Entanglement of indistinguishable particles in condensed-matter physics

Mark R. Dowling,[1,*] Andrew C. Doherty,[1,†] and Howard M. Wiseman[2,‡]

[1]*School of Physical Sciences, The University of Queensland, Queensland 4072, Australia*

[2]*Centre for Quantum Computer Technology, Centre for Quantum Dynamics, School of Science, Griffith University, Brisbane 4111, Australia*

The concept of entanglement in systems where the particles are indistinguishable has been the subject of much recent interest and controversy. In this paper we study the notion of entanglement of particles introduced by Wiseman and Vaccaro [Phys. Rev. Lett. **91**, 097902 (2003)] in several specific physical systems, including some that occur in condensed-matter physics. The entanglement of particles is relevant when the identical particles are itinerant and so not distinguished by their position as in spin models. We show that entanglement of particles can behave differently than other approaches that have been used previously, such as entanglement of modes (occupation-number entanglement) and the entanglement in the two-spin reduced density matrix. We argue that the entanglement of particles is what could actually be measured in most experimental scenarios and thus its physical significance is clear. This suggests that entanglement of particles may be useful in connecting theoretical and experimental studies of entanglement in condensed-matter systems.

I. INTRODUCTION

Recently there has been much interest in understanding and quantifying the entanglement present in quantum many-body systems. The aim of this program of research is to shed new light on systems, particularly strongly correlated systems, that are difficult to treat with conventional approaches. Most studies have focused on quantum spin systems, especially near quantum phase transitions, see for example Refs. [1–6] and references therein. The concept of entanglement is well defined in these systems as the spins can be considered distinguishable.

The subject of entanglement becomes more subtle when the system to be studied consists of many *indistinguishable* particles. Examples of such systems span many fields of physics: quantum optics, ultracold atomic gases, itinerant electrons, and superconductors. Even the question of which states are entangled is the subject much recent debate [7–18]. The difficulty arises from the lack of individual identity of the particles that are supposed to be entangled, which is manifest as the necessary symmetrization or antisymmetrization of the quantum wave function.

Wiseman and Vaccaro [17] have recently proposed a measure of entanglement for systems of indistinguishable particles that is operational in the sense that it quantifies the amount of "accessible" entanglement in the system where a local particle number superselection rule restricts the possible operations that may be performed. This is in contrast to other measures such as the mode entanglement, where the physical meaning of the entanglement measure is not so clear as the measurements required to demonstrate entanglement are not obviously possible. The rapidly developing field of

mesoscopic electronics may provide a useful testing ground for comparing different notions of entanglement in condensed-matter systems as experiments to demonstrate entanglement may be feasible in the near future [19–24].

The accessible entanglement, which is referred to as the "entanglement of particles" in Ref. [17], is defined as the amount of entanglement that could be extracted from the system and placed in conventional quantum registers, from which it could be used to perform quantum information processing tasks, such as teleportation. In many physical systems it may be difficult to extract all, or even some, of this entanglement, but the quantity itself may still give insight into the physical properties of the system. An analogy with thermodynamics is helpful. In thermodynamics it is often fruitful to consider quantities such as the amount of free energy in a system, even in the absence of an explicit scheme to extract that free energy. If the total entanglement is taken to be analogous to the total internal energy, then the accessible entanglement is analogous to the free energy.

In Ref. [17] the entanglement of particles was defined and evaluated for a number of states of indistinguishable particles. However, there is a lack of studies of entanglement of particles in explicit physical models. In this work we aim to fill this gap by investigating the entanglement of particles in a number of simple physical systems, and compare and contrast to other approaches to studying entanglement.

We begin in Sec. II by reviewing the definition of entanglement of particles and explaining its motivation in terms of superselection rules and measurements. In Sec. III we study ground and thermal states of systems of bosons and fermions with a small number of modes. We show that for any number of modes noninteracting bosons have zero entanglement of particles, as one might intuitively expect. However, noninteracting fermions can have nonzero entanglement of particles. We then study the effect of interactions on the entanglement of particles using the Bose-Hubbard and Fermi-Hubbard models as examples. We contrast the behavior of the entanglement of particles with

----

*Electronic address: dowling@physics.uq.edu.au

†Electronic address: doherty@physics.uq.edu.au

‡Electronic address: h.wiseman@griffith.edu.au

the entanglement of modes and show that the two measures can display opposite behavior as one varies the interaction parameter.

In Sec. IV we turn to multimode systems. In Sec. IV A we show how to calculate the entanglement of particles from correlation functions. A particularly striking example of entanglement of indistinguishable particles is the noninteracting electron gas as studied in Refs. [15,25]. In those works the "two-spin reduced density matrix"—a concept common in many-body physics—is used to study entanglement. It is shown that there is a finite length over which the noninteracting electrons are entangled. In Sec. IV B we show a similar effect in a lattice model of noninteracting electrons, where the entanglement persists over many lattice sites. In Sec. IV C we make the connection to the continuum explicit and argue that writing down a two-spin reduced density matrix on the lattice leads to difficulties in interpreting the entanglement. The subtle difficulty stems from the indeterminate number of particles at any particular location. Our results show that the phenomenon of entanglement of noninteracting electrons may feasibly be observed in an experiment.

II. SUPERSELECTION RULES, MEASUREMENTS, AND ACCESSIBLE ENTANGLEMENT

In this section we review the concept of entanglement of particles, as defined by Wiseman and Vacarro [17] and explain why we consider it an appropriate measure of entanglement in condensed-matter systems.

In many-body physics it is common to represent the state of a system in the *occupation-number representation*. If $\{\psi_j\}$ is a complete set of single-particle wave functions (for example, modes localized in position or momentum) then a many-particle state is written,

$$|\Psi\rangle = \sum_{\vec{n}} c_{\vec{n}} |\vec{n}\rangle, \tag{1}$$

where $\vec{n} = (n_1, n_2, \dots)$ is a set of occupation numbers for the single-particle modes (for fermions the occupation numbers are restricted to be 0 or 1 due to the Pauli exclusion principle), and the $c_{\vec{n}}$ are coefficients in the superposition. Formally, the space of occupation-number states is equivalent to a tensor product space where each mode is a factor (subsystem), and the occupation number of each mode represents a distinct state in that subsystem. It is thus tempting to define the "entanglement" in a many-body state as being with respect to this mode decomposition.

Following Ref. [17], for bipartite systems we may quantify the *entanglement of modes*, E_M, as

$$E_M(\rho_{AB}) = M(\rho_{AB}), \tag{2}$$

where M is some bipartite measure of entanglement (e.g., entanglement of formation, entanglement of distillation, negativity), A and B each control some subset of the total modes, and ρ_{AB} is the total state shared by A and B. This approach is advocated in, for example, Refs. [16,26,27]. The entanglement of modes depends on which modes A and B

control, as discussed in Refs. [28,29], but not on the local mode decomposition that they choose.

The difference between entanglement of particles, which we define shortly, and entanglement of modes stems from the local particle-number superselection rule which may apply to systems of massive particles. Operationally, a superselection rule (SSR) is a restriction on the allowed physical operations (closed or open evolution, preparation, measurement, etc.) on a system [30].

It is sometimes asserted that certain superselection rules apply *in principle* due to some underlying symmetry of the system, e.g., a SSR for charge that appears in Lorentz-invariant quantum field theories. However, it is possible to lift superselection rules by constructing an appropriate reference frame for the quantity in question, the most well-known example of this procedure being the thought experiment of Aharonov and Susskind [31].

Whether or not superselection rules apply in principle is not important for our purposes. We simply note that often a superselection rule applies in practice due to the lack of an appropriate reference frame. The example we will be concerned with is the superselection rule for *local* particle number. Consider a bipartite state of one particle superposed over two modes, where each party controls one of the modes:

$$|\psi_\theta\rangle_{AB} = (|1\rangle_A |0\rangle_B + e^{i\phi}|0\rangle_A |1\rangle_B)/\sqrt{2}. \tag{3}$$

The phase ϕ in this superposition is only meaningful relative to some shared reference frame. Two examples of systems that could act as a reference frame for this phase are a large coherent state of light if the particle were a photon, or a Bose-Einstein condensate if it were a Bosonic atom. However, without such a reference frame, as is generally the case in condensed-matter systems, the phase is not accessible to experiment and the state $|\psi_\theta\rangle$ is indistinguishable from the averaged state,

$$\bar{\rho}_{AB} = \int_0^{2\pi} \frac{d\theta}{2\pi} |\psi_\theta\rangle_{AB}\langle\psi_\theta|$$

$$= (|1\rangle_A\langle1| \otimes |0\rangle_B\langle0| + |0\rangle_A\langle0| \otimes |1\rangle_B\langle1|)/2, \tag{4}$$

which is an incoherent mixture of the particle being in one mode or the other.

Notice that in the above example averaging over the unknowable phase ϕ is equivalent to projecting onto fixed local particle numbers. This is a general result—if two parties, A and B, share a multimode state of indistinguishable particles, ρ_{AB}, and a local particle number superselection rule applies, then this state is indistinguishable from the averaged state,

$$\bar{\rho}_{AB} = \sum_{n_A, n_B} \Pi_{n_A, n_B} \rho_{AB} \Pi_{n_A, n_B}, \tag{5}$$

where Π_{n_A, n_B} projects onto fixed particle number n_A and n_B at A and B, and the sum runs over all possible local particle numbers [17].

