Particle partitioning entanglement in itinerant many-particle systems

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For itinerant fermionic and bosonic systems, we study "particle entanglement," defined as the entanglement between two subsets of particles making up the system. We formulate the general structure of particle entanglement in many-fermion ground states, analogous to the "area law" for the more usually studied entanglement between spatial regions. Basic properties of particle entanglement are uncovered by considering relatively simple itinerant models.

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I. 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, $S_A = -\mathrm{tr}[\rho_A \ln \rho_A]$, is defined in terms of the reduced density matrix $\rho_A = \mathrm{tr}_B \rho$ 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 wave function 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 wave functions, 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.

Particle partitioning entanglement in a many-particle system is generally quite different from the entanglement between spatial partitions of the same system. The investigation of particle partitioning entanglement has started relatively recently [1–3]. In work reported since then, particle entanglement has been shown to be a promising novel measure of correlations [2–6]. In fractional quantum Hall states and in the ground state of the Calogero-Sutherland model, this type of entanglement reveals the *exclusion statistics* inherent in excitations over such states [2,4,5]. For one-dimensional anyon states, particle entanglement is found to be sensitive to the anyon statistics parameter [6,7].

Clearly, entanglement between particles in itinerant systems is a promising 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 been studied up to now mostly in relatively exotic models, so that the literature lacks simple intuition about these quantities. This paper fills that 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 next present results for a 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 wave functions, 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.

II. GENERIC CONSIDERATIONS

Before analyzing specific systems, we start with some results that we expect to be universal for itinerant quantum many-particle states.

Bounds. A generic itinerant lattice system has N particles in L sites; we consider bosons or spinless fermions so that $N \leqslant L$. 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 ρ_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 wave function is simply a product state of individual boson wave functions, each identical. For fermions, however, antisymmetrization requires the superposition of product states; for free fermions, this causes ρ_n to have $C(N,n)$ equal eigenvalues. This provides a nonzero lower bound for S_n in a fermionic system.

$$0 \leqslant S_n \leqslant \ln C(L-1+n,n) \quad \text{for bosons}, \tag{1}$$

$$\ln C(N,n) \leqslant S_n \leqslant \ln C(L,n) \quad \text{for fermions.} \tag{2}$$

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:

$$S_n(N) = \ln C(N,n) + \alpha_n + O(1/N^\gamma) = n \ln N + \alpha'_n + O(1/N^\gamma), \tag{3}$$

with $\gamma > 0$. This form is suggested by results reported in Refs. [2,4–6], and in this paper. For example, $\alpha_n = n \ln m$ for the Laughlin state at filling $\nu = 1/m$ [2]. The same canonical behavior seems to hold for bosonic systems that lack macroscopic condensation into a single mode, e.g., bosonic Laughlin states [4], 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 α_n, and sometimes also the $O(1/N^\gamma)$ term. Our calculations provide important intuition about how such effects show up in α_n, as we summarize at the end of this paper.

Note that, for lattice sizes larger than N, the generic behavior (3) indicates that the entanglement entropy does not saturate the upper bound (1) or (2) obtained from the size of the reduced Hilbert space.

III. 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

$$\hat{H} = -(\hat{b}_1^\dagger \hat{b}_2 + \hat{b}_2^\dagger \hat{b}_1) + \frac{1}{2} U(\hat{b}_1^\dagger \hat{b}_1^\dagger \hat{b}_1 \hat{b}_1 + \hat{b}_2^\dagger \hat{b}_2^\dagger \hat{b}_2 \hat{b}_2). \tag{4}$$

For $U=0$, the system is a noninteracting Bose condensate, with each boson packed into the state $\frac{1}{\sqrt{2}}(|1\rangle + |2\rangle)$. In the $U \to +\infty$ 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 wave function), but involves symmetrization in the "particle" basis (first-quantized wave function), leading to nonzero particle entanglement entropy. Finally, the $U \to -\infty$ 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 two-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 the "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 $\ln 2 \simeq 0.6931$ in both positive and negative directions (Fig. 1).

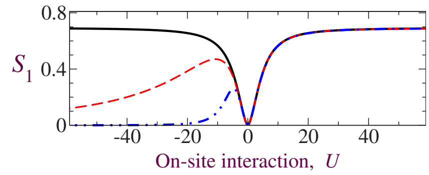

FIG. 1. (Color online) Entanglement between two bosons, in the ground state of a two-site lattice model with on-site repulsion. The solid curve is for the basic Bose-Hubbard model. Dashed ($\epsilon = 0.1$) and dash-dotted ($\epsilon = 0.1U$) curves illustrate the fragility of the "cat" state via an $\epsilon \hat{b}_1^\dagger \hat{b}_1$ term.

