Single-Site Entanglement of Fermions at a Quantum Phase Transition

Daniel Larsson\textsuperscript{1,2} and Henrik Johannesson\textsuperscript{2}

\textsuperscript{1}Fachbereich Physik, Philipps Universität Marburg, D-35032 Marburg, Germany and
\textsuperscript{2}Department of Physics, Göteborg University, SE-412 96 Göteborg, Sweden

We show that the single-site entanglement of a generic spin-1/2 fermionic lattice system can be used as a reliable marker of a finite-order quantum phase transition, given certain provisos. We discuss the information contained in the single-site entanglement measure, and provide illustrations from the Mott-Hubbard metal-insulator transitions of the one-dimensional (1D) Hubbard model, and the (1D) Hubbard model with long-range hopping.

PACS numbers: 71.10.Fd,03.65.Ud,03.67.Mn,05.70.Jk

Introduction. The study of entanglement properties of many-particle systems has become a subject of intense interest. Much of the motivation comes from quantum information theory where entanglement is made the key physical resource for a variety of information-processing tasks \cite{1}. In recent work it has been suggested that this resource may be efficiently extracted from a solid, or from some other many-particle system, by scattering particles off the system \cite{2}. Thermodynamic properties of solids have also been shown to be crucially influenced by entanglement properties of their microscopic degrees of freedom \cite{3}. Moreover, a rapidly growing body of results \cite{3,4,5,6,7} suggests that a properly chosen measure of entanglement may serve as a precise and convenient physical resource for a variety of information processing tasks \cite{1}. In recent work it has been suggested that this resource may be efficiently extracted from a solid, or from some other many-particle system, by scattering particles off the system \cite{2}. Thermodynamic properties of solids have also been shown to be crucially influenced by entanglement properties of their microscopic degrees of freedom \cite{3}. Moreover, a rapidly growing body of results \cite{3,4,5,6,7} suggests that a properly chosen measure of entanglement may serve as a precise and convenient physical resource for a variety of information processing tasks \cite{1}. The recent proof that any entanglement measure can be expanded as a unique functional of the first derivatives of the ground state energy (with respect to the parameters that control the QPT) puts this intuition on firm ground \cite{12}.

The connection between entanglement and QPTs can also be cast in the language of statistical mechanics, as pointed out recently by Campos Venuti et al. \cite{13}. As an example, consider the Hamiltonian density \( \mathcal{H}(g) \) of a system that undergoes a continuous second-order QPT when changing a parameter \( g \): \( \mathcal{H}(g) = \mathcal{H}_0 + g \Lambda \). Differentiating the energy density \( \langle \psi_0 | \mathcal{H}(g) | \psi_0 \rangle \) of the ground state \( | \psi_0 \rangle \) with respect to \( g \), its singular part \( \mathcal{O}_g \sim \langle \psi_0 | \Lambda | \psi_0 \rangle \) will behave as \( \mathcal{O}_g \sim \text{sgn}(g-g_c)|g-g_c|^\rho \) as \( g \) approaches \( g_c \), implying a divergence of \( \partial \mathcal{O}_g / \partial g \sim |g-g_c|^{\rho-1} \) at criticality. The singular term \( \mathcal{O}_g \) enters every reduced density matrix that contains a site where the operator \( \Lambda \) is defined, and it follows that any entanglement measure constructed from such a density matrix exhibits a singularity with an exponent related to \( \rho \) (barring accidental cancellations).

Having established this linkage, one may ask how it can be exploited for a specific problem. For example, in the case of a continuous second (or higher) order QPT, is it possible to “read off” the critical exponent \( \rho \) from the singularity of the entanglement measure? Conversely, is the information provided by the singular behavior of a local entanglement measure already contained in the scaling of observables – as predicted within the usual statistical mechanics framework?