For these reasons Wiseman and Vaccaro [17] argue that the entanglement of modes does not capture the true amount of entanglement that the two parties, A and B, share since in order to take advantage of it they would need to be able to

perform arbitrary local operations on the modes. In general such local operations would violate the local particle number superselection rule and are hence not possible in practice.

Wiseman and Vaccaro give an operational definition of bipartite entanglement of indistinguishable particles by using the concept of a *standard quantum register*—a set of distinguishable qubits [32]—which each party possesses. They define the *entanglement of particles* as the maximal amount of entanglement that the two parties can produce between their standard quantum registers by local operations on the modes that they have access to. Because the standard quantum registers consist of distinguishable qubits their entanglement may be measured by any standard measure of bipartite entanglement.

In Ref. [17] only pure states are considered, however, a definition of entanglement of particles E_P that applies for mixed states as well is

$$E_P(\rho_{AB}) = \sum_{n_A,n_B} P_{n_A,n_B} E_M(\rho_{AB}^{(n_A,n_B)}),\qquad(6)$$

where $\rho_{AB}^{(n_A,n_B)} = \Pi_{n_A,n_B}\rho_{AB}\Pi_{n_A,n_B}$ is the (unnormalized) state conditioned on obtaining the results n_A and n_B for a measurement of local particle number at A and B, $P_{n_A,n_B} = \mathrm{Tr}(\rho_{AB}^{(n_A,n_B)})$ is the probability of obtaining that result, and $E_M(\rho_{AB}^{(n_A,n_B)})$ is the entanglement of modes in $\rho^{(n_A,n_B)}$ [33]. In words, the entanglement of particles is the weighted sum of the entanglement of modes when local particle number is measured. It is sensitive, for example, to entanglement in spin between two particles at distinct spatial locations, but not to "occupation-number entanglement" such as exists mathematically in the state $|\psi_\theta\rangle$ above but would be impossible to extract in an experiment without a shared reference frame.

It would be most in the spirit of the operational definition to use the *distillable entanglement* [34] as the entanglement measure E_M. However, this measure is often difficult to calculate, so throughout this paper we use *entanglement of formation* instead, as it is generally easier to calculate. In general the distillable entanglement is less than the entanglement of formation, and it is possible for a quantum state to have nonzero entanglement of formation but zero distillable entanglement.

The effective measurement of local particle number that appears in the definition of entanglement of particles is formally due to a lack of phase reference, as discussed above. However, in many experimental scenarios the measurement does actually occur. For example, in measuring correlations in spin between electrons in a mesoscopic conductor a measurement of spin (up or down) simultaneously implies that an electron was also measured at the location of the detector. In measuring a mode or modes, e.g., momentum mode(s) in a mesoscopic conductor, the Hamiltonian coupling the measuring apparatus to the mode will typically commute with the total occupation number for the mode(s). It is straightforward to show that under these circumstances the set of generalized measurements (POVMs) [35] that can be implemented have Kraus operators that commute with the total occupation number. This implies that the generalized measurements obey

the superselection rule. An example of a measurement that does not commute with local particle number, and therefore does not obey the superselection rule, is a projective measurement in the basis $\{(|0\rangle + |1\rangle)/\sqrt{2}, (|0\rangle - |1\rangle)/\sqrt{2}\}$.

Practically it is often convenient to use entanglement witness to prove that a certain state is entangled. We note that entanglement of particles could be detected by measuring an entanglement witness that commutes with local particle number, as discussed for optical lattices in Ref. [36]. In other words states which are entangled in modes but not in particles are not detected by this type of entanglement witness.

III. SOME SIMPLE SYSTEMS

We now study some simple systems using the entanglement of particles in order to build intuition for its behavior before moving to multimode systems in the next section.

In order to share a state with nonzero entanglement of particles A and B must each be in control of at least two modes, and there must be at least two particles in the system. Therefore the simplest possible system in which there is entanglement of particles is two particles in four modes.

In these minimal systems the entanglement of particles is due solely to entanglement of the modes at A and B when there is one particle at each location [i.e., only the $n=1$ term from Eq. (6) contributes]. Because there are two modes at A and B we have an effective two qubit system for which it is possible to calculate the entanglement of formation in closed form as a function of the density matrix for pure [37] or mixed states [38].

A. Two bosons in four modes

Perhaps the simplest model for interacting bosons on a lattice is the Bose-Hubbard model. For four lattice sites (modes) the Hamiltonian is

$$\hat{H} = -t\sum_{j=0}^{3}(\hat{b}_j^\dagger\hat{b}_{j+1} + \hat{b}_{j+1}^\dagger\hat{b}_j) + U\sum_{j=0}^{3}\hat{n}_j(\hat{n}_j - 1),\qquad(7)$$

where $\hat{b}_j$, $\hat{b}_j^\dagger$ are the usual boson annihilation and creation operators that satisfy $[\hat{b}_j,\hat{b}_{j'}^\dagger]=\delta_{j,j'}$, $\hat{n}_j = \hat{b}_j^\dagger\hat{b}_j$ is the number operator for site j, and we have imposed periodic boundary conditions, $j+1=0$ for $j=3$.

For a fixed total number of bosons, $N=2$ say, we write out the Hamiltonian matrix in the Fock basis and calculate the eigenvalues and eigenstates. Figure 1 shows the entanglement of particles in the (nondegenerate) ground state of Eq. (7) as a function of U/t, where both A and B's sites are adjacent to one another. The other distinct partition, where A and B control diagonally opposite modes, never contains entanglement in either the ground or thermal state. At $U=0$ we have no entanglement of particles, as seems reasonable since the bosons are noninteracting.

In fact it is possible to show that the ground state of the noninteracting Bose-Hubbard model with an arbitrary number of sites has zero entanglement of particles for any possible bipartition. Consider an N-mode ring containing M noninteracting bosons. The ground state is
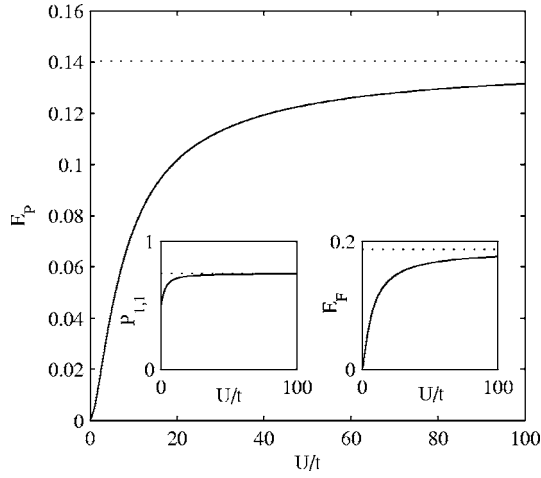
FIG. 1. Bipartite entanglement of particles in the ground state of two bosons in four modes with Bose-Hubbard Hamiltonian and periodic boundary conditions. A and B control adjacent modes in the ring. E_P is zero at $U=0$ (noninteracting bosons) and saturates at $(3/4)h(1/2+\sqrt{2}/3)\simeq 0.1405$ for large U/t corresponding to $P_{1,1}=3/4$ and $E_F=h(1/2+\sqrt{2}/3)$.

$$|g(N,M)\rangle = \frac{1}{\sqrt{N^M M!}}\left(\sum_{j=0}^{N-1}\hat{b}_j^\dagger\right)^M |\mathrm{vac}\rangle, \quad (8)$$

where $|\mathrm{vac}\rangle$ is the vacuum state containing zero particles in each mode. If A controls n_A modes and B n_B modes ($n_A+n_B=N$), and we project onto A and B having m_A and m_B bosons, respectively ($m_A+m_B=M$), then using the commutation relations amongst the boson modes,

$$\Pi_{m_A,m_B}|g(N,M)\rangle \propto \left(\sum_{j\in A}\hat{b}_j^\dagger\right)^{m_A}\left(\sum_{j\in B}\hat{b}_j^\dagger\right)^{m_B}|\mathrm{vac}\rangle,$$

$$\propto |g(n_A,m_A)\rangle|g(n_B,m_B)\rangle. \quad (9)$$

In words, the projected wave function is proportional to a factorized wave function where A or B's wave function is the ground state of their m_A or m_B noninteracting bosons as if their n_A or n_B modes were arranged in a ring. Therefore there is no entanglement of particles for any division of the lattice into A and B. By contrast the entanglement of modes is nonzero between any two partitions with respect to this spatial mode decomposition, even for noninteracting bosons.

