anymore. To exemplify this point let us consider the case $L=3$. It is not difficult to see that all the states in $\mathcal{H}_3(2)$, seen as elements of $h_3^{\otimes 2}$, have the *same* entanglement. Indeed all of them can be written as $|a\rangle\otimes|b\rangle-|b\rangle\otimes|a\rangle$ for suitable $|a\rangle$ and $|b\rangle$ [11]. On the other hand both the "separable" state $|1\rangle\otimes|1\rangle\otimes|0\rangle$ and the "entangled" $(|0\rangle\otimes|1\rangle-|1\rangle\otimes|0\rangle)\otimes|1\rangle$ belongs to $\Lambda(\mathcal{H}_3(2))$. This kind of puzzle is solved by observing that the entanglement of, say $|a\rangle\otimes|b\rangle-|b\rangle\otimes|a\rangle$, is not *physical*. Indeed the involved subsystems, i.e., individual "labeled" particles, due to the very notion of indistinguishability, are physically not *accessible*.

This situation is just an illustration of the relativity of the notion of entanglement [8]. The latter crucially depends on the choice of a particular partition into physical subsystems. In this case "good" subsystems are associated with the set of single-particle modes (labeled by $l\in\mathbf{N}_L$) whose occupation numbers are physical observables and *not* with the particles themselves. From this perspective one can have entanglement *without* entanglement. For instance, a one-particle state, e.g., $|0\rangle\otimes|1\rangle+|1\rangle\otimes|0\rangle$, can be—with respect to the partition into mode subsystems—entangled. It is important to stress that such a kind of one-particle entanglement (or correlation), despite its paradoxical nature, has been recently proven to allow for quantum teleportation [12]; therefore it has to be regarded as a genuine *resource* for QIP.

The Fock space $\mathcal{H}_L$, since it allows for a varying particle occupation, does *not* correspond generally to the state space of a physical system. For charged fermions coherent superpositions of vectors belonging to different particle-number sectors are forbidden due to the charge superselection rule [5]. In this sense our qubits are *unphysical*. Only qubit states in the $\Lambda(\mathcal{H}_L(N))$ are associated with (N-particle) physical states. Accordingly not all the elements of $\mathrm{End}(\mathcal{H}_L)$ correspond to physical observables: the latter span the subalgebra $\mathcal{F}$ of number-conserving operators, i.e., $\mathcal{F}:=\{X/[X,N]=0\}=\oplus_N\mathrm{End}(\mathcal{H}_L(N))$.

LOCAL ENTANGLEMENT

Let $|\Psi\rangle\in\mathcal{H}_L(N)$ be the associated jth *local*-density matrix given by $\rho_j:=\mathrm{Tr}_{\underline{j}}|\Psi\rangle\langle\Psi|$, where $\mathrm{Tr}_{\underline{j}}$ denotes the trace over all but the jth sites. For any $j\in\mathbf{N}_L$ one obtains a bipartition of $\mathcal{H}_L$, i.e., $\mathbb{C}^2\otimes(\mathbb{C}^2)^{\otimes(L-1)}$ therefore the entropy S (von Neumann as well as linear) of ρ_j is a measure of the entanglement of the jth site with the remaining $N-1$ ones.

Local entanglement is *relative* to the decomposition into subsystems, i.e., sites defined by mapping (2) [8]. One could consider different isomorphisms giving rise to *inequivalent* partitions into "local" subsystems. This fact can be clearly seen by introducing creation and annihilation operators $\{c_j\}_{j=1}^L\subset\mathrm{End}(\mathcal{H}_L)$ ($[a,b]_\pm=ab\pm ba$), which satisfy canonical (anti) commutation relations for (fermions) bosons,

$$[c_i,c_j]_\pm=0,\quad [c_i,c_j^\dagger]_\pm=\delta_{ij},\quad c_j|0\rangle=0\,(j\in\mathbf{N}_L). \tag{3}$$