In this article we address these questions by studying the single-site entanglement of a generic fermionic lattice system. We do so by constructing and analyzing its explicit representation using the Hellman-Feynman theorem. We find that the single-site entanglement measure can be used as reliable marker of a finite-order QPT (given certain provisos) and that it contains unique and useful information about the transition. The questions raised above will both turn out to have negative answers. As illustrations we use our construction to obtain the single-site entanglement at the Mott-Hubbard metal-
insulator transitions of the 1D Hubbard model [15], and
the 1D Hubbard model with long-range hopping [16], ex-
ploring exact results for the ground state properties of
these models. We stress that our analysis can be easily
adapted so as to apply to a system of localized spins,
with no change in the general results. Specifically, the
questions raised above are answered in the negative also
for coupled qubit (spin-1/2) systems. Our reason for fo-
cusing on fermionic systems is simply that these are less
well understood. With our contribution we hope to dis-
pel some of the perceived difficulties attached to their

treatment.

**Single-site entanglement and QPTs.** Let us first
recall that the concept of quantum entanglement of in-
distinguishable fermions [bosons] suffers from a certain
ambiguity since the accessible state space contains only
antisymmetrized [symmetrized] states and hence lacks a
direct product structure. The simplest way around this
problem is to use an occupation number representation
[17]. For spin-1/2 fermions one thus takes \( |n\rangle_j = |0\rangle_j,\)
\(|\uparrow\rangle_j,|\downarrow\rangle_j\) as local basis states, with \(j = 1,2,\ldots,L\)
indexing the corresponding lattice sites. In this way the
product structure of the state space is manifestly recov-
ered, with the representation spanned by the \(4^L\) basis
states \(|n_1\rangle \otimes |n_2\rangle \otimes \ldots \otimes |n_L\rangle\). One may now proceed
as usual and partition the system into two parts A and
B, with the entanglement (von Neumann) entropy \(\mathcal{E}\)
of a pure state \(|\psi\rangle\) defined by

\[
\mathcal{E} = - \text{Tr}(\rho_A \log_2 \rho_A). \tag{1}
\]

The reduced density matrix \(\rho_A\) is calculated from the
full density matrix \(\rho = |\psi\rangle \langle \psi|\) by taking the trace over
the local states belonging to B: \(\rho_A = \text{Tr}_B(\rho)\). By choos-
ing A as a single site (assuming translational invariance)
with B the rest of the system, one obtains the **single-site
entanglement**. One should note that in the occupation
number representation the subsystems A and B corre-
pond to fermionic modes (empty sites, singly occupied
sites with spin up or down, doubly occupied sites) and
not to particles. In this sense the notion of fermionic
(and similarly, bosonic) entanglement is different from
the text book example with spatially separated particles.

Given the occupation number representation it is
straightforward to verify that the reduced ground state
density matrix \(\rho_j\) for a single site \(j\) is diagonal, provided
that the ground state \(|\psi_0\rangle\) is a superposition of basis
states with the same number of particles and the same
total spin. Introducing the ground state expectation
values for a single site to be doubly occupied \(w_2\), singly
occupied by a fermion with spin-up [spin-down], \((w_{\uparrow\downarrow}),\)
or empty \((w_0)\), and assuming that the system is transla-
tionally invariant, we write:

\[
\begin{align*}
w_2 &= \langle \psi_0 | \hat{n}_j \hat{n}_j | \psi_0 \rangle \\
w_{\uparrow\downarrow} &= \langle \psi_0 | \hat{n}_j ^\dagger \hat{n}_j | \psi_0 \rangle - w_2 = \frac{n}{2} + m - w_2 \\
w_\downarrow &= \langle \psi_0 | \hat{n}_j \downarrow | \psi_0 \rangle - w_2 = \frac{n}{2} - m - w_2 \\
w_0 &= 1 - n + w_2
\end{align*}
\]

where in Eq. (2) \(\hat{n}_{j\sigma} = \hat{c}_{j\sigma} ^\dagger \hat{c}_{j\sigma}\) is the number
operator that samples site \(j\) for a fermion of spin \(\sigma = \uparrow, \downarrow, n =
\langle \psi_0 | \hat{n}_{j\uparrow} + \hat{n}_{j\downarrow} | \psi_0 \rangle\) is the average single site occupation
in the ground state, and \(m = (1/2) \langle \psi_0 | \hat{n}_{j\uparrow} - \hat{n}_{j\downarrow} | \psi_0 \rangle\) is the
ground state magnetization per site. It follows that

\[
\rho_j = \sum_{\alpha=0,\uparrow,\downarrow} w_{\alpha} |\alpha\rangle_j \langle \alpha |_j + w_2 |\uparrow\downarrow\rangle_j \langle \uparrow\downarrow |_j. \tag{3}
\]

