Particle partitioning entanglement in itinerant many-particle systems

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Introduction — In recent years, concepts from quantum information have proved useful for condensed matter systems. One prominent example is the study of the entanglement between a part (A) and the rest (B) of the many-particle system, measured by the entanglement entropy $S_A$. The entanglement entropy, $S_A = -\text{tr} [\rho_A \ln \rho_A]$, is defined in terms of the reduced density matrix $\rho_A = \text{tr}_B \rho$ obtained by tracing out $B$ degrees of freedom.

To define a bipartite entanglement, one has to first specify the partitioning of the system into $A$ and $B$. The most commonly used scheme is to partition space, e.g., partition the lattice sites into $A$ sites and $B$ sites. However, for itinerant particles, with the wavefunction expressed in first-quantized form, one can meaningfully partition particles rather than space, and calculate entanglements between subsets of particles. Since each particle has a label in first-quantized wavefunctions, indistinguishability does not preclude well-defined subsets of particles. Note that, with such partitioning, $A$ or $B$ do not correspond to connected regions of space.

The distinction between particle entanglement and spatial entanglement was made relatively recently [1, 2, 3]. In work reported since then, particle entanglement has been shown to be a promising novel measure of correlations [2, 3, 4, 5, 6]. In fractional quantum Hall states this type of entanglement reveals the exclusion statistics inherent in excitations over such states [2, 3]. Similar insight arises from particle entanglement calculations in the Calogero-Sutherland model [4]. For one-dimensional anyon states, particle entanglement is found to be sensitive to the anyon statistics parameter [2, 3].

Clearly, entanglement between particles in itinerant systems is a promising new concept, potentially useful for describing subtle correlations and the interplay between statistics and interaction effects. A broad study of the concept and its utility is obviously necessary. Unfortunately, particle entanglement has till now been studied mostly in relatively exotic models, so that the literature lacks simple intuition about these quantities. This Letter fills this gap. We provide results for the simplest nontrivial itinerant fermionic and bosonic models, and present generic behaviors by generalizing available results.

We first present upper and lower bounds for the entropy of entanglement $S_n$ between a subset of $n$ particles and the remaining $N - n$ particles. We formulate a ‘canonical’ asymptotic form for fermionic and some bosonic systems. We present results for the two-site Bose-Hubbard model. Through this toy model, we identify two general mechanisms of obtaining nonzero particle entanglement in many-particle models. One mechanism is simply that of (anti-)symmetrization of wavefunctions, while the other is due to the formation of ‘Schrödinger cat’-like states. The second mechanism is shown to be fragile, in the same sense that cat states are fragile in macroscopic settings. We next switch to true lattice models, focusing on spinless fermions on a one-dimensional (1D) lattice with nearest-neighbor repulsion, sometimes known as the $t$-$V$ model. We find similar mechanisms at work, in a nontrivial setting. In addition, our study of the $t$-$V$ model enables us to present generic intuition about particle entanglement in many-particle systems, expressed in our canonical asymptotic language.

Bounds — A generic itinerant lattice system has $N$ particles in $L$ sites; we consider bosons or spinless fermions so that $N \leq L$. In every case, a natural upper bound for $S_n$ is provided by the (logarithm of the) size of the reduced density matrix $\rho_A = \rho_n$, i.e., the dimensions of the reduced Hilbert space of the $A$ partition. This size is $\binom{L}{n} = C(L, n)$ for fermions and $C(L - 1 + n, n)$ for bosons. The actual rank of $\rho_n$ can be much smaller due to physical reasons, so that the entanglement entropies are usually significantly smaller than the upper bounds, as we shall see in the examples we treat.

In a bosonic system, $S_n$ can vanish, since a Bose condensate wavefunction is simply a product state of individual boson wavefunctions, each identical. For fermions, however, anti-symmetrization requires the superposition of product states; for free fermions this causes $\rho_n$ to have $C(N, n)$ equal eigenvalues. This provides a nonzero lower bound for $S_n$ in a fermionic system.

Bosons: $0 \leq S_n \leq \ln C(L - 1 + n, n)$, \hspace{1cm} (1)

Fermions: $\ln C(N, n) \leq S_n \leq \ln C(L, n)$, \hspace{1cm} (2)

Canonical form — For large fermion number, $N \gg 1$,
we propose the following canonical form for the entanglement of \( n \ll N \) fermions with the rest:

\[
S_n(N) = \ln C(N,n) + \alpha_n + O(1/N) \\
= n \ln N + \alpha'_n + O(1/N).
\] (3)

This form is suggested by results reported in Refs. 2, 3, 4, 5, and in this Letter. For example, \( \alpha_n = n \ln m \) for the Laughlin state at filling \( v = 1/m \) 2. The same canonical behavior seems to hold for bosonic systems which lack macroscopic condensation into a single mode, \textit{e.g.}, bosonic Laughlin states 3, or hard-core repulsive bosons in one dimension 8.