Of course $\mathcal{H}_L=\mathrm{span}\{\Pi_{j=1}^L(c_j^\dagger)^{n_j}|0\rangle/n_1,\ldots,n_L\in\mathbf{N}_\infty\}$. If U is a $L\times L$ unitary matrix then it is well known that the following (Bogoliubov) transformation

$$c_i\rightarrow\tilde{c}_i:=\sum_{j=1}^L U_{ij}c_j\quad (i\in\mathbf{N}_L) \tag{4}$$

maps fermions (bosons) onto fermions (bosons) giving rise to an automorphism of the observable algebra. Accordingly new occupation-number representations $\Lambda_U:\Pi_{i=1}^L(\tilde{c}_i^\dagger)^{n_i}|0\rangle\mapsto\otimes_{i=1}^L|n_i\rangle$ ($n_i=0,1$) are defined. Clearly entanglement is strongly *relative* to the decompositions associated with different Λ_U's. Notice that even though automorphisms (4) have a single-particle origin, they define *nonlocal* transformations of the Fock space onto themselves. Indeed a mapping $W\in\mathcal{U}(\mathcal{H}_L)$ is local with respect to the subsystem decomposition associated with Λ_U iff $\Lambda_U W\Lambda_U^{-1}\in\Pi_{i=1}^L\mathcal{U}(\mathbb{C}^2)_i$.

As a particular, though quite relevant, case one can consider Fourier transformation, i.e., $U_{kj}:=e^{ikj}$, $k:=2\pi(l-1)/L$ ($l\in\mathbf{N}_L$). The wave vectors k label the so-called reciprocal lattice (Λ_U is denoted by Λ^*) and represent physical modes delocalized over the spatial lattice. It is obvious that states that are entangled (nonentangled) with respect Λ can be nonentangled (entangled) with respect Λ^*.

The situation we shall investigate in this paper is the following. Suppose $H\in\mathrm{End}(\mathcal{H}_L)$ is a nondegenerate (grand-canonical) Hamiltonian and $H=\Sigma_m\epsilon_m|\epsilon_m\rangle\langle\epsilon_m|$ is its spectral decomposition. If ρ_j^m denotes the jth local-density matrix associated with the energy eigenstate ϵ_m, one can compute the quantity

$$S_{1/\beta}:=\frac{1}{ZL}\sum_{m=1}^{2^L}e^{-\beta\epsilon_m}\sum_{j=1}^L S(\rho_j^m), \tag{5}$$

where Z is the (grand-canonical) partition function, i.e., $Z:=\Sigma_{m=1}^{2^L}e^{-\beta\epsilon_m}$. Equation (5) is the thermal expectation value of the local entanglement averaged over the whole lattice [13]. In particular, we will be interested in the limit $\beta\mapsto\infty$, i.e., local entanglement S_0 in the *ground state*.

When the energy spectrum shows degeneracies, Eq. (5) is no longer well defined. We assume that there is a "natural" (see examples below) way to select a complete set of commuting observables containing H, whose joint eigenvectors provide the ϵ_m's to be used in Eq. (5).

To begin with, we observe that

$$\rho_i=|1\rangle\langle1|\langle\Psi|n_i|\Psi\rangle+|0\rangle\langle0|\langle\Psi|\mathbb{1}-n_i|\Psi\rangle, \tag{6}$$

where $n_i:=c_i^\dagger c_i=|1\rangle\langle1|_i\otimes\mathbb{1}_{\underline{i}}$ is the local occupation-number projector. Indeed $\langle1|\rho_i|1\rangle=\mathrm{Tr}(|1\rangle\langle1|,\rho_i)=\mathrm{Tr}(n_i\rho_i)=\langle\Psi|n_i|\Psi\rangle$ in the same way one obtains the other diagonal element of ρ_i. Moreover, $\langle0|\rho_i|1\rangle=\mathrm{Tr}(|1\rangle\langle0|\rho_i)=\mathrm{Tr}(c_i^\dagger\rho_i)=\langle\Psi|c_i^\dagger|\Psi\rangle=0$, the last equality is due to the fact that $|\Psi\rangle$ is a particle-number eigenstate, i.e., an eigenstate of the operator $\hat{N}:=\Sigma_{j=}^L n_j$.

