Entanglement of two delocalized electrons

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Several convenient formulas for the entanglement of two indistinguishable delocalized spin-1/2 particles are introduced. These generalize the standard formula for concurrence, valid only in the limit of localized or distinguishable particles. Several illustrative examples are given.

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Entanglement is a well-defined quantity for two distinguishable qubits in a nonfactorizable quantum state, where it may be uniquely defined through von Neumann entropy and concurrence [1–4]. However, among the realistic systems of major physical interest, electron qubits have the potential for a much richer variety of entanglement measure choices due to both their charge and spin degrees of freedom. For example, in lattice fermion models such as the Hubbard dimer, entanglement is sensitive to the interplay between charge hopping and the avoidance of double occupancy due to Hubbard repulsion, which results in an effective Heisenberg interaction between adjacent spins [5]. In systems of identical particles the main challenge is to define an appropriate entanglement measure that adequately deals with multiple-occupation states [6–11]. In the case of fermions such a measure must also account for the effect of exchange [12] as well as of mutual electron repulsion.

Entangled fermionic qubits can be created with electron-hole pairs in a Fermi sea [13] and in the scattering of two distinguishable particles [14]. A spin-independent scheme for detecting orbital entanglement of two-quasiparticle excitations of a mesoscopic normal-superconductor system was also proposed recently [15].

A consensus regarding the appropriate generalization of entanglement measure which would consider spin and orbital entanglement of electrons on the same footing has not, however, been reached yet. In any realistic solid-state device, spin entanglement is intimately related to the orbital degrees of freedom of the carriers, which cannot be ignored, even in otherwise pure spin-entanglement observations. In this paper we introduce spin-entanglement measure formulas valid for real electrons and show how, in general, spin entanglement depends in an essential way on spatially delocalized orbitals.

For two distinguishable particles A and B, each described with single spin-1/2 (or pseudospin) states $s = \uparrow$ or $\downarrow$ and in a pure state $|\Psi_{AB}\rangle = \sum_{\alpha,\alpha'} \alpha_{\alpha}\alpha'_{\alpha'} |\alpha\alpha'\rangle_B$ concurrence as a measure of entanglement is given by [2]

$$C = 2|\alpha_{\uparrow}\alpha_{\downarrow} - \alpha_{\downarrow}\alpha_{\uparrow}|.$$

(1)

Concurrence is related to the density matrix of a pair of spins [4] and can be expressed in terms of spin-spin correlators $\langle \Psi_{AB} | S^x_A S^y_B | \Psi_{AB} \rangle$ and expectation values $\langle \Psi_{AB} | S^z_A | \Psi_{AB} \rangle$, where $S^\lambda_{A(B)}$ for $\lambda = x, y, z$ are spin operators corresponding to spin A or B, respectively. This approach has proved to be efficient in the analysis of entanglement in various spin-chain systems with interaction [16–19].

Consider now the general problem of two interacting electrons in a pure state. It is clear that in some circumstances this system reduces approximately to an equivalent system of two interacting spins, for which the above entanglement formula is appropriate. Furthermore, in the general case, entanglement between the spins of the fermions relates to measurements of spin irrespective of their orbital motion. We consider therefore spin entanglement for a general class of two-electron states on a lattice of the form

$$|\Psi\rangle = \sum_{i,j=1}^N \left( \psi_{ij}^0 c_{i\uparrow} c_{j\uparrow} + \frac{1}{2} \left( \psi_{ij}^1 c_{i\uparrow} c_{j\downarrow}^\dagger + \psi_{ij}^0 c_{i\downarrow} c_{j\uparrow}^\dagger \right) \right) |0\rangle,$$

(2)

where $c_{ia}$ creates an electron with spin $s$ on site $i$ and $N$ is the total number of sites. The system in question could be, for example, a tight-binding lattice containing two valence electrons occupying nondegenerate atomic orbitals, or two electrons in the conduction band of a semiconductor, for which the sites represent finite-difference grid points. In either case, the interaction between the electrons is included together with any externally applied potential.

The two electrons are in separate regions of space (measurement domains) [A] and [B] as illustrated in Fig. 1(a). Entanglement might be produced, for example, when two initially unentangled electrons in wave packets approach each other and interact [Fig. 1(b)] and then again become well separated into distinct regions [A] and [B] [Fig. 1(c)]. Here one should realize that in real measurements of entanglement, indistinguishable electrons would be detected and the formalism relevant to distinguishable spins is not directly applicable. Nevertheless, complete information regarding the spin properties of such a fermionic system is contained in spin correlation functions for the two domains. The spin-measuring apparatus would measure spin correlation functions for two domains [A] and [B] rather than for two distinguishable spins A and B.

Concurrence as a measure of entanglement for two electrons is related to the eigenvalues of the non-Hermitian matrix $\rho$ where $\rho$ is reduced density matrix given in terms of the electron spin correlations corresponding to the domains, and $\tilde{\rho}$ is the time-reversed density matrix as in Ref. [4]. In general the eigenvalues of $\rho$ can be determined only numerically and a closed form for concurrence cannot be ob-
tained, unless the system exhibits additional symmetries. Possible symmetries are conveniently studied through 
spin–spin correlation functions. We express spin operators for do-
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when the electrons are far apart. However, Eq. which in our case is strictly satisfied only asymptotically with $\frac{U}{\Delta k}$.

In Fig. 2 for which concurrence oscillates as $C(t) = 2$ approximately mapped onto an effective Heisenberg model, function of electron-electron interaction and the model can be directly from Eq. (6).