Subtle correlation and statistics effects can be contained in the behavior of the \( O(1) \) term \( \alpha_n \), and sometimes also the \( O(1/N) \) term. Our calculations provide important intuition about how such effects show up in \( \alpha_n \), as we summarize at the end of this Letter.

Note that, for lattice sizes larger than \( N \), the generic behavior 8 indicates that the entanglement entropy does not saturate the upper bound (1) or 2 obtained from the size of the reduced Hilbert space.

Two-site Bose-Hubbard model — We start with a toy lattice model, with only two sites. We will consider \( N \) bosons on this ‘lattice’, subject to a Bose-Hubbard model Hamiltonian, to elucidate the basic mechanisms by which an itinerant quantum system can possess particle entanglement. The Hamiltonian is

\[
\hat{H} = -\left(\hat{b}_1^\dagger \hat{b}_2 + \hat{b}_2^\dagger \hat{b}_1\right) + \frac{1}{2} U \left(\hat{b}_1^\dagger \hat{b}_1 \hat{b}_2 \hat{b}_2^\dagger + \hat{b}_2^\dagger \hat{b}_2 \hat{b}_1 \hat{b}_1^\dagger\right).
\] (4)

For \( U = 0 \), the system is a non-interacting Bose condensate, with each boson packed into the state \( \frac{1}{\sqrt{2}} \left(\left| 1 \right> + \left| 2 \right>\right) \). In the \( U \rightarrow +\infty \) case, the system is a Mott insulator, with half the particles in site 1 and the other half in site 2. Such a state is simple in the “site” basis (second-quantized wavefunction), but involves symmetrization in the “particle” basis (first-quantized wavefunction), leading to nonzero particle entanglement entropy. Finally, the \( U \rightarrow -\infty \) limit involves all particles in either site 1 or site 2. The ground state is a linear combination of these two possibilities, which for large \( N \) is a macroscopic ‘Schrödinger cat’ state. Such a state is somewhat artificial, because an infinitesimal energy imbalance between the two states will ‘collapse’ this state. For example, a ‘symmetry-breaking’ term of the form \( \epsilon \hat{b}_1^\dagger \hat{b}_1 \), added to the Hamiltonian 4, would favor site 2 and destroy the cat state. The resulting state is a product state with zero particle entanglement.

Incidentally, a 2-site model with off-site interaction \( V \) (instead of on-site \( U \)) has similar physics, with negative (positive) \( V \) playing the role of positive (negative) \( U \).

Two bosons in two sites — There is only one way of partitioning two particles (\( n = 1 \)), so the only \( S_n \) is \( S_1 \). We expect \( S_1 = 0 \) at \( U = 0 \), and maximal entanglement \( S_1 = \ln 2 \) for both ‘Mott’ state at \( U = +\infty \) and the ‘Schrödinger cat’ state at \( U = -\infty \). The Hilbert space is small; one can diagonalize the problem and calculate \( S_1 \) analytically as a function of \( U \). We find \( S_1(U) = S_1(-U) \) interpolating smoothly between zero and \( \ln 2 \approx 0.6931 \) in both positive and negative directions (Fig. 1).

We also demonstrate the fragility of the cat state by showing the effect of an \( \hat{b}_1^\dagger \hat{b}_1 \) term. There is no appreciable effect for \( U > 0 \), but for \( U < 0 \) the cat state is destroyed and we get \( S_1 \rightarrow \infty \) for \( U \rightarrow -\infty \).

Many bosons in two sites — For \( N \) bosons, it is meaningful to study \( S_n \) with \( n > 1 \). Labeling the basis states by site occupancies, \textit{i.e.}, as \( |N_1, N_2\rangle \), the Mott and cat ground states are respectively \( |N/2, N/2\rangle \) and \( (|N,0\rangle + |0, N\rangle)/\sqrt{2} \). The \( n \)-particle reduced Hilbert space has dimension \( n + 1 \); the reduced-space basis states can be labeled by the number of \( A \) bosons in site 1. In the Mott state \(|N/2, N/2\rangle\), only the diagonal elements of \( \rho_n \) are nonzero and they are all equal; hence \( S_n(U \rightarrow -\infty) = \ln(n + 1) \). In the cat state, only two elements are nonzero, both on the diagonal; hence \( S_n(U \rightarrow -\infty) = \ln 2 \), independent of \( n \). Fig. 2 demonstrates, via calculation from wavefunctions obtained by numerical diagonalization, that \( S_n \) increases to \( \ln(n + 1) \) and \( \ln 2 \) in the \( U \rightarrow \pm \infty \) limits.