For $U\neq 0$ we have nonzero entanglement of particles in the ground state, which increases with U/t and plateaus at approximately 0.1405. The limit of large U or small t, sometimes referred to as the hard-core boson limit, displays interesting behavior in terms of entanglement of particles. At precisely $t=0$ the ground state is sixfold degenerate corresponding to the six ways of arranging the two bosons in four modes such that no mode contains two bosons. Each of these canonical ground states has zero entanglement of particles. However, there are linear superpositions of these ground states that have nonzero E_P. In particular, using degenerate perturbation theory we find the $t\rightarrow 0$ limit of the (nondegenerate) ground state is the superposition

$$|g\rangle\rightarrow\left[|1,0,1,0\rangle + |0,1,0,1\rangle - \frac{1}{\sqrt{2}}(|1,1,0,0\rangle + |0,1,1,0\rangle\right.$$

$$\left.+|0,0,1,1\rangle + |1,0,0,1\rangle)\right]\Big/2. \quad (10)$$

The different coefficients in this sum can be understood as due to suppressed ability to tunnel when the particles are in adjacent modes; because U is much larger than t tunneling such that two particles end up on the same site is energetically unfavorable. From this expression we can see why the ground state has zero entanglement of particles in the diagonal partition ($A=\{1,3\}, B=\{2,4\}$) but nonzero E_P in the adjacent partition ($A=\{1,2\}, B=\{3,4\}$). The projected state for the diagonal partition is

$$\Pi_{1,1}|g\rangle\propto|1,1,0,0\rangle + |0,1,1,0\rangle + |0,0,1,1\rangle + |1,0,0,1\rangle$$

$$=(|0,1\rangle + |1,0\rangle)_A(|0,1\rangle + |1,0\rangle)_B, \quad (11)$$

which is separable. For the adjacent partition the projected state is

$$\Pi_{1,1}|g\rangle=\left[|1,0,1,0\rangle + |0,1,0,1\rangle + \frac{1}{\sqrt{2}}(|0,1,1,0\rangle\right.$$

$$\left.+|1,0,0,1\rangle)\right]\Big/2 \quad (12)$$

which is nonseparable—it has $E_F=h(1/2+\sqrt{2}/3)$, where $h(x)=-x\log_2(x)-(1-x)\log_2(1-x)$ is the binary entropy, and normalization $P_{1,1}=3/4$. Therefore entanglement of particles is

$$E_P(|g\rangle)=\frac{3}{4}h(1/2+\sqrt{2}/3)\simeq 0.1405. \quad (13)$$

At nonzero temperature T the canonical-ensemble thermal state is

$$\rho=\exp(-H/k_BT)/\mathcal{Z}, \quad (14)$$

where k_B is Boltzmann's constant. As $T\rightarrow 0$ the thermal state approaches Eq. (10) for small nonzero t, and so should contain entanglement of particles below some temperature. In particular, for the ground state to have the majority of the weight in the thermal-state mixture we need k_BT to be of order or less than the energy gap to the first excited state.

There are four states in the $t=0$ ground-state manifold that remain at energy 0 for small t. To first order in t, the state (10) has energy

$$E_g=-2\sqrt{2}t. \quad (15)$$

Therefore the energy gap for small t is of order $2\sqrt{2}t$, and the condition for entanglement of particles is

$$k_BT\lesssim 2\sqrt{2}t. \quad (16)$$

In Fig. 2 we plot the entanglement of particles in the thermal state as a function of the inverse temperature and the tunneling, both scaled by U to obtain dimensionless quantities. The plot is for small t/U and we see the type of scaling we expect—entanglement of particles appears at inverse
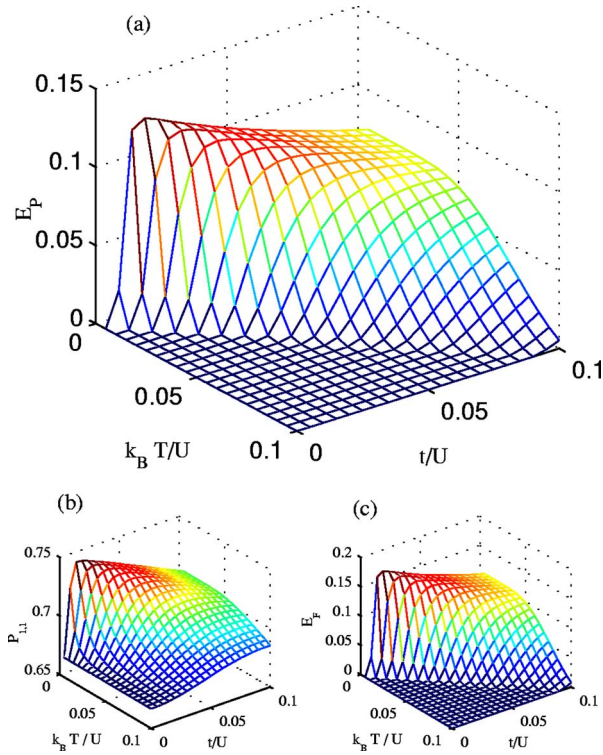
FIG. 2. (Color online) (a) Bipartite entanglement of particles in the canonical-ensemble thermal state of two bosons in four modes with Bose-Hubbard Hamiltonian and periodic boundary conditions. A and B each control adjacent modes in the ring, as in Fig. 1. (b) Probability of finding one particle at A and one at B, $P_{1,1}$. (c) Entanglement of formation of the *a posteriori* state $\rho_{AB}^{(1,1)}$.

temperatures proportional to the inverse of the tunneling, as in Eq. (16).

B. Two spinless fermions in four modes

We now study a precisely analogous model for fermions—noninteracting spinless fermions in a four-mode ring. The Hamiltonian is

$$\hat{H} = -t \sum_{j=0}^{3} (\hat{c}_j^\dagger \hat{c}_{j+1} + \hat{c}_{j+1}^\dagger \hat{c}_j), \qquad (17)$$

where $\hat{c}_j$, $\hat{c}_j^\dagger$ are fermion annihilation and creation operators, satisfying anticommutation relations $\{\hat{c}_j, \hat{c}_{j'}^\dagger\} = \delta_{jj'}$. Due to the Pauli exclusion principle it is not possible to have two spinless fermions on the same site so there can be no on-site interaction term.

It is straightforward to calculate the spectrum by Fourier transforming the annihilation operators, $\hat{C}_k = \frac{1}{2} \sum_{j=0}^{3} e^{2\pi i jk/4} \hat{c}_j$, $k = 0, \ldots, 3$. For $N = 2$ particles the ground state is twofold degenerate—a basis is

$$\{|g_1\rangle = C_1^\dagger C_0^\dagger |\text{vac}\rangle, \quad |g_2\rangle = C_3^\dagger C_0^\dagger |\text{vac}\rangle\}. \qquad (18)$$

As for bosons, the entanglement of particles in the ground or thermal state is zero for the diagonal partition. However, for the adjacent partition these basis states each have $P_{1,1} = 3/4$.

and $E_F = h(1/2 + \sqrt{2}/3)$. Furthermore, the equal mixture of these two states, i.e., the $T \to 0$ limit of the canonical-ensemble thermal state, has the same values for $P_{1,1}$ and E_F [39]. So we have the somewhat surprising result that even *noninteracting* fermions can have nonzero entanglement of particles in the ground state. This is in stark contrast to bosons, where in the noninteracting limit the entanglement of particles was zero. Mathematically the reason that noninteracting fermions can have nonzero entanglement of particles but noninteracting bosons cannot is that the commutation relations needed to obtain Eq. (9) as a local particle number projection from Eq. (8) do not hold for fermions.

Motivated by this counterintuitive behavior of noninteracting fermions we now turn to another simple, and perhaps more experimentally relevant, model of two fermions in four modes—the Hubbard dimer.

C. Hubbard dimer

The two-site Hubbard model (Hubbard dimer) for fermions with spin (e.g., electrons) is defined by the Hamiltonian

$$\hat{H} = -t \sum_{\sigma=\uparrow,\downarrow} (\hat{c}_{L\sigma}^\dagger \hat{c}_{R\sigma} + \hat{c}_{R\sigma}^\dagger \hat{c}_{L\sigma}) + U \sum_{j=L,R} \hat{n}_{j\uparrow} \hat{n}_{j\downarrow}, \qquad (19)$$

where $j = L, R$ is a position label and $\sigma = \uparrow, \downarrow$ is a spin label. The t term describes hopping between the two sites while conserving spin, and the U term is a Coloumb interaction between fermions on the same site.

The Hubbard dimer is a simple model for a number of physical systems, including the electrons in a H_2 molecule [40]. By varying t we have a model of bond breaking as the two atoms are separated.

The ground state may be calculated exactly as a function of U/t, see, e.g., Ref. [26],

$$|g\rangle \propto \hat{G}_0 |\text{vac}\rangle, \qquad (20)$$

where

$$\hat{G}_0 = \hat{c}_{L\uparrow}^\dagger \hat{c}_{L\downarrow}^\dagger + \hat{c}_{R\uparrow}^\dagger \hat{c}_{R\downarrow}^\dagger + \alpha(U/4t)(\hat{c}_{L\uparrow}^\dagger \hat{c}_{R\downarrow}^\dagger - \hat{c}_{L\downarrow}^\dagger \hat{c}_{R\uparrow}^\dagger), \qquad (21)$$

and $\alpha(x) = x + \sqrt{1+x^2}$.