An interesting observation here is substantial reduction of concurrence due to the coherent amplitudes for transmission (into region $[C]$) and reflection (back into region $[A]$), as shown in Fig. 1(d).

Let the initial state be prepared as $\psi^+_0 = (b_0 \phi_0 \pm g \phi_0) / \sqrt{2}$, where $g$ is the orbital state of the bound electron with spin $\downarrow$ centered around $i \sim 0$. Similarly, $g_x \propto \int \phi_{0x}^{(k)}(x) \phi_{0x}^{(k+\Delta k)} dx$ is the initial orbital state of the propagating electron with spin $\uparrow$, centered around $i \sim \ell$ and moving in the positive $i$ direction with momentum amplitude $\phi_0$ peaked at $k \sim k_0$, and with momentum uncertainty $\Delta k \sim 0$. Here we consider elastic scattering with amplitudes after the collision, $\psi^{+}_0 = r_s(b_0 \phi_0 \pm a \phi_0) + t_s(b_0 \phi_0 \pm a \phi_0)$, where $r_s(k_0)$ and $t_s(k_0)$ are singlet (triplet) reflection and transmission amplitudes and $b_0$ are normalized wave packets with mean momentum $-k_0$ and $k_0$, respectively.

Two basic experimental setups are possible when electrons are detected in different measurement domains, $[AB]$ or $[BC]$. The concurrence corresponding to reflected qubits is then

$$C_{AB} = \frac{2|\langle S^z A S^z B \rangle|}{n_{AB}} \sim \frac{|r_s^2(k_0) - r_s^2(k_0)|}{|r_s(k_0)|^2 + |r_s(k_0)|^2},$$

where $n_{A} = \langle \Sigma_{i \in [A]} n_i \rangle$, $n_i = 1$ [26]. The concurrence for transmitted qubits, $C_{BC}$, is given by an analogous expression with $A \rightarrow C$, and consequently with $r_s$ replaced with $t_s$. If the measuring apparatus captures both reflected and transmitted electrons ($i \in [A] \cup [C], j \in [B]$), the concurrence is given by $C_{AC,B} = (r_s - r_s)^2(r_s + r_s + t_s - t_s + t_s + t_s)^2$ and no additional renormalization is required. Equation (7) also follows directly from Eq. (1) if appropriately applied to scattering states [22,23]. However, for finite $\Delta k$, $C_{AB}$ (and correspondingly $C_{BC}$ or $C_{AC,B}$) has to be rederived from Eq. (5),

$$C_{AB} = \frac{\int [r_s^2(k) - r_s^2(k)] \phi_b^2 \, dk}{\int [r_s^2(k) + r_s^2(k)] \phi_b^2 \, dk}.$$
In order to demonstrate the basic properties of $C_{AB}$ and $C_{BC}$ we consider here the Anderson model, $H=H_0+\sum_{i}(\epsilon_n e_{i0}-(\epsilon_i -\epsilon_0)(c^\dagger_{i1}c_{i0}+c^\dagger_{i0}c_{i1}+H.c.))$, where $H_0$ is the Hubbard Hamiltonian in which $U=0$ except for the impurity site, $\epsilon<0$ is the impurity energy level, and $t_1$ is the hopping matrix element connecting the impurity site $i=0$ with left and right leads.

In the large-$U$ regime, $U,-\epsilon \gg t_0$, the static electron is strongly localized, $b_1 - \delta_0$. Electrons in the triplet channel are reflected, $r_1 = -\frac{1}{2}$, $t_1 = 0$, while singlet scattering amplitudes exhibit “charge transfer” resonance:

$$t_1 = \frac{1}{2} + r_1 = \frac{1}{2} \Gamma_k / (\epsilon_k - \omega_0 + i \Gamma_k)$$

with $\epsilon_k = -2t_0 \cos k$, $\omega_0 = (\epsilon + U)/(1 - 2 t_1^2 / t_0^2)$, and $\Gamma_k = 2t_0^2 (4t_0^2 - \omega_k^2)^{1/2} / (t_0^2 - 2t_1^2)$ [27]. “Transmitted” concurrence is due to the missing triplet amplitude, trivially, $C_{BC} = 1$. Reflected electrons are completely entangled at the singlet resonance energy but “total” concurrence $C_{AB} = 0$ there, as shown in Fig. 3.

The main result of this work is the closed-form formulas of the Wootters entanglement measure defined for two delocalized electrons. The proposed approach enables simple analysis of entanglement for a variety of realistic problems, from scattering of flying and static qubits represented as wave packets with finite energy resolution, to time evolution of static qubits due to electron-electron interaction or to externally applied fields. Further application to systems described with mixed states or with more than two electrons is possible; however, an appropriate definition of entanglement valid also for systems with non-negligible double occupancy remains open.


[20] This symmetry is conserved, e.g., in various electron-electron processes with Coulomb interaction.

[21] $\lvert ij, 1(2) = [1(\epsilon_1/\sqrt{2})c_{i1}^\dagger c_{i2}^\dagger \pm c_{i2}^\dagger c_{i1}^\dagger]0 \rangle \text{ and } \lvert ij, 3(4) = [\epsilon(1/\sqrt{2})\times c_{i1}^\dagger c_{i2}^\dagger \pm c_{i2}^\dagger c_{i1}^\dagger]0 \rangle \text{ [12].}$


[26] $n_A = \sum_{\epsilon(A)} \sum_{\epsilon(B)} \epsilon_{\epsilon_1} (\psi_1^\dagger)^2 + (\psi_2^\dagger)^2 + (\psi_3^\dagger)^2 + (\psi_4^\dagger)^2$.