Both \( \rho_n(U) \) and \( S_n(U) \) can be understood in greater detail using approximations available in the literature 4. For \( U > 0 \), the coefficients \( \Psi_{N_1} \) of the ground state \(|GS\rangle = \sum_{N_1} \Psi_{N_1} |N_1, N - N_1\rangle \) can be approximated by a gaussian \( \Psi_{N_1} \propto \exp \left[ (N_1 - \frac{1}{2} N)^2/\sigma^2 \right] \), with \( N_0 = (1 + U N)^{1/2} \). The reduced density matrix then has off-diagonal elements of the form \( \exp(-\epsilon/\sigma^2) \), which vanish as \( U \) increases to the Mott limit. For \( U < 0 \) and \(|U|N \geq 2 \), the function \( \Psi_{N_1} \) can be approximated by two gaussians centered at separate points around \( N_1 = N/2 \). As the two peaks sharpen, we converge to the two-eigenvalue case described for \( U \rightarrow -\infty \). Fig. 2 shows that \( S_n \) changes rather sharply around \( U \sim -2/N \), for large \( N \).

To summarize our findings from the bosonic model, we note that the Mott state for \( U > 0 \) and Schrödinger cat state for \( U < 0 \) both possess particle entanglement. We have thus identified two generic mechanisms for generat-
ing particle entanglement in itinerant systems.

Spinless fermions in one dimension — We will now consider the 1D \( t-V \) model: \( N \) spinless fermions on \( L \) sites with periodic boundary conditions:

\[
H = -t \sum_{<ij>} \left( c_i^\dagger c_{i+1} + c_{i+1}^\dagger c_i \right) + VN_i n_{i+1}.
\]

We will use \( t = 1 \) units. For repulsive interactions at half filling \( (N = \frac{1}{2}L) \), this model has a quantum phase transition at \( V = 2 \), from a Luttinger-liquid phase at small \( V \) to a charge density wave (CDW) phase at large \( V \). We will focus mainly on \( V > 0 \). This model is solvable by the Bethe ansatz; however, calculating particle entanglement entropies \( S_n \) using the Bethe ansatz is a nontrivial problem which we do not address here.

Limits — For \( V = 0 \) (free fermions), the ground state is simple in terms of momentum-space modes: a Slater determinant of the \( N \) fermions occupying the \( N \) lowest-energy modes. The \( n \)-particle reduced density matrix has \( C(N,n) \) equal eigenvalues, so that \( S_n = \ln [C(N,n)] \), independent of the lattice size \( L \).

In the infinite-\( V \) limit, the ground state and hence particle entanglement can be simply understood for the case of half filling, \( N = \frac{1}{2}L \). The ground state is an equal superposition of two ‘crystal’ states, and each of them gives a separate contribution to the reduced density matrix. The reduced density matrix has rank \( 2C(N,n) \) and equal eigenvalues: \( S_n = \ln [2C(N,n)] \). In the notation of Eq. (3), the subleading term \( \alpha_n \) interpolates between \( \alpha_n = 0 \) at \( V = 0 \) and \( \alpha_n \to \ln 2 \) for \( V \to \infty \) for half filling. The interpolation details depend on \( n \) and \( N \).

Numerical results — For half-filling \( (N = \frac{1}{2}L) \), Fig. 3 presents \( S_n(V) \), calculated from wavefunctions obtained by direct numerical diagonalization. The \( S_n(V) \) function evolves from \( S_{FF} = \ln [C(N,n)] \) to \( \ln [2C(N,n)] \simeq S_{FF} + 0.6931 \). For \( n > 1 \), we see non-monotonic behavior in some cases. At present we have no detailed understanding of the states or particle entanglements at finite nonzero \( V \).

As in our bosonic model, we see Schrödinger cat physics in the \( t-V \) model also: the \( V = +\infty \) ground state is a superposition of two CDW states of the form [101010...10] and [010101...01]. The fragility of this cat state can be seen by adding a single-site potential, \( \epsilon c_1^\dagger c_1 \), or a staggered potential, \( \epsilon \sum_i c_i^\dagger c_{i+1} \). The ground state then collapses to a single crystal wavefunction, and \( S_n \) drops to \( \ln [C(N,n)] \) (Fig. 3 top panel).

Phase transition — The particle entanglement entropy shows no strong signature of the phase transition at \( V = 2 \). This is also true after extrapolating to the \( N \to \infty \) limit. (The extrapolated curves are very close to the largest-\( N \) curves displayed in Fig. 3 and so are not shown.) The lack of transition signature is not too surprising, because in the definition of the particle entanglement, the notion of distances (space) enters rather weakly. Thus \( S_n \) is not sensitive to characteristics of phase transitions, such as diverging correlation length or large-scale fluctuations.