For the purposes of calculating entanglement of particles it seems most natural to imagine party A controlling the up and down modes of one site and party B the up and down modes of the other site. With this partition we see that the entanglement of particles in the ground state comes entirely from the second term in Eq. (21), where there is one fermion at each site forming a singlet. The projected state, the singlet, has entanglement of formation equal to 1, and as U/t increases the probability $P_{1,1}$ increases from $1/2$ to 1 as the fermions are forced to localize on each site. At a fixed temperature we see that the entanglement of particles reaches a peak as a function of U/t. When interpreted as a model for H_2 bond-breaking the peak corresponds to an optimal distance at which the tradeoff between entanglement and probability of measuring one electron at each atom is maximized. However, in reality the Hubbard model is only a good approximation to the molecule when U/t is not too large or small [40], and at finite temperature vibrational modes will
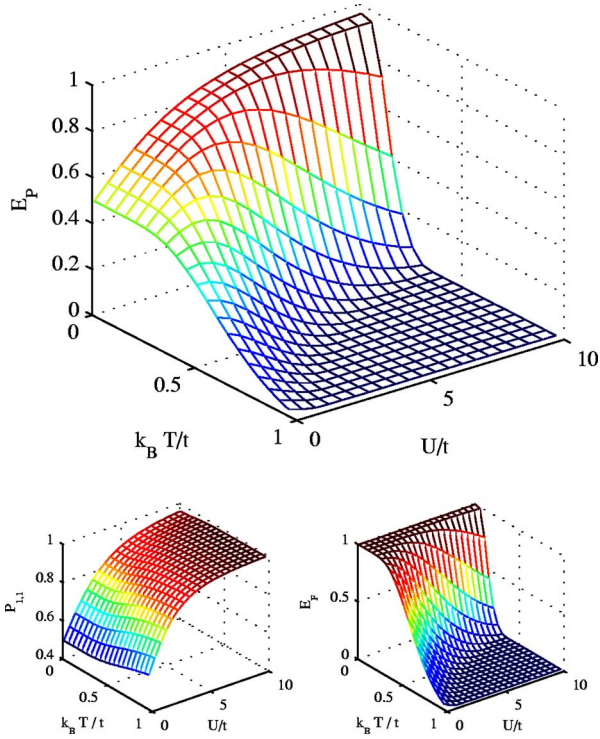
FIG. 3. (Color online) Bipartite entanglement of particles in the canonical-ensemble thermal state of the Hubbard dimer as a function of the scaled temperature $k_B T/t$ and on-site interaction U/t. A controls the up and down modes of one site and B the up and down modes of the other. The color represents the probability of finding one particle at each site and the height represents the entanglement of formation of the *a posteriori* state.

become relevant, so it is unclear whether this effect could actually be observed in H_2.

The behavior of the canonical-ensemble thermal state is plotted in Fig. 3. For any U/t the entanglement of formation of the projected state approaches 1 (singlet) as the system is cooled to the ground state ($k_B T/t \rightarrow 0$), whereas the probability $P_{1,1}$ approaches some value between 0 and 1 that increases with U/t (as the particles become more localized).

In Ref. [26] Zanardi performed a similar calculation of entanglement in the ground state of the Hubbard dimer. He calculates what we refer to as the entanglement of modes between the two sites, which does not distinguish local entropy arising from indefinite local particle number ("charge fluctuations") and that from entanglement of the spins ("spin fluctuations"). From his point of view the ground state becomes less entangled as one increases U/t as it goes from a superposition over four local states at each site ($0, \uparrow, \downarrow, 2$) to a superposition over just two ($\uparrow, \downarrow$). From the entanglement of particles viewpoint it is only the "spin fluctuations" that are due to accessible entanglement between the two sites, and these increase with U/t.

Zanardi also considers the entanglement of modes in the reciprocal (momentum) space, where the Fourier-transformed mode operators are $\hat{C}_{k\sigma} = (\hat{c}_{L\sigma} + e^{ik\pi} \hat{c}_{R\sigma})/\sqrt{2}$, for $k=0,1$, $\sigma = \uparrow, \downarrow$. In this mode representation the operator that creates the ground state, $\hat{G}_0$, may be written

$$\hat{G}_0 = \sum_{k=0,1} [1 + e^{ik\pi} \alpha(U/4t)] \hat{C}_{k\uparrow}^\dagger \hat{C}_{k\downarrow}^\dagger. \qquad (22)$$

We can see from this expression that the two fermions are perfectly correlated in momentum for any U/t—both terms create the two fermions in the same k mode, one up and one down. Therefore if A controls one k mode and B the other there is no entanglement of particles in this state.

Finally, one could imagine A controlling both up modes and B both down modes. To observe this type of entanglement we could, for example, use a magnetic field to separate up and down fermions. We could then look for entanglement of particles in the position or momentum degrees of freedom, post-selected on having one up and one down. From Eq. (21) or Eq. (22) we see that each term in the superposition has one fermion up and one fermion down, so $P_{1,1}=1$ and the entanglement of particles coincides with the entanglement of modes. Since we are guaranteed to have one up and one down, the change between position and momentum bases is a "local" change of basis [41] and the entanglement is therefore independent of this choice. It is equal to the mode entanglement between the momentum modes, as calculated in Ref. [26,42]—it increases from $E_F=0$ at $U/t=0$ to $E_F \rightarrow 1$ as $U/t \rightarrow \infty$.

The fact that one sees entanglement in position when the particles are distinguished by spin or entanglement in spin when the particles are distinguished by position may be viewed as a type of "dualism of entanglement," as addressed in Ref. [43].

Thus we see that there is rather subtle structure to the entanglement in the ground state of the Hubbard dimer that is not revealed by simply calculating the entanglement of modes. The subtlety is above and beyond the dependence of the mode entanglement on the choice of modes—it arises from considering how one might perform a measurement in practice to reveal this entanglement and is captured by the entanglement of particles.

IV. MULTIMODE SYSTEMS

Having studied the behavior of the entanglement of particles in a few small systems we now move to more-realistic systems containing many particles in many modes. This is typically the situation studied in condensed-matter physics; a Hamiltonian is specified in terms of annihilation and creation operators for bosons or fermions on a discrete set of lattice sites labeled by an index, say j. In order to begin to get a feel for the role of entanglement in such systems one may ask simple questions such as: is there entanglement between the spins of fermions on two distinct lattice sites, j_A and j_B? If we imagine A to have control of site j_A and B to have control of site j_B then this is precisely the situation addressed by the entanglement of particles—A and B share a state of indistinguishable particles of indefinite local particle number.

A. Entanglement of particles from correlation functions

We restrict our attention to fermions for the remainder of the paper as we have seen in Sec. III that they can display counterintuitive features of entanglement of particles that are

not seen for bosons. As an aid in answering questions such as the one posed above we show how to write the projected density matrices that appear in the definition of entanglement of particles in terms of correlation functions.

First note there are four possible local states at each site: $|0\rangle$, $|\uparrow\rangle$, $|\downarrow\rangle$, and $|2\rangle$ corresponding to zero fermions on the site, a single fermion with spin up, a single fermion with spin down and a doubly occupied site. Hence if one traces out the rest of the lattice besides two sites one obtains a 16×16 reduced density matrix between those two sites. We refer to this matrix as the *full two-site matrix* in the following.

When a local particle number superselection rule applies, the only accessible entanglement is between the projected state with one and only one particle at each site—if even one of the sites contains either zero or two fermions then there is no room for entanglement as there is then only one possible local state at that site. This projected state $\rho^{(1,1)}$ is a 4×4 matrix that we refer to as the *projected two-site matrix*. It may be calculated as

$$\rho^{(1,1)} = \text{Tr}_{\overline{j_A, j_B}}[\Pi_{1,1} \rho \Pi_{1,1}], \qquad (23)$$

where ρ is the total state of the system (e.g., in the next subsection we will take ρ to be the grand canonical ensemble thermal density matrix), $\text{Tr}_{\overline{j_A, j_B}}$ indicates the trace over all sites in the lattice besides j_A and j_B, and $\Pi_{1,1}$ is the projector onto the subspace where there is one and only one fermion at both j_A and j_B. The normalization (trace) of $\rho^{(1,1)}$ corresponds to the *a priori* probability of detecting one and only one particle at each site, $P_{1,1}$.

The projector $\Pi_{1,1}$ may be written in terms of number operators as

$$\begin{aligned}
\Pi_{1,1} = {} & \hat{n}_{j_A\uparrow}(1 - \hat{n}_{j_A\downarrow})\hat{n}_{j_B\uparrow}(1 - \hat{n}_{j_B\downarrow}) + \hat{n}_{j_A\uparrow} \\
& \times (1 - \hat{n}_{j_A\downarrow})\hat{n}_{j_B\downarrow}(1 - \hat{n}_{j_B\uparrow}) \\
& + \hat{n}_{j_A\downarrow}(1 - \hat{n}_{j_A\uparrow})\hat{n}_{j_B\uparrow}(1 - \hat{n}_{j_B\downarrow}) \\
& + \hat{n}_{j_A\downarrow}(1 - \hat{n}_{j_A\uparrow})\hat{n}_{j_B\downarrow}(1 - \hat{n}_{j_B\uparrow}).
\end{aligned} \qquad (24)$$

The matrix elements of $\rho^{(1,1)}$ may be written as averages over creation and annihilation operators as

$$\begin{aligned}
\rho^{(1,1)}_{ss',tt'} &= \text{Tr}_{j_A,j_B}[\rho^{(1,1)} \hat{c}^\dagger_{j_A t} \hat{c}^\dagger_{j_B t'} \hat{c}_{j_B s'} \hat{c}_{j_A s}], \\
&= \langle \Pi_{1,1} \hat{c}^\dagger_{j_A t} \hat{c}^\dagger_{j_B t'} \hat{c}_{j_B s'} \hat{c}_{j_A s} \Pi_{1,1} \rangle,
\end{aligned} \qquad (25)$$

where s, s', t, t' take the values $\uparrow, \downarrow$. In Table I these correlation functions are simplified where possible by substituting Eq. (24) into Eq. (25).