Itinerant Fermions. We now consider free (spinless) fermions hopping in the lattice. The Hamiltonian is given by

$$H_{\mathrm{Free}}=-t\sum_{j=1}^{L-1}(c_{j+1}^\dagger c_j+\mathrm{H.c.})-\mu\hat{N}. \tag{7}$$

Introducing the Fourier fermionic operators $c_k:=1/\sqrt{L}\Sigma_{j=1}^L e^{ikj}c_j$, it is a textbook exercise to prove that Eq. (7) has eigenstates given by the N-particle vectors $|\mathbf{k}\rangle:=\Pi_{m=1}^L c_{k_m}^\dagger|0\rangle$ ($\mathbf{k}:=(k_1,\ldots,k_N)\in\mathbf{R}^N$ with eigenvalues $\epsilon_{\mathbf{k}}:=-2t\Sigma_{m=1}^N\cos(k_m)-\mu N$.

The local-density matrix is easily obtained by using Eq. (6) and the translational properties of the $|\mathbf{k}\rangle$'s. If T denotes the natural representation in $\mathcal{H}_L$ of the cyclic permutations $i \mapsto i+1 \pmod L$, i.e., the translation operator, one has $T|\mathbf{k}\rangle = \exp(\Sigma_{m=1}^N k_m)|\mathbf{k}\rangle$. Therefore

$$\langle \mathbf{k}|n_j|\mathbf{k}\rangle = (1/L)\Sigma_{i=1}^L \langle \mathbf{k}|n_i|\mathbf{k}\rangle = N/L =: n.$$

Whereby

$$E = (1/Z)\sum_{N=0}^{L} S(N/L)e^{\beta\mu N}Z_N(\beta)$$

$$= (1/Z)\mathrm{Tr}[S(\hat{N}/L)e^{-\beta H_{\mathrm{Free}}}],$$

in which $S(n) = -n\ln n - (1-n)\ln(1-n)$ and $Z_N(\beta) := \mathrm{Tr}_{\mathcal{H}_L(N)} e^{-\beta(H_{\mathrm{Free}}+\mu\hat{N})}$ is the (N-particle) canonical partition function.

The fraction $p(N) := e^{\beta\mu N} Z_N/Z$ gives of course the probability of having any N-particle configuration. In the thermodynamical limit $(N, L \mapsto \infty, N/L = \mathrm{const})$ $p(N)$ becomes strongly peaked around the expectation value N_0 of $\hat{N}$. In this case local entanglement is simply given by the Shannon function $E \sim S(n_0)$; it readily displays an intuitive feature: local entanglement vanishes for the empty (fully filled) lattice being the unique associated state, given the product $|0\rangle$ $(\otimes_l |1\rangle_l)$; moreover, E is maximal at half-filling, i.e., $n_0 = 1/2$. Notice that for the states $|\mathbf{k}\rangle$ entanglement associated with the Λ^* partition is obviously zero.

SPIN-(1/2) FERMIONS

Here we consider the lattice models of the spin-(1/2) fermion model. We have then to introduce an extra dicothomic variable $\sigma = \uparrow, \downarrow$ to label the single-particle state vectors. As usual, fermionic operators corresponding to different σ's always anticommute. In this case it is convenient to consider the 2^{2L}-dimensional Fock space as the isomorphic L-fold tensor power of four-dimensional space, i.e., $\mathcal{H}_F \cong (\mathbb{C}^4)^{\otimes L}$. The local state space is spanned by the vacuum $|0\rangle$ and the vectors

$$|\uparrow\rangle_j := c_{j\uparrow}^\dagger |0\rangle, \quad |\downarrow\rangle_j := c_{j\downarrow}^\dagger |0\rangle, \quad |\uparrow\downarrow\rangle_j := c_{j\downarrow}^\dagger c_{j\uparrow}^\dagger |0\rangle. \quad (8)$$

The $\rho_j = \mathrm{Tr}\, \underline{j}|\Psi\rangle\langle\Psi|$ is now a 4×4 matrix. If the N-particle state $|\Psi\rangle$ is (a) translational invariant and (b) an eigenstate of $S^z := \Sigma_{j=1}^L (n_{j\uparrow} - n_{j\downarrow})$, it is easy to see that $\rho_j = 1/L\ \mathrm{diag}(1 - N_\uparrow - N_\downarrow - N_l, N_\uparrow, N_\downarrow, N_l)$, where $N_\sigma := \Sigma_{j=1}^L \langle\Psi|n_{j\sigma}(1-n_{j-\sigma})|\Psi\rangle$ $(\sigma = \uparrow, \downarrow)$ is the number of lattice sites singly occupied by a σ fermion and $N_l := \Sigma_{j=1}^L \langle\Psi|n_{j\uparrow}n_{j\downarrow}|\Psi\rangle$ is the number of doubly occupied sites. We see that local entanglement in state $|\Psi\rangle$ is a function just of the occupation numbers N_α $(\alpha = \uparrow, \downarrow, l)$; in particular, it follows that Eq. (5) can be effectively computed for Hamiltonians commuting with the N_α's, i.e., $E = \Sigma_{\{N_\alpha\}} e^{\beta\mu N} S(\{N_\alpha\}) Z(\{N_\alpha\})/Z$. An instance of this case is illustrated in the following.