Combining Eqs. (1), (2), and (3) the single-site entan-
glement takes the form

\[
\mathcal{E} = - \left( \frac{n}{2} + m - w_2 \right) \log_2 \left( \frac{n}{2} + m - w_2 \right) - \left( \frac{n}{2} - m - w_2 \right) \log_2 \left( \frac{n}{2} - m - w_2 \right) - w_2 \log_2 w_2 - w_2 \log_2 (1 - n + w_2).
\]

Let us now consider a fermion system with Hamiltonian
density \(\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda\) that exhibits a QPT for
some value \(g_c\) of \(g\) (with \(\Lambda\) the conjugate operator,
and with all other control parameters kept fixed and
absorbed as part of \(\mathcal{H}_0\)). By definition, a QPT of
\(k\)th order implies a divergence or a discontinuity in
the \(k\)th derivative \(\partial^k e_0 / \partial g^k\) of the ground state
energy density \(e_0 = \langle \psi_0 | \mathcal{H}(g) | \psi_0 \rangle\), with all derivatives
of order \(k < \) being finite and continuous. Defining
\(O_g \equiv \langle | \psi_0 \rangle | \mathcal{A} | \psi_0 \rangle - \) regular terms] (equal to \(\partial^k e_0 / \partial g^k -\) regular terms) by the Hellman-Feynman theorem,
it follows that \(\partial^k e_0 / \partial g^{k-1}\) has a divergence or a
discontinuity at \(g = g_c\). With these preliminaries we can
now prove the following

**Proposition**

Consider a spin-1/2 translationally invariant fermionic
system with a Hamiltonian density \(\mathcal{H}(g) = \mathcal{H}_0 + g\Lambda\)
that conserves particle number and total spin, and where
\(O_g \equiv \langle | \psi_0 \rangle | \mathcal{A} | \psi_0 \rangle - \) regular terms] is a linear combination
of \(m\) and/or \(w_2\). It follows that a divergence or a dis-
continuity in the \((k - 1)\)th derivative of the single-site
entanglement with respect to \(g\) (with all derivatives of
order \(k < k - 1\) being finite and continuous) signals that the
system undergoes a \(k\)th order QPT.

**Proof**

The proof is elementary. Repeated differentiation of Eq.
(1) yields

\[
(2)
\]

\[
(3)
\]

\[
(4)
\]
\[
\frac{\partial^{k-1} \mathcal{E}}{\partial g^{k-1}} = \left( \frac{\partial^{k-1}}{\partial g^{k-1}} \frac{n}{2} + m - w_2 \right) \log_2 \left( \frac{n}{2} + m - w_2 \right) - \left( \frac{\partial^{k-1}}{\partial g^{k-1}} \frac{n}{2} - m - w_2 \right) \log_2 \left( \frac{n}{2} - m - w_2 \right)
\]

\[
- \frac{\partial^{k-1} w_2}{\partial g^{k-1}} \log_2 (w_2) + \left( \frac{\partial^{k-1}}{\partial g^{k-1}} [n - w_2] \right) \log_2 (1 - n + w_2) + \text{terms containing lower-order derivatives.}
\]

By assumption all derivatives with respect to \( g \) of order \(< k - 1 \) are finite and continuous. Any singularity in \( \partial^{k-1} \mathcal{E}/\partial g^{k-1} \) must hence reside in terms containing derivatives of order \( k - 1 \). Since \( O_g \) is a linear combination of \( m, n \) and \( w_2 \), the proposition follows. \( \blacksquare \)