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

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, i.e., as $|N_1, N_2\rangle$, the Mott and cat ground states are, respectively, $|N/2, N/2\rangle$ and $(|0,N\rangle + |N,0\rangle)/\sqrt{2}$. 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 ρ_n are nonzero and they are all equal; hence $S_n(U \to \infty) = \ln(n+1)$. In the cat state, only two elements are nonzero, both on the diagonal; hence $S_n(U \to -\infty) = \ln 2$, independent of n. Figure 2 demonstrates, via calculation from wave functions obtained by numerical diagonalization, that S_n increases to $\ln(n+1)$ and $\ln 2$ in the $U \to \pm\infty$ limits.

Both $\rho_n(U)$ and $S_n(U)$ can be understood in greater detail using available approximations [9]. For $U>0$, the coefficients Ψ_{N_1} of the ground state $|\mathrm{GS}\rangle = \Sigma_{N_1} \Psi_{N_1} |N_1, N-N_1\rangle$ can be approximated by a Gaussian $\Psi_{N_1} \propto \exp[(N_1 - \frac{1}{2}N)^2/\sigma^2]$, with $N\sigma^{-2} = (1+UN)^{1/2}$. The reduced density matrix then has off-diagonal elements of the form $\exp(-c/\sigma^2)$, which vanish as $U \to \infty$. For $U<0$ and $|U|N \gtrsim 2$, the function Ψ_{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 $U \to -\infty$. Figure 2

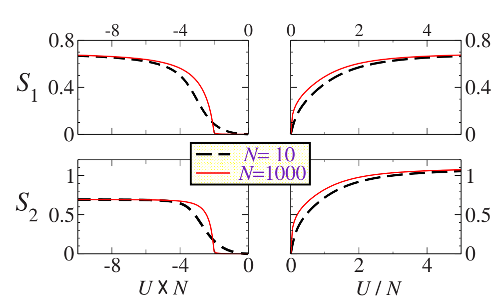

FIG. 2. (Color online) One- and two-particle entanglement entropies for N bosons in two sites.

shows that S_n changes rather sharply around $U\sim -2/N$ for large N.

Incidentally, the particle entanglements of this toy model are equivalent to the entanglements between spins in the Lipkin-Meshkov-Glick (LMG) model; our $UN=-2$ features appear at a field-driven phase transition in the LMG case [10]. For lattice models, however, particle entanglements generally have no simple spin analogies.

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

IV. SPINLESS FERMIONS IN ONE DIMENSION

We will now consider the 1D t-V model: N spinless fermions on L sites with periodic boundary conditions,

$$H = -t\sum_{\langle ij\rangle} (c_i^{\dagger}c_{i+1} + c_{i+1}^{\dagger}c_i) + Vn_in_{i+1}.$$

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. This model is solvable by the Bethe ansatz; however, calculating particle entanglement entropies S_n using the Bethe ansatz is a highly nontrivial problem.

Limits. For $V=0$ [free fermions (FF)], 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 α_n intrapolates 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 wave functions obtained by direct numerical diagonalization. The $S_n(V)$ function evolves from $S_{\mathrm{FF}}=\ln[C(N,n)]$ to $\ln[2C(N,n)]\simeq S_{\mathrm{FF}}+0.6931$. For $n>1$, we see nonmonotonic behavior in some cases. At present, we have no detailed understanding of the states or S_n 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 $|101010\ldots10\rangle$ and $|010101\ldots01\rangle$. 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, $\epsilon'\Sigma_i c_{2i}^{\dagger}c_{2i}$. The ground state then collapses to a single-crystal wave function, and S_n drops to $\ln[C(N,n)]$ (Fig. 3, top panel).