SUPERSYMMETRIC DIMER

We consider here a two-site, i.e., a *dimer*, version of the so-called supersymmetric Essler-Korepin-Schoutens (EKS) model [14]. For zero chemical potential, i.e., half-filling the EKS Hamiltonian acts on the basis states as follows:

$$H|\alpha\rangle \otimes |\beta\rangle = (-1)^{|\alpha||\beta|}|\beta\rangle \otimes |\alpha\rangle, \quad (9)$$

where $|\alpha|$ is the *parity* of the single-site state $|\alpha\rangle$, i.e., $|\uparrow| = |\downarrow| = 1$, $|0| = |\uparrow\downarrow| = 0$. Since H is just a *graded* permutator the relations $[H, N_\alpha] = 0$ hold true. The state space splits according to the N_α configurations $\mathcal{H}_L = \oplus_{\{N_\alpha\}} \mathcal{H}(\{N_\alpha\})$, and the Hamiltonian can be diagonalized within each sector. Notice that Eq. (9) is also invariant under a global *particle-hole* transformation, i.e., $|\sigma\rangle \leftrightarrow |-\sigma\rangle$, $|0\rangle \leftrightarrow |\uparrow\downarrow\rangle$.

It is straightforward to check that H admits four singlets nonentangled [the configurations (0, 0, 0), (2, 0, 0) along with their particle-hole conjugates] and six doublets [(1, 0, 0), (0, 1, 0) and conjugates and the self-conjugated (1, 1, 0), (0, 0, 1)] with entanglement ln 2. Moreover, since $H^2 = \mathbb{1}$, one gets an energy spectrum given by $\{-1, 1\}$, both being eigenvalues that are eightfold degenerate. Therefore $E = 12 \ln 2 \cosh\beta/16 \cosh\beta = 3/4 \ln 2$: the local entanglement (at half-filling) is temperature independent.

This very simple result is due to the large symmetry group of the Hamiltonian (9). A more interesting case is obtained introducing a model in which a free parameter controls the competition between the localized and itinerant nature of the lattice fermions.

HUBBARD DIMER

If H_{Free}^σ simply denotes Eq. (7) with an extra spin index, then the Hubbard Hamiltonian [15] reads

$$H_{\mathrm{Hubb}} = \sum_{\sigma=\uparrow,\downarrow} H_{\mathrm{Free}}^\sigma + U\sum_{j=1}^{L} n_{j\uparrow}n_{j\downarrow}. \quad (10)$$

The new local terms added account for the on-site interaction, e.g., Coulomb repulsion experienced by pairs of (opposite) spin fermions sitting on the same lattice site. By introducing the total fixed spin-number operators $\hat{N}_\sigma := \Sigma_{j=1}^L n_{j\sigma}$ $(\sigma = \uparrow, \downarrow)$ is easy to check that both of them commute with the Hubbard Hamiltonian (10). This implies that H_{Hubb} can be separately diagonalized in each joint eigenspace $\mathcal{H}(N_\uparrow, N_\downarrow)$ of the $\hat{N}_\sigma$'s. In the the dimer case, i.e., the *dimer*, one finds

$$\dim \mathcal{H}(N_\uparrow, N_\downarrow) = \Pi_\sigma \binom{2}{N_\sigma};$$

then at most (for $N_\uparrow = N_\downarrow = 1$) one has to solve a four-dimensional diagonalization problem.