Several comments are in order. First note that the constraint that \( O_g \) should be some linear combination of \( m, n \) and \( w_2 \) is much less restrictive than may first appear to be the case. In fact, for a generic fermionic QPT caused by a change of an interaction or an external perturbation that couples only to single sites, \( O_g \) is identical to \( w_2 \) (with the transition driven by an on-site fermion-fermion interaction, \( g \equiv u \), \( m \) (with the transition driven by a magnetic field, \( g \equiv h \), or \( n \) (with the transition driven by a chemical potential, \( g \equiv \mu \)). One may think that the tight link between the scaling of \( \partial^{k-1} \mathcal{E}/\partial g^{k-1} \) and that of \( \partial^{k-1} O_g/\partial g^{k-1} \) would allow for the critical exponent that controls \( O_g \) to be immediately extracted from \( \partial^{k-1} \mathcal{E}/\partial g^{k-1} \). This is not so, however. As an example, take a second order QPT \((k = 2)\) with \( O_g = w_2 \), where \( \partial w_2/\partial u \sim |u - u_c|^{\rho - 1} \rightarrow \infty \) as \( g \rightarrow g_c = u_c \). By inspection of Eq. (5) one then notes that the leading scaling of \( \partial \mathcal{E}/\partial g \) will be governed by the same exponent \( \rho \) only if \( m \) and \( n \) are independent of \( w_2 \), or, depend on \( w_2 \) as a power with exponent \( \geq 1 \). Whether this is the case typically requires that one has access to an exact solution of the model, and in any event can only be determined on a case-to-case basis. Turning to the logarithmic factors in (5) one realizes that these will cause logarithmic divergences if one or several of the occupation parameters \( w_0, w_1, w_\downarrow, w_\uparrow \) vanish at the transition (cf. the parameterization in (2)). Such logarithmic corrections, multiplying the leading scaling of \( \partial^{k-1} \mathcal{E}/\partial g^{k-1} \) inherited from \( O_g \), thus signal a change of the dimension of the accessible local Hilbert space as the system undergoes the transition. This is a useful and important property of the single-site entanglement scaling not shared by the scaling of \( O_g \) or its derivatives. One should here note that a spurious signaling of a \( k^{\text{th}} \) order QPT by a divergence in \( \partial^{k-1} \mathcal{E}/\partial g^{k-1} \) caused by a vanishing occupation parameter is blocked by the constraint in the proposition that all lower-order derivatives of \( \mathcal{E} \) are finite. (Although maybe hard to realize, one may envision a system where one or several local basis states get excluded when tuning some parameter in the Hamiltonian [implying the vanishing of an occupation parameter] without the occurrence of a QPT.)

Using the diagnostics supplied by our proposition, are we guaranteed to catch all fermionic QPTs? The answer is negative. First, the diagnostics obviously fails for a QPT of infinite order [18], a Berezinskii-Kosterlitz-Thouless (BKT) type transition being a case in point [19]. Second, and more insidious, a system may exhibit a QPT of finite order, but with the single-site entanglement and its derivatives still remaining regular. This happens if all local basis states \( |n\rangle_j = |0\rangle_j, |\uparrow\rangle_j, |\downarrow\rangle_j \), and \( |\uparrow\downarrow\rangle_j \) become equally populated as one approaches the transition. As seen from (5), the \((k - 1)^{\text{st}}\) derivative terms then vanish identically, killing the signal of the QPT. The simultaneous vanishing of \( \partial \mathcal{E}/\partial g \) implies that \( \mathcal{E} \) has a local extremum at the transition (expected to be a maximum since in this case all local basis states are equally represented in the make-up of the many-particle ground state). However, one cannot a priori exclude that \( \mathcal{E} \) is at an extremum without the occurrence of a QPT. Hence, an extremum of the single-site entanglement does not necessarily signal a QPT. Whether a QPT is present or not in this case requires information beyond that provided by the entanglement measure.

Having exposed the general features of entanglement scaling at a fermionic QPT, let us look at two examples.