B. Noninteracting electrons on a lattice

Perhaps the simplest multimode Fermionic system one can imagine is noninteracting electrons in thermal equilibrium at zero or finite temperature. We will be interested in the thermodynamic limit—large lattice size—which is of relevance to condensed-matter physics, and serves as the starting point for more realistic, interacting, models of real materials such as superconductors. We aim to clarify issues of entanglement in this simple case in order that the same issues can be addressed in interacting systems.

TABLE I. Above double space: the elements of the projected two-site matrix, $\rho^{(1,1)}$, written as correlation functions. Below double space: elements of the full two-site matrix that contribute to the two-spin reduced density matrix, but are not in the projected state. The elements below the diagonal are obtained by complex conjugation.

Site element	Correlation function
$(\uparrow\uparrow, \uparrow\uparrow)$	$\langle \hat{n}_{j_A\uparrow}(1 - \hat{n}_{j_A\downarrow})\hat{n}_{j_B\uparrow}(1 - \hat{n}_{j_B\downarrow}) \rangle$
$(\uparrow\uparrow, \uparrow\downarrow)$	$\langle \hat{n}_{j_A\uparrow}(1 - \hat{n}_{j_A\downarrow})\hat{c}^\dagger_{j_B\downarrow}\hat{c}_{j_B\uparrow} \rangle$
$(\uparrow\uparrow, \downarrow\uparrow)$	$\langle \hat{c}^\dagger_{j_A\downarrow}\hat{c}_{j_A\uparrow}\hat{n}_{j_B\uparrow}(1 - \hat{n}_{j_B\downarrow}) \rangle$
$(\uparrow\uparrow, \downarrow\downarrow)$	$\langle \hat{c}^\dagger_{j_A\uparrow}\hat{c}_{j_A\downarrow}\hat{c}^\dagger_{j_B\uparrow}\hat{c}_{j_B\downarrow} \rangle$
$(\uparrow\downarrow, \uparrow\uparrow)$	$\langle \hat{n}_{j_A\uparrow}(1 - \hat{n}_{j_A\downarrow})\hat{n}_{j_B\uparrow}(1 - \hat{n}_{j_B\uparrow}) \rangle$
$(\uparrow\downarrow, \downarrow\uparrow)$	$\langle \hat{c}^\dagger_{j_A\uparrow}\hat{c}_{j_A\downarrow}\hat{c}^\dagger_{j_B\downarrow}\hat{c}_{j_B\uparrow} \rangle$
$(\uparrow\downarrow, \downarrow\downarrow)$	$\langle \hat{c}^\dagger_{j_A\uparrow}\hat{c}_{j_A\downarrow}\hat{n}_{j_B\downarrow}(1 - \hat{n}_{j_B\uparrow}) \rangle$
$(\downarrow\uparrow, \downarrow\uparrow)$	$\langle \hat{n}_{j_A\downarrow}(1 - \hat{n}_{j_A\uparrow})\hat{n}_{j_B\uparrow}(1 - \hat{n}_{j_B\downarrow}) \rangle$
$(\downarrow\uparrow, \downarrow\downarrow)$	$\langle \hat{n}_{j_A\downarrow}(1 - \hat{n}_{j_A\uparrow})\hat{c}^\dagger_{j_B\downarrow}\hat{c}_{j_B\uparrow} \rangle$
$(\downarrow\downarrow, \downarrow\downarrow)$	$\langle \hat{n}_{j_A\downarrow}(1 - \hat{n}_{j_A\uparrow})\hat{n}_{j_B\downarrow}(1 - \hat{n}_{j_B\uparrow}) \rangle$
$(\uparrow 2, \uparrow 2)$	$\langle \hat{n}_{j_A\uparrow}(1 - \hat{n}_{j_A\downarrow})\hat{n}_{j_B\uparrow}\hat{n}_{j_B\downarrow} \rangle$
$(\uparrow 2, \downarrow 2)$	$\langle \hat{c}^\dagger_{j_A\downarrow}\hat{c}_{j_A\uparrow}\hat{n}_{j_B\uparrow}\hat{n}_{j_B\downarrow} \rangle$
$(\downarrow 2, \downarrow 2)$	$\langle \hat{n}_{j_A\downarrow}(1 - \hat{n}_{j_A\uparrow})\hat{n}_{j_B\uparrow}\hat{n}_{j_B\downarrow} \rangle$
$(2\uparrow, 2\uparrow)$	$\langle \hat{n}_{j_A\uparrow}\hat{n}_{j_A\downarrow}\hat{n}_{j_B\uparrow}(1 - \hat{n}_{j_B\downarrow}) \rangle$
$(2\uparrow, 2\downarrow)$	$\langle \hat{n}_{j_A\uparrow}\hat{n}_{j_A\downarrow}\hat{c}^\dagger_{j_B\downarrow}\hat{c}_{j_B\downarrow} \rangle$
$(2\downarrow, 2\downarrow)$	$\langle \hat{n}_{j_A\uparrow}\hat{n}_{j_A\downarrow}\hat{n}_{j_B\downarrow}(1 - \hat{n}_{j_B\uparrow}) \rangle$
$(22, 22)$	$\langle \hat{n}_{j_A\uparrow}\hat{n}_{j_A\downarrow}\hat{n}_{j_B\uparrow}\hat{n}_{j_B\downarrow} \rangle$

The Hamiltonian for noninteracting electrons is

$$\hat{H} = -t \sum_{\substack{\langle j,k \rangle \\ \sigma = \uparrow, \downarrow}} \hat{c}^\dagger_{j\sigma} \hat{c}_{k\sigma}, \qquad (26)$$

where $\langle j, k \rangle$ indicates that the sum runs over nearest neighbors j and k as defined by a link in the lattice. If we were to add an on-site interaction between electrons of opposite spin (i.e., a Coloumb interaction), $U\sum_j \hat{n}_{j\uparrow}\hat{n}_{j\downarrow}$, we would have the well-studied Hubbard model, the two-site version of which was studied in Sec. III C. This simple type of interaction might be a good starting point for studying how interactions affect the entanglement of particles.

One's immediate reaction may be that there can be no entanglement in this system as the fermions are noninteracting and the up and down spins are independent. However, this intuition was shown to be incorrect in Sec. III C, where we saw that the two-site version of this model ($U=0$) contained entanglement of particles in the ground state. Furthermore, in Refs. [15,25] it is argued that it is indeed possible to have "entanglement of spins in a noninteracting electron gas," which is roughly the continuum limit of our discrete model. There are subtle differences between the entanglement as studied in those works and the concept of entanglement of particles that we have focused on here. Section IV C contains a detailed comparison of this previous work to the current entanglement-of-particles approach.

We now explicitly calculate the entanglement of particles for noninteracting fermions on a lattice, Eq. (26), in thermal

and chemical equilibrium. We choose the simple case of a one-dimensional (1D) lattice of M sites with closed boundary conditions (i.e., a ring) for the purpose of illustration. The state of the system at temperature T and chemical potential μ is given by the grand canonical ensemble density matrix,

$$\rho_T = \exp[-(\hat{H} - \mu\hat{N})/k_B T]/\mathcal{Z}, \qquad (27)$$

where $\hat{N}$ is the total number operator and $\mathcal{Z}$ is the grand canonical partition function, $\mathcal{Z} = \text{Tr}[\exp(-(\hat{H} - \mu\hat{N})/k_B T)]$.

In order to explicitly calculate $\rho^{(1,1)}$ we use the fact that the grand canonical ensemble density matrix, Eq. (27), is a Gaussian state when the system is described by the noninteracting fermion Hamiltonian, Eq. (26). For this reason higher-order correlation functions, as in Table I, factorize into second-order correlation functions.

Another simplifying feature is that many of the matrix elements are zero due to the collective SU(2) rotational symmetry of the model. In fact the only nonzero elements are those along the diagonal, and the off-diagonal elements $\rho_{\uparrow\downarrow,\downarrow\uparrow}^{(1,1)} = \rho_{\downarrow\uparrow,\uparrow\downarrow}^{(1,1)*}$. A way to see this is via the well-known result due to Weyl that states invariant under collective SU(2) rotations of the spin have the form

$$\rho = \int dU U \otimes U \rho U^\dagger \otimes U^\dagger = p_A \Pi_A + p_S \Pi_S, \qquad (28)$$

where $\Pi_{A/S}$ are the projectors onto the antisymmetric (spanned by the singlet) and symmetric (spanned by the three triplet states) subspaces, and $p_{A/S}$ are the weights of these projectors. In our case $p_A + p_S = P_{1,1}$. States of this form are known as *Werner states* in quantum information theory.