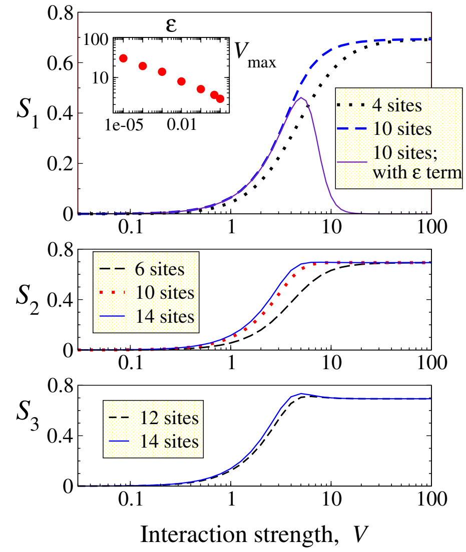

FIG. 3. (Color online) $n=1$, 2, and 3 entanglement entropy in the half-filled t-V model ($N=L/2$). The free-fermion contribution $\ln[C(N,n)]$ has been subtracted off. The $n=1$ plot also displays the effect of a symmetry-breaking $\epsilon c_1^{\dagger}c_1$ term, with $\epsilon=0.1$. Inset: position of the maximum as a function of ϵ.

Phase transition. The small-n particle entanglement entropies show no strong signature of the phase transition at $V=2$, even 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.) This is not too surprising because the notion or space enters rather weakly in the definition of particle entanglement; thus S_n is not too sensitive to diverging correlation length or large-scale fluctuations. It remains unclear whether sharper signatures appear for finite n/N (as opposed to our $n\ll N$).

Away from half-filling. For $N\neq L/2$, the behavior is qualitatively similar to the half-filled case, α_n increasing from zero to an $O(1)$ 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 superpo-

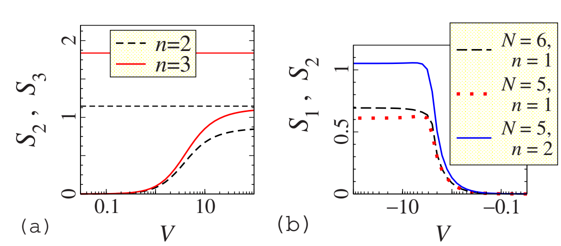

FIG. 4. (Color online) (a) S_n for $N=7$, $L=12\neq 2N$. Horizontal lines are corresponding maximal bounds $\ln[C(L,n)]$. (b) Negative V, half-filling. Free-fermion contribution $\ln[C(N,n)]$ has been subtracted off in each case.

sition (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 $V\to-\infty$ wave function yields $S_1=\ln N+\ln 2$. There are $O(N^{-1})$ corrections for odd $N=L/2$.

Eigenvalue spectrum (majorization). The full eigenvalue spectrum of the reduced density matrices (ρ_n) of course contains more information than the S_n alone. For $n=1$, where $S_1(V>0)$ is monotonic, we numerically observe "majorization" (e.g., Ref. [11]) of spectra. Obviously, there are many other aspects of the full spectra that remain unexplored.

Hardcore bosons. An important issue concerns bosonic systems that 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 [12], which we exploited to find

$$S_n = \nu n \ln N + O(N^0),$$

where $\nu=N/L$ is the filling fraction. A natural interpretation is that the prefactor represents the uncondensed fraction. Whether this is generic for bosonic systems with partial condensation remains an open question.

V. MANY-PARTICLE CORRELATIONS

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 α_n. For free fermions, for CDW states of the t-V model, and for Laughlin states [2,4], we have

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

where FQH denotes fractional quantum Hall. We note that states that are intuitively "more nontrivially correlated" have a stronger n dependence in α_n. This strongly suggests that the α_n function is a measure of correlations in itinerant fermionic states. It is natural to conjecture that the linear behavior of α_n is symptomatic of intricately correlated states like quantum Hall states, and that in generic itinerant states α_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. [4], 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.

VI. 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 α_n describes correlations. More concretely, one could ask "how correlated" a state needs to be in order to have a linear α_n function.

We have demonstrated that particle-partitioning entanglement tends not to saturate the upper bound provided by the size of the reduced Hilbert space. This is reminiscent of the "area law" for spatial entanglement, where the entropy of entanglement between a spatial block and the rest of the system is much smaller than the upper bound arising from the volume of the block.

Generally speaking, the information contained in particle-partitioning entanglement is very different from that contained in spatial entanglement. At this stage, we are not aware of applications of particle partitioning to specific condensed-matter issues or to the simulation of many-particle quantum states. However, given the conceptual richness of the findings on this quantity to date, particle-partitioning entanglement is likely to establish itself as an important tool in the description of quantum many-particle states.

Finally, we note that we have focused on $n\ll N$; S_n for finite n/N remain relatively unexplored. For example, one unanswered question is whether such S_n show clearer signatures of phase transitions compared to $S_{n\ll N}$.

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