**Case studies.** Consider first the ordinary 1D Hubbard model

\[
H = - \sum_{\sigma = \uparrow, \downarrow} L_{\sigma} \left( \hat{c}_{i\sigma}^\dagger \hat{c}_{i+1\sigma} + \text{h.c.} \right) + u \sum_{i=1}^L \hat{n}_{i\uparrow} \hat{n}_{i\downarrow}
\]

with the first term describing hopping of electrons between neighboring sites, and with the second term an effective on-site interaction of strength \( u \). At half-filling of the lattice, \( n = 1 \), the model exhibits a QPT at \( u = 0 \), separating a Mott insulating phase \((u > 0)\) from a metallic phase \((u < 0)\). The ground state energy density becomes non-analytic at the transition, but allows for an asymptotic power series expansion with all derivatives being finite and continuous [20]. The QPT is thus of infinite order, and can be shown to belong to the BKT universality class [21]. As found by Gu et al., the single-site entanglement has a maximum at the transition. This reflects the equipartition of empty-, singly- and doubly occupied local states when \( u = 0 \) (non-interacting fermions). The transition is thus special on two counts: it is of infinite order and it supports an equipartition of
local states. This makes it an exceptional example of a fermionic QPT, where no information can be deduced from the entanglement measure.

A metal-insulator transition can also be triggered when \( u > 0 \) by connecting the system to a particle reservoir and tuning the chemical potential \( g = \mu \). When \( n < 1 \) the system is metallic, but turns into an insulator at the critical charge \( \mu_c = 2 - 4 \int_0^\infty J_1(\omega)\omega[1+\exp(\omega u/2)]^{-1} \) where \( n = 1 \). The transition is second order with a logarithmic divergent susceptibility \( \chi_c = \partial n/\partial \mu \sim (\mu - \mu_c)^{-1/2} \). As shown in Ref. 2, the derivative of the critical single-site entanglement for finite \( u \) is precisely given by \( \chi_c \), up to a multiplicative constant: \( \partial \mathcal{E}/\partial \mu = -C(u)\chi_c \). In the limit \( u \to \infty \) the empty local states get suppressed at the transition and the scaling of \( \partial \mathcal{E}/\partial \mu \) picks up a logarithmic correction \( \chi_c \approx \chi_c(\ln |\mu - \mu_c| + \text{const.})/2\ln 2 \). Both behaviors well illustrate our general discussion above: For finite \( u \) the logarithms in Eq. 5 add up to the \( u \)-dependent constant \( C(u) \), whereas in the limit \( u \to \infty \) the entanglement measure detects a change in the logarithmic correction to the leading scaling.

As a second example, let us consider the 1D Hubbard model with long-range hopping, introduced by Gebhard and Ruckenstein: 16

\[
H = \sum_{\ell \sigma = u, l} t_{\ell m} \hat{c}_\ell^{\dagger} \hat{c}_m \sigma + u \sum_{l=1}^L \hat{n}_{\ell l} \hat{n}_{l \ell} \quad (7)
\]

with \( t_{\ell m} = i(-1)^{(l-m)}(l-m)^{-1} \). The ground state energy density at half-filling is given by \( e_0 = (un - u_c(1-2n))/4 - (1/(24uw_c))((u + u_c)^3 - ((u + u_c)^2 - 4uu_c n)^3/2) \) with \( u_c = 2\pi \) the critical point 16. This implies that \( w_2 = \partial e_0/\partial u \) has a discontinuity in its second order derivative with respect to \( u \) at \( u_c \), and hence the transition is third order. From Eq. 4 with \( n = 1 \) it follows that the single site entanglement can be written as

\[
\mathcal{E} = -(1 - 2w_2) \log_2(1/2 - w_2) - 2w_2 \log_2(w_2)
\]

when no magnetic field is present (i.e. \( m = 0 \), and one immediately verifies that \( \partial^2 \mathcal{E}/\partial u^2 \) is also discontinuous at the transition point \( u_c \). Since the local basis states do not become equally populated at \( u_c \) — in contrast to the \( u = 0 \) metal-insulator transition of the ordinary Hubbard model — the single-site entanglement here provides an accurate diagnostics of the transition.