Away from half-filling — For \( N \neq L/2 \), the behavior is qualitatively similar to the half-filled case, \( \alpha_n \) increasing from zero to an \( \mathcal{O}(1) \) value as \( V \) increases from zero to infinity. (Fig. 4) However, there is no simple picture for the \( V \to \infty \) limit. Also, \( \alpha_n(V) \) appears to be monotonic, perhaps because \( \alpha_n(V \to \infty) \) is not constrained as in the half-filled (CDW) case.

Note that, except for \( S_{n=1} \) in the half-filled case, the particle entanglement never saturates the upper bound, \( \ln [C(L,n)] \), dictated by Hilbert space size.

Negative \( V \) — An attractive interaction causes the fermions to cluster. In the \( V \to -\infty \) limit, the ground state is a superposition (cat state) of \( L \) terms, each a cluster of the \( N \) fermions. The cat state can be destroyed as in the positive-\( V \) case. For half-filling with even \( N \), the \( V \to -\infty \) wavefunction yields \( S_1 = \ln N + \ln 2 \). There are \( \mathcal{O}(N^{-1}) \) corrections for odd \( N = L/2 \).

Eigenvalue spectrum (majorization) — The full eigen-
value spectrum of the reduced density matrices ($\rho_n$) of course contain more information than the $S_n$ alone. For $n = 1$ where $S_1(V > 0)$ is monotonic, we numerically observe ‘majorization’ (e.g., Ref. [10]) of spectra. Obviously, there are many other aspects of the full spectra that remain unexplored.

Bosons — An important issue concerns bosonic systems which have partial condensation into a single mode, so that the leading asymptotic term is not $\ln N$. We have treated one example, closely related to the fermionic t-$V$ model: hard-core bosons on a 1D lattice (forbidden multiple occupancy, $U = \infty$) with nearest-neighbor interaction $V$. The point $V = -2$ has a ‘simple’ ground state [11], which we exploited to find

$$S_n = \nu n \ln N + \mathcal{O}(N^0)$$

where $\nu = N/L$ is the filling fraction. A natural interpretation is that the pre-factor represents the un-condensed fraction. Whether this is generic for bosonic systems with partial condensation remains an intriguing open question.

Correlations in subleading term — The canonical relation $S_n(N) = \ln |C(N, n)| + \alpha_n$ allows us to formulate correlation effects in terms of the function $\alpha_n$. For free fermions, for CDW states of the $t - V$ model, and for Laughlin states [2, 3], we have

$$\alpha_n(\text{FF}) = 0, \quad \alpha_n(\text{CDW}) = \ln 2, \quad \alpha_n(\text{FQH}) = n \ln m.$$

We note that states which are intuitively ‘more nontrivially correlated’ have stronger $n$-dependence in $\alpha_n$. This strongly suggests that the $\alpha_n$ function is a measure of correlations in itinerant fermionic states. It is natural to conjecture that the linear behavior of $\alpha_n$ is symptomatic of intricately correlated states like quantum Hall states, and that in generic itinerant states $\alpha_n$ will have sublinear dependencies on $n$.

Equal partitions — In addition to the $n \ll N$ behavior we have focused on here, another promising quantity is $S_{n=N/2}$. In Ref. [2] we presented close bounds for this quantity, showing that for fractional quantum Hall states of given filling $S_{n=N/2}$ tends to be higher for more correlated states. For example $S_{n=N/2}$ for a Moore-Read state is higher than that for a Laughlin state.

Conclusions — Particle entanglement is an emerging important measure of correlations in itinerant many-particle quantum systems. In this work, we have set the framework for future studies of the asymptotic behavior of particle entanglement. We have also explored these quantities in relatively simple itinerant models. We have pointed out several different mechanisms for particle entanglement in itinerant quantum states, such as localization, Schrödinger cat states, and of course antisymmetrization of fermionic systems. Since particle entanglement is a relatively new quantity on which little intuition is available, these results will form a much-needed basis for future studies.

Our work opens up a number of questions. Our considerations have led to an intriguing speculation for bosonic systems, relating the leading term in the asymptotic ($N \to \infty$) expression for $S_n(N)$ to the extent of Bose condensation. A thorough study, addressing several bosonic systems, is clearly necessary. In the same asymptotic form, one would also like to have a detailed characterization of how the subleading term $\alpha_n$ describes correlations. More concretely, one could ask “how correlated” a state needs to be, in order to have a linear $\alpha_n$ function.

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