The nonzero matrix elements are all determined by two second-order correlation functions

$$\bar{n} = \langle \hat{n}_{j_A\uparrow} \rangle = \langle \hat{n}_{j_A\downarrow} \rangle = \langle \hat{n}_{j_B\uparrow} \rangle = \langle \hat{n}_{j_B\downarrow} \rangle, \qquad (29)$$

$$c_{j_A,j_B} = \langle \hat{c}_{j_A\uparrow}^\dagger \hat{c}_{j_B\uparrow} \rangle = \langle \hat{c}_{j_A\downarrow}^\dagger \hat{c}_{j_B\downarrow} \rangle, \qquad (30)$$

where for the first line we have also used the translational invariance of the lattice. The average occupation of any individual up or down mode which we call the *filling factor* in the following, is given by $\bar{n}$, and c_{j_A,j_B} is an exchange correlation between the two sites. Explicitly the matrix elements are

$$\rho_{\uparrow\uparrow,\uparrow\uparrow}^{(1,1)} = \rho_{\downarrow\downarrow,\downarrow\downarrow}^{(1,1)} = (\bar{n}^2 - |c_{j_A,j_B}|^2)((1-\bar{n})^2 - |c_{j_A,j_B}|^2),$$

$$\rho_{\uparrow\downarrow,\uparrow\downarrow}^{(1,1)} = \rho_{\downarrow\uparrow,\downarrow\uparrow}^{(1,1)} = (\bar{n}(1-\bar{n}) + |c_{j_A,j_B}|^2)^2,$$

$$\rho_{\uparrow\downarrow,\downarrow\uparrow}^{(1,1)} = -|c_{j_A,j_B}|^2. \qquad (31)$$

For noninteracting fermions we can actually calculate the two correlation functions, $\bar{n}$ and c_{j_A,j_B}, explicitly as a function of μ and T. The Hamiltonian (26) is diagonal when written in terms of momentum creation and annihilation operators

$$\hat{H} = -2t \sum_{\substack{k=0 \\ \sigma=\uparrow,\downarrow}}^{M-1} \cos(2\pi k/M) \hat{C}_{k\sigma}^\dagger \hat{C}_{k\sigma}, \qquad (32)$$

where

$$\hat{C}_{k,\sigma} = \frac{1}{\sqrt{M}} \sum_{j=0}^{M-1} e^{2\pi i jk/M} \hat{c}_{j\sigma}. \qquad (33)$$

The occupation of the momentum-space modes is therefore

$$n_k = \langle \hat{C}_{k\uparrow}^\dagger \hat{C}_{k\uparrow} \rangle = \langle \hat{C}_{k\downarrow}^\dagger \hat{C}_{k\downarrow} \rangle = \frac{1}{e^{-(E_k-\mu)/k_B T} + 1}, \qquad (34)$$

where $E_k = -2t\cos(2\pi k/M)$ is the energy of the kth mode. By inverse Fourier transforming back to the position-space modes we obtain

$$\bar{n} = \frac{1}{M} \sum_{k=0}^{M-1} n_k, \qquad (35)$$

$$c_{j_A,j_B} = \frac{1}{M} \sum_{k=0}^{M-1} e^{2\pi i(j_A-j_B)k} n_k. \qquad (36)$$

Figure 4(a) illustrates entanglement of particles between two sites as the system is cooled from high temperature down to zero temperature (the ground state) as a function of the inverse temperature $t/k_B T$, for a fixed chemical potential (which determines the $T \to 0$ filling factor). At high temperature ($t/k_B T = 0$) the probability of each up or down mode being occupied is 0.5 and completely uncorrelated with any other mode, so $P_{1,1} = 0.25$ and there is no entanglement. As we cool to lower temperatures entanglement appears between increasingly distant sites in the lattice, but the probability $P_{1,1}$ decreases because the mean atom number is decreasing. The entanglement in $\rho^{(1,1)}$ decreases with the separation between the two sites and goes to zero at some finite separation between the sites that depends on the temperature. We call this distance the *entanglement length r_e* in anticipation of a relationship to previous work on the free Fermi gas to be discussed in the next section. In this case the entanglement length is five sites in the $T \to 0$ limit (ground state).

Figure 5 illustrates the entanglement of particles between sites in the ground state as a function of the filling factor $\bar{n}$. For filling factors less than one half the entanglement length decreases with increasing filling factor, and by the time half filling is reached there is only entanglement between neighboring sites. For filling factors greater than one-half the entanglement length increases again due to the particle-hole symmetry of the model—the filling factor for holes is decreasing. By contrast the probability that one particle will be found at each site reaches a maximum at half filling, as indicated by greyscale in the figure.

When there are only two electrons or holes in the lattice $[\bar{n} = 2/(2 \times 30) = 1/30]$ they form a singlet with $E_F = 1$ independent of the separation between the sites—i.e., the entanglement length is infinite. This effect is rather more subtle than simply entanglement between sites as may be seen in
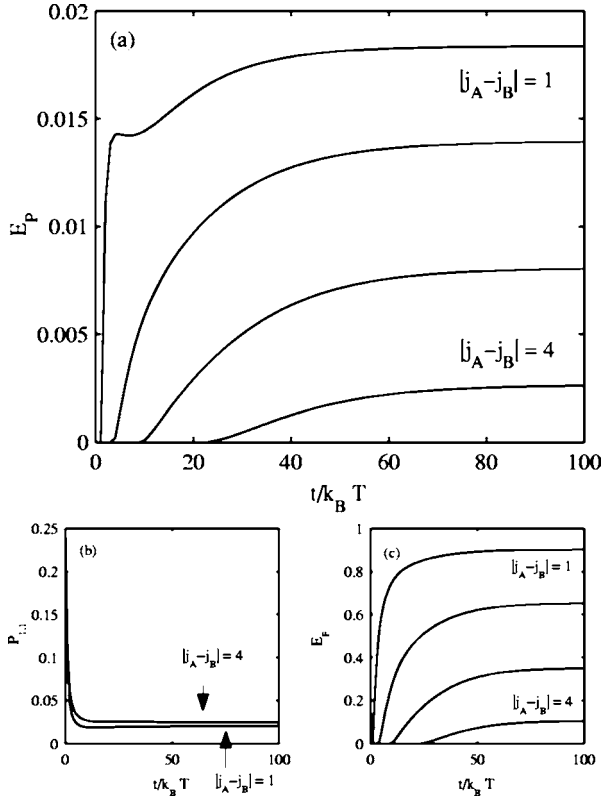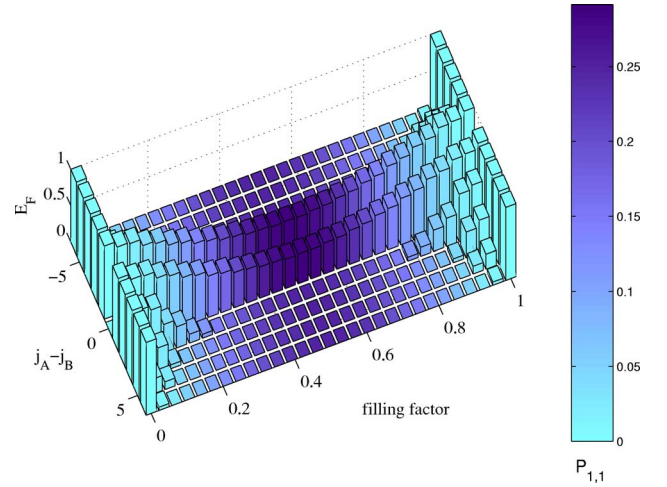
FIG. 5. (Color online) Bipartite entanglement of formation (height) and probability $P_{1,1}$ (greyscale) as a function of separation and filling factor in the $T \to 0$ limit of the grand canonical-ensemble thermal state of the Fermi-Hubbard model with 30 sites and periodic boundary conditions. The chemical potential was varied from -2 to 2 to achieve different filling factors.

FIG. 4. (a) Entanglement of particles for noninteracting fermions on a $1-D$ lattice with 30 sites as a function of inverse temperature ($t/k_B T$) and separation between the sites ($|j_A - j_B|$). The subfigures (b) and (c) indicate the contributions to E_P from the probability of finding one particle at each site, $P_{1,1}$, and the entanglement of formation in the *a posteriori* state, respectively. The chemical potential was $\mu \simeq -1.89$ corresponding to a $T \to 0$ filling factor of $\bar{n} = 0.2$. In the $T \to 0$ limit we therefore roughly expect that $P_{1,1} \sim (0.2)^2 = 0.04$.

spin models. The wave function is such that the fermions are equally likely to be found anywhere in the lattice (apart from on top of each other which is slightly more likely), but wherever they are found they must be in a singlet.

Note that from the entanglement of particles perspective entanglement is only possible if A and B each control both up and down modes of *distinct* sites. If A controlled the up mode and B the down mode of the *same* site they could never share any entanglement as they each only have one mode. This is why $|j_A - j_B| = 0$ is not plotted in these figures.

C. Continuum limit

We now discuss the continuum limit of the noninteracting fermion lattice model and contrast the entanglement of particles with another approach that has been used in recent work—the so-called two-spin reduced density matrix [15,25].

The *two-spin reduced density matrix* between two points $\vec{r}$ and $\vec{r}'$ is defined as

$$\rho_{ss',tt'}^{\text{spin}} = \langle \hat{\psi}_t^\dagger(\vec{r}) \hat{\psi}_{t'}^\dagger(\vec{r}') \hat{\psi}_{s'}(\vec{r}') \hat{\psi}_s(\vec{r}) \rangle, \qquad (37)$$

where $\hat{\psi}_s(\vec{r}), \hat{\psi}_s^\dagger(\vec{r})$ are field annihilation or creation operators for a particle with spin s located at position $\vec{r}$ satisfying

$\{\hat{\psi}_s(\vec{r}), \hat{\psi}_{s'}^\dagger(\vec{r}')\} = \delta_{ss'}\delta(\vec{r} - \vec{r}')$. We refer to this matrix as the *spin-correlation matrix* in what follows as we believe the name is more appropriate.