One can also drive a Mott-Hubbard metal-insulator transition by tuning the chemical potential when \( u > u_c \), in exact analogy with the ordinary Hubbard model. Expressing \( n \) as a function of \( \mu \), and applying the Hellman-Feynman theorem to the ground state energy \( e_0 \) above, one obtains a discontinuity in \( \partial n/\partial \mu \) at \( \mu = \mu_c = \pm 2\pi \). Eq. 4 immediately implies that \( \partial \mathcal{E}/\partial \mu \) is also discontinuous at \( \mu = \mu_c \), with the transition being second order. In the limit \( u \to \infty \) this discontinuity is multiplied by a logarithmic divergent factor when \( \mu \to \mu_c \), reflecting the suppression of empty states in this case.

**Summary.** We have shown that a generic finite-order quantum phase transition in a spin-1/2 fermionic lattice system can be consistently identified and characterized by studying the behavior of the single-site entanglement and its derivatives with respect to the parameter that controls the transition. Extensions to cases where the transition is driven by an interaction or a field that couples to pairs or clusters of lattice sites (like the extended Hubbard model 23) is conceptually straightforward, albeit technically more demanding. We hope to return to this problem in a future publication.

**Acknowledgments.** We thank F. Gebhard and W. Metzner for valuable discussions. D.L. thanks the Physics Department at Phillips Universität Marburg for its hospitality. H.J. acknowledges support from the Swedish Research Council under grant no. 621-2002-4947.

---

1. M. A. Nielsen and I. L. Chuang, *Quantum Computation and Quantum Information* (Cambridge University Press, Cambridge, 2000).
2. G. De Chiara et al., quant-ph/0505107.
3. S. Ghosh, T. F. Rosenbaum, G. Aeppli, and S. N. CooperSmith, Nature 425, 48 (2003).
4. A. Osterloh, L. Amico, G. Falci, and R. Fazio, Nature 416, 608 (2002).
5. T. J. Osborne and M. A. Nielsen, Phys. Rev. A 66, 032110 (2002).
6. L.-A. Wu, M. S. Sarandy, and D. A. Lidar, Phys. Rev. Lett. 93, 250404 (2004).
7. W. K. Wootters, Phys. Rev. Lett. 80, 2245 (1998).
8. S.-J. Gu et al., Phys. Rev. Lett. 93, 086402 (2004).
9. D. Larsson and H. Johannesson, Phys. Rev. Lett. 95, 196406 (2005).
10. By the term local we mean that the entanglement measure is defined with respect to local observables.
11. S. Sachdev, *Quantum Phase Transitions* (Cambridge University Press, Cambridge, 1999).
12. G. Vidal and R. F. Werner, Phys. Rev. A 65, 032314 (2002).
13. L.-A. Wu et al., quant-ph/0512031.
14. L. Campos Venuti et al., Phys. Rev. A 73, 010303 (2006).
15. E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. 20, 1445 (1968); Physica A 321, 1 (2003).
16. F. Gebhard and A. E. Ruckenstein, Phys. Rev. Lett. 68, 244 (1992).
17. F. Zanardi, Phys. Rev. A 65, 042101 (2002).
18. C. Itoh and H. Mukaida, Phys. Rev. E 60, 3688 (1999).
19. V. L. Berezinskii, Zh. Eksp. Teor. Fiz. 59, 907 (1970) [Sov. Phys. JETP 32, 493 (1971)]; J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973).
20. W. Metzner and D. Vollhardt, Phys. Rev. B 39, 4462 (1989).
21. T. Giamarchi, Physica B 230, 975 (1997).
22. F. Gebhard, A. Girndt and A.E. Ruckenstein, Phys. Rev. B 49, 10926 (1994).
23. A. Anfossi, P. Giraud, A. Montorsi, and F. Traversa, Phys. Rev. Lett. 95, 056402 (2005).