The (unnormalized) ground state for the repulsive case $U > 0$ is given by $-G_0|0\rangle$, where

$$G_0 := c_{1\uparrow}^\dagger c_{1\downarrow}^\dagger + c_{2\uparrow}^\dagger c_{2a\downarrow}^\dagger + \alpha_+ (U/4t)(c_{1\uparrow}^\dagger c_{2\downarrow}^\dagger - c_{1\downarrow}^\dagger c_{2\uparrow}^\dagger), \quad (11)$$

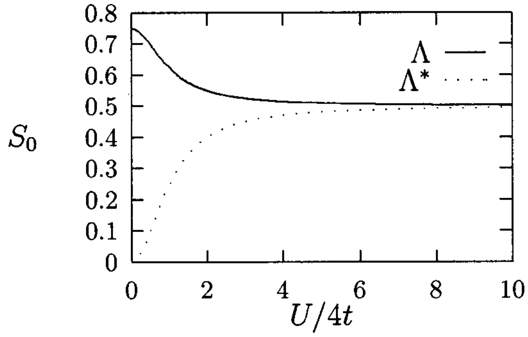

FIG. 1. Entanglement of the Hubbard dimer ground state as a function of $U/4t$ for decomposition associated with real and reciprocal lattice.

where $\alpha_{\pm}(x)=x\pm\sqrt{1+x^2}$, and the associated eigenvalue is given by $E_0=-2t\alpha_{-}$. The entanglement of the state (11) is easily studied as a function $U/4t$. Using linear entropy as an entanglement measure one finds $S_0(U/t)=1-\mathrm{Tr}\,\rho_0^2=1-1/2(\alpha_+^4+1)(\alpha_+^2+1)^{-2}$. Local entanglement is monotonically decreasing as a function of $U/4t$ (Fig. 1). In particular, one obtains the free limit $S_0(0)=3/4$ and the strong coupling limit $S_0(\infty)=1/2$ that correspond to ground states given by uniform superpositions of, respectively, four and two states [see Eq. (11)]. Of course the physical interpretation is quite simple: the higher the on-site repulsion U the more local charge fluctuations are suppressed and the smaller the number of available states. Eventually for infinite repulsion doubly occupied sites get decoupled and only spin fluctuations survive. In this regime the Hubbard model is known to be equivalent to an *antiferromagnetic* Heisenberg model for spin 1/2 [16]. The ground state as well as thermal entanglement for these (and related) models have been quite recently studied [17].

It is instructive to write the dimer ground-state creator (11) in terms of the Fourier operators $c_\sigma^{(\pm)}:=1/\sqrt{2}(c_{1\sigma}\pm c_{2\sigma})$ $(\sigma=\uparrow,\downarrow)$, from Eq. (11) one finds

$$G_0(\alpha)=\sum_{k=\pm}(1+k\alpha)c_\uparrow^{(k)\dagger}c_\downarrow^{(k)\dagger}. \qquad (12)$$

With respect to this reciprocal decomposition local entanglement is an *increasing* function of $U/4t$. From the free case, $\alpha=1$, which is unentangled up to strong coupling $\alpha=\infty$, which gives $S_0^*(\infty)=1/2$ (see Fig. 1).

The example of the Hubbard dimer shows that, not surprisingly, entanglement is well suited to analyze the interplay between itinerant and localized features of the Hubbard Model (10): the hopping term t (repulsion U) term is responsible for entanglement in the real (reciprocal) lattice decomposition.

CONCLUSIONS

In this paper we discussed some issues related to entanglement in the system of indistinguishable particles. For these systems quantum statistics applies and therefore their state space is not naturally endowed with a tensor-product structure.

Nevertheless, mappings between their Fock spaces and multipartite state spaces can be established (the well-known occupation-number representation) and then the usual definition of entanglement can be applied. For systems with L single-particle states available, the set of possible inequivalent decompositions into L subsystems (modes) is parameterized by the group $U(L)$ of Bogoliubov transformations.

We focused on simple, e.g., Hubbard, models of fermions on lattices, studying how, as a function of the model parameters, local entanglement varies both with respect to real and reciprocal lattice decomposition. Results suggest that this notion of entanglement is well suited to describe interplay between localization and itinerancy in these systems.

We believe that the approach pursued in this paper—besides establishing a connection between the field of quantum-information processing and condensed-matter physics—can provide physical insight into the study of interacting ensembles of indistinguishable particles.

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