It was shown in Refs. [15,25] that for a free Fermi gas in thermal equilibrium the spin-correlation matrix takes the form of a Werner state, for the same reasons as for the lattice model in the previous section. After normalization, let $p = p_A$ be the weight of the singlet. The function p depends on the relative distance $r = |\vec{r} - \vec{r}'|$ and temperature T; $p = 1$ at $r = 0$ and $p \to 0$ as $r \to \infty$. The *entanglement length* r_e is uniquely determined by

$$p(r_e, T) = 1/3, \qquad (38)$$

and the spins are entangled for $r < r_e$ and separable for $r \geq r_e$. At zero temperature the relevant parameter is the Fermi momentum k_F and the entanglement length scales as

$$r_e \propto 1/k_F. \qquad (39)$$

One might expect to see similar behavior in a lattice model of noninteracting fermions, and indeed we saw in the previous section that the concept of an entanglement length persists when one considers entanglement of particles on a lattice. We will see subsequently that the lattice filling factor $\bar{n}$ plays the role of the Fermi momentum in a certain limit. However, first we discuss the precise relationship between the spin correlation matrix and the projected two-site matrix.

In analogy to Eq. (37) one may be tempted to write down

$$\rho_{ss',tt'}^{\text{spin}} = \langle \hat{c}_{j_A t}^\dagger \hat{c}_{j_B t'}^\dagger \hat{c}_{j_B s'} \hat{c}_{j_A s} \rangle \qquad (40)$$

as a "two-spin reduced density matrix" in the lattice. However, from the results of the previous section this matrix does not correspond to the density matrix of a two-component quantum system in the usual sense of quantum information theory—the central reason being that the two subsystems are

TABLE II. Mapping the full two-site matrix onto the spin-correlation matrix. The left column represents the elements of the spin-correlation matrix, which are obtained by summing elements of the full two-site matrix represented in the right-hand column.

Spin element	Sum of site elements
$(\uparrow\uparrow, \uparrow\uparrow)$	$(\uparrow\uparrow, \uparrow\uparrow)+(\uparrow2, \uparrow2)+(2\uparrow, 2\uparrow)+(2\,2, 2\,2)$
$(\uparrow\uparrow, \uparrow\downarrow)$	$(\uparrow\uparrow, \uparrow\downarrow)+(2\uparrow, 2\downarrow)$
$(\uparrow\uparrow, \downarrow\uparrow)$	$(\uparrow\uparrow, \downarrow\uparrow)+(\uparrow2, \downarrow2)$
$(\uparrow\uparrow, \downarrow\downarrow)$	$(\uparrow\uparrow, \downarrow\downarrow)$
$(\uparrow\downarrow, \uparrow\downarrow)$	$(\uparrow\downarrow, \uparrow\downarrow)+(\uparrow2, \uparrow2)+(2\uparrow, 2\downarrow)+(2\,2, 2\,2)$
$(\uparrow\downarrow, \downarrow\uparrow)$	$(\uparrow\downarrow, \downarrow\uparrow)$
$(\uparrow\downarrow, \downarrow\downarrow)$	$(\uparrow\downarrow, \downarrow\downarrow)+(\uparrow2, \downarrow2)$
$(\downarrow\uparrow, \downarrow\uparrow)$	$(\downarrow\uparrow, \downarrow\uparrow)+(\downarrow2, \downarrow2)+(2\uparrow, 2\uparrow)+(2\,2, 2\,2)$
$(\downarrow\uparrow, \downarrow\downarrow)$	$(\downarrow\uparrow, \downarrow\downarrow)+(2\uparrow, 2\downarrow)$
$(\downarrow\downarrow, \downarrow\downarrow)$	$(\downarrow\downarrow, \downarrow\downarrow)+(\downarrow2, \downarrow2)+(2\downarrow, 2\downarrow)+(2\,2, 2\,2)$

not well defined. By contrast the entanglement in Eq. (25) is experimentally accessible.

To see this point first note that Eq. (25) has the same form as Eq. (40) but with projectors onto the one-particle subspace inserted. As we have argued in Sec. II the projector is necessary in order to define the subsystems; without it multiparticle correlations contribute. If one were to imagine extracting entangled fermions from the lattice then the very act of extracting is implicitly a measurement of local particle number, and entanglement can then exist only if precisely one fermion is found per site.

Of course the correlation functions that make up the matrix could, in principle, be measured without actually extracting fermions [44]. Moreover, it is not difficult to show that entanglement in the matrix (40) (normalized, and treated as if it were a density matrix) provides a lower bound on the entanglement in the projected two-site matrix [45]. Therefore if the matrix (40) were reconstructed experimentally, as may be possible in the near future in mesoscopic systems [24], then a calculation of nonzero entanglement in this matrix would imply that the accessible entanglement would be nonzero (but the converse is not true). Nevertheless, it would, in our opinion, still be wrong to call the spin correlation matrix (40) a density matrix, for the reasons given above.

There are some more intuitive reasons why we should not expect correlations between two fermions on one site and one or two fermions on the other to contribute to entanglement. The spatial wave functions of two fermions on the same site are identical and therefore their spin wave function is a singlet (as in Refs. [15,25]). By the monogamy of entanglement neither can be entangled in spin with any other. In this sense a doubly occupied site is like an unoccupied site—one should not include correlations from it in the calculation of a density matrix. The projected two-site matrix respects particle-hole symmetry in this sense and therefore fits in naturally with experimental considerations in mesoscopic systems [22], whereas the spin-correlation matrix does not.

In Table II we show precisely the relationship between the two matrices by writing the elements of the spin correlation

matrix as sums of elements of the full two-site matrix. This mapping is not a "coarse graining" in the sense that each element of the full two-site matrix contributes to only one element in the spin-correlation matrix—certain elements, for example (22, 22) map to many of the spin elements. Therefore the spin-correlation matrix is not the "density matrix" of a well defined two-component system in the sense that is used in quantum information. We conclude that, at least in lattice models, the entanglement of particles—i.e., the entanglement in the projected two-site matrix, is what should be used instead of the entanglement in the spin-correlation matrix.

Despite these problems with using the spin-correlation matrix to calculate entanglement for discrete lattice models, in the continuum limit Eq. (37) recovers a interpretation as a density matrix of two spins. The reason for this is basically that the probability of finding two electrons at a particular location in space is negligible compared with the probability of finding one electron.

To see this in more detail, let N noninteracting electrons be confined to a region $[0, L]$ in one dimension. Define a set of M orthonormal wave functions, $\{\psi_j(x), j=0 \dots M-1\}$, on the region by

$$\psi_j(x) = \begin{cases} 1/\sqrt{\epsilon}, & x \in [j\epsilon, (j+1)\epsilon] \\ 0, & x \notin [j\epsilon, (j+1)\epsilon] \end{cases}, \qquad (41)$$

where $\epsilon = L/M$. Let $\hat{c}_{j\sigma}$ be the annihilation operator that destroys an electron in the jth region with spin σ. For noninteracting electrons in thermal equilibrium the probability of finding one electron in the jth region is $\langle \hat{n}_{j\sigma} \rangle = N\epsilon/L$, while the probability of finding two electrons, one up and one down, scales as $\langle \hat{n}_{j\uparrow} \hat{n}_{j\downarrow} \rangle = O(\epsilon^2)$. Therefore in the $\epsilon \to 0$ limit, where $\psi_j(x)$ approaches a delta function at $x = j\epsilon$, the probability of finding two electrons at the same site becomes negligible compared to the probability of finding one. Hence the projector in Eq. (25) has no effect, and the projected two-site matrix approaches the spin-correlation matrix (37) in the continuum limit.

The question of using Eq. (37) as a density matrix was considered in the appendix of Ref. [46]. Their explanation agrees with ours for the case where there is one and only one particle in each of local modes. Our results show why this is a valid assumption in the continuum limit, but also apply to more general situations when there is a nonzero probability of finding two electrons in the same local mode.

With this calculation in mind we should expect that in the limit of low filling factor on the lattice the difference between Eqs. (25) and (40) will be negligible. We define the entanglement length for the lattice as the smallest $|j_A - j_B|$ for which the entanglement of the two-site matrix is zero. Figure 6 shows the entanglement length versus the inverse of the filling factor alongside the "entanglement" length calculated from the spin-correlation matrix. We see that in the limit of small filling factor ($1/\bar{n}$ large) the entanglement length scales linearly with $1/\bar{n}$, as one might expect from Refs. [15,25] since $k_F \propto \bar{n}$ in one dimension.

For noninteracting electrons we see from Table II that the many-electron correlations simply add a term proportional to
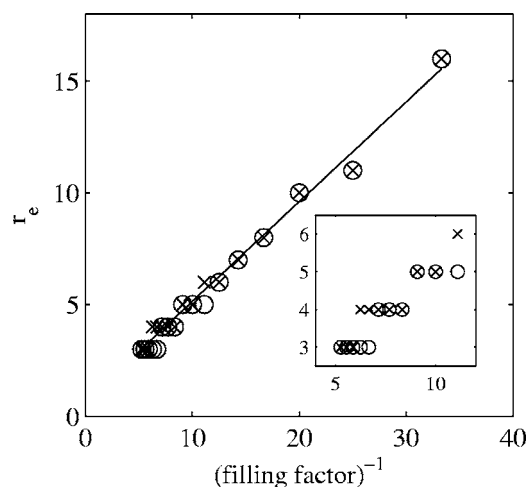
FIG. 6. Entanglement length (crosses) r_e vs inverse filling factor $1/\bar{n}$ for noninteracting fermions on a $1-D$ lattice. The circles show what the entanglement length would have been if it were defined using the spin-correlation matrix, Eq. (40), instead of the projected matrix, Eq. (25). The line is a linear least-squares fit to the crosses. The inset shows that the projected matrix predicts a longer entanglement length for some values of the filling factor.

the identity to the density matrix. This can only have the effect of diluting the entanglement and decreasing the entanglement length. We see from the inset in the figure that the projected matrix therefore predicts a longer entanglement length than for the spin-correlation matrix for some values of the filling factor approaching half filling ($\bar{n}=1/2$). For $0.45 \leqslant \bar{n} \leqslant 0.55$ (not plotted in the figure) the spin-correlation matrix would have predicted an entanglement length of 1 site (i.e., not even nearest neighbors are entangled), whereas the projected matrix gives $r_e=2$ (nearest neighbors are entangled). This is precisely the limit where there is a good chance of finding two electrons at the same site.

V. SUMMARY AND CONCLUSION

An idea that has attracted much attention recently from the quantum information theory community is that the improved understanding of entanglement that has been developed may lead to new insights into the physics of strongly correlated systems in condensed matter. Typically in these systems the particles are itinerant and so must be treated as indistinguishable. Thus if one wishes to explore the role of entanglement one must have a good understanding of what it means for indistinguishable particles to be entangled.

We have argued that in many situations of interest in condensed matter a local particle number superselection rule applies to operations, such as measurements, that can be performed on the system. Thus the notion of entanglement of particles, introduced in Ref. [17], may be a more appropriate measure of entanglement to use in studying these systems than the entanglement of modes which appears in many previous studies. The physical meaning of entanglement of particles is clear—the subsystems that are supposed to be en-

tangled are established by measurement of local particle number by the two parties. The mathematical entanglement in occupation number (mode entanglement) may still display interesting behavior, however, its physical significance is less clear as the measurements that could be performed to observe it are unspecified.

In order to get a feel for how the entanglement of particles compares with the entanglement of modes we began by studying some simple systems that are analytically solvable. The minimal situation in which entanglement of particles is possible is two particles in four modes. We found that the entanglement of particles was zero for bosons but nonzero for fermions for two noninteracting particles in a four-mode ring. In both cases the mode entanglement was nonzero. For the Hubbard dimer we calculated the entanglement of particles according to a number of different mode decompositions and compared with previous studies of mode entanglement [26].

Finally we studied noninteracting fermions on a lattice and compared with previous results for this system. We first showed how to write the projected matrix for one fermion on each of two distinct sites in terms of correlation functions. In agreement with previous results regarding the free Fermi gas [15,25] we found an "entanglement length" in the system beyond which the fermions are not entangled. It is intriguing that this length extends over multiple lattice sites and persists even when one considers the more restrictive criteria of entanglement of particles where real measurements are considered. Thus the phenomena of entanglement of noninteracting fermions should be experimentally observable, perhaps in optical lattice setups where condensed-matter Hamiltonians may be engineered. It cannot be dismissed as trivially due to the antisymmeterization of the wave function and unobservable. Finally we showed precisely how the entanglement of particles relates to the two-spin spin reduced density matrix [15,25] in the continuum limit.

Recently there has been interest in studying scaling laws for entanglement entropy in arbitrary dimensions [47,48]. The entanglement entropy corresponds to the entanglement of modes for pure states when entanglement of formation is used as the measure. An interesting direction for future research would be to see if such scaling laws persist when the more-restrictive criteria of entanglement of particles is used, rather than entanglement of modes.

In conclusion, we believe that the entanglement of particles may be a useful concept to consider alongside mode entanglement in studying systems of indistinguishable particles that are central to condensed-matter physics. We have showed that it is physically well motivated by measurement considerations and leads to distinct phenomenology of entanglement in a few simple systems.

[1] T. J. Osborne and M. A. Nielsen, Phys. Rev. A **66**, 032110 (2002).

[2] A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature (London) **416**, 608 (2002).

[3] G. Vidal, J. I. Latorre, E. Rico, and A. Kitaev, Phys. Rev. Lett. **90**, 227902 (2003).

[4] J. I. Latorre, E. Rico, and G. Vidal, Quantum Inf. Comput. **4**, 048 (2004).

[5] F. Verstraete, M. A. Martin-Delgado, and J. I. Cirac, Phys. Rev. Lett. **92**, 087201 (2004).

[6] M. Popp, F. Verstraete, M. A. Martin-Delgado, and J. I. Cirac, Phys. Rev. A **71**, 042306 (2005).

[7] S. M. Tan, D. F. Walls, and M. J. Collett, Phys. Rev. Lett. **66**, 252 (1991).

[8] L. Hardy, Phys. Rev. Lett. **73**, 2279 (1994).

[9] D. M. Greenberger, M. A. Horne, and A. Zeilinger, Phys. Rev. Lett. **75**, 2064 (1995).

[10] S. J. van Enk, Phys. Rev. A **72**, 064306 (2005).

[11] R. Paškauskas and L. You, Phys. Rev. A **64**, 042310 (2001).

[12] J. Schliemann, J. I. Cirac, M. Kus, M. Lewenstein, and D. Loss, Phys. Rev. A **64**, 022303 (2001).

[13] Y. S. Li, B. Zeng, X. S. Liu, and G. L. Long, Phys. Rev. A **64**, 054302 (2001).

[14] J. R. Gittings and A. J. Fisher, Phys. Rev. A **66**, 032305 (2002).

[15] V. Vedral, Cent. Eur. J. Phys. **1**, 289 (2003).

[16] Yu Shi, Phys. Rev. A **67**, 024301 (2003).

[17] H. M. Wiseman and John A. Vaccaro, Phys. Rev. Lett. **91**, 097902 (2003).

[18] T. A. Kaplan, Fluct. Noise Lett. **5**, C15 (2005).

[19] P. Samuelsson, E. V. Sukhorukov, and M. Buttiker, Phys. Rev. Lett. **91**, 157002 (2003).

[20] C. W. J. Beenakker, C. Emary, M. Kindermann, and J. L. van Velsen, Phys. Rev. Lett. **91**, 147901 (2003).

[21] P. Samuelsson, E. V. Sukhorukov, and M. Buttiker, Phys. Rev. Lett. **92**, 026805 (2004).

[22] C. W. J. Beenakker, cond-mat/0508488.

[23] P. Samuelsson, E. V. Sukhorukov, and M. Buttiker, New J. Phys. **7**, 176 (2005).

[24] P. Samuelsson and M. Buttiker, Phys. Rev. B **73**, 041305(R) (2006).

[25] Sangchul Oh and Jaewan Kim, Phys. Rev. A **69**, 054305 (2004).

[26] Paolo Zanardi, Phys. Rev. A **65**, 042101(R) (2002).

[27] A. P. Hines, R. H. McKenzie, and G. J. Milburn, Phys. Rev. A **67**, 013609 (2003).

[28] P. Zanardi, Phys. Rev. Lett. **87**, 077901 (2001).

[29] S. J. van Enk, Phys. Rev. A **67**, 022303 (2003).

[30] Stephen D. Bartlett and H. M. Wiseman, Phys. Rev. Lett. **91**, 097903 (2003).

[31] Y. Aharonov and L. Susskind, Phys. Rev. **155**, 1428 (1967).

[32] The qubits could be distinguished, for example, by their fixed positions in space.

[33] We first normalize the state, $\rho_{AB}^{(n_A, n_B)}/P_{AB}$, before calculating the standard bipartite measure of entanglement, M.

[34] C. H. Bennett, D. P. DiVincenzo, J. A. Smolin, and W. K. Wootters, Phys. Rev. A **54**, 3824 (1996).

[35] Michael A. Nielsen and Isaac L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, England, 2000).

[36] G. Tóth, Phys. Rev. A **69**, 052327 (2004).

[37] For pure states it is equal to the distillable entanglement, and given by the von Neumann entropy of the reduced state of either party.

[38] William K. Wootters, Phys. Rev. Lett. **80**, 2245 (1998).

[39] It may seem unusual that a mixture of two pure states can have the same entanglement of formation as either of them individually; in this case it is because these two pure states coincidentally achieve the minimum in the definition of E_F for the mixed state [38]. Using the negativity, which is an upper bound for the entanglement of distillation, E_D [49], it is possible to show that E_D is strictly less for the mixed state than for either pure state.

[40] Neil W. Ashcroft and N. David Mermin, *Solid State Physics* (Saunders College, Philadelphia, 1976).

[41] Where "local" is defined by the spin variable, as that is what A or B each control, even though they are not local in space.

[42] Zanardi uses the local entropy as his measure of entanglement.

[43] S. Bose and D. Home, quant-ph/0505217.

[44] For example by using detectors sensitive to the presence of either up spins or down fermions independent of whether the other is present.

[45] P. Samuelsson and M. Büttiker (private communication).

[46] D. Cavalcanti, M. F. Santos, M. O. Terra Cunha, C. Lunkes, and V. Vedral, Phys. Rev. A **72**, 062307 (2005).

[47] M. B. Plenio, J. Eisert, J. Dreissig, and M. Cramer, Phys. Rev. Lett. **94**, 060503 (2005).

[48] M. M. Wolf, Phys. Rev. Lett. **96**, 010404 (2006).

[49] G. Vidal and R. F. Werner, Phys. Rev. A **65**, 032314 (2002).