



Measuring Entanglement in Condensed Matter Systems

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We show how entanglement may be quantified in spin and cold atom many-body systems using standard experimental techniques only. The scheme requires no assumptions on the state in the laboratory, and a lower bound to the entanglement can be read off directly from the scattering cross section of neutrons deflected from solid state samples or the time-of-flight distribution of cold atoms in optical lattices, respectively. This removes a major obstacle which so far has prevented the direct and quantitative experimental study of genuine quantum correlations in many-body systems: The need for a full characterization of the state to quantify the entanglement contained in it. Instead, the scheme presented here relies solely on global measurements that are routinely performed and is versatile enough to accommodate systems and measurements different from the ones we exemplify in this work.

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Interacting quantum many-body systems generally exhibit correlations between its constituents. At sufficiently low temperatures, these correlations possess quantum mechanical features—entanglement. Compared to its classical counterpart, entanglement is extremely complex. Its full characterization generally requires the measurement of a number of observables that grows exponentially with the number of constituents of the systems. The ability to create entanglement merely by cooling an interacting quantum many-body system provides the attractive opportunity of carrying out quantum information processing tasks which gain their power exactly because of the complex structure of entanglement. However, the very same setting offers significant challenges, as it is much harder to analyze theoretically and, crucially, experimentally: While for the few-particle systems that can now be prepared in highly controlled environments such as ion traps, it is possible to fully characterize the state in the laboratory by quantum state tomography [1], the situation in condensed matter systems is far more challenging. Firstly, the number of subsystems tends to be much larger, the level of control over states and Hamiltonians is more restricted, and, crucially, the available measurements for condensed matter systems are much less general: Local measurements addressing individual constituents are usually not available and one has to rely on global measurements such as those obtained in scattering experiments to draw conclusions about the system. These are of course by no means sufficient to fully characterize the state in the laboratory. How might one still be able to say something about the entanglement that is available? One approach could be to, e.g., model the system with a certain quantum Hamiltonian and compare it to a classical model. If the predictions from the quantum model match the measurement results while the classical does not, and the simulated quantum state displays entanglement, one might conclude

that the state in the laboratory is indeed entangled. This, however, is a fallacy. Consider the following example of two spins [2]: Suppose one measures the correlation $\langle \hat{\sigma}_1^z \hat{\sigma}_2^z \rangle - \langle \hat{\sigma}_1^z \rangle \langle \hat{\sigma}_2^z \rangle$ and obtains the result -1 . This measurement is consistent with both the maximally entangled state $|\psi\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$ and the separable state $\hat{\rho} = (|\uparrow\uparrow\rangle\langle\uparrow\uparrow| + |\downarrow\downarrow\rangle\langle\downarrow\downarrow|)/2$. Hence, without further assumptions, one may not decide whether the state in the laboratory is entangled or not. A possible assumption may be that the system is in thermal equilibrium at some known temperature and that the Hamiltonian that governs the system is known precisely. But obtaining knowledge about the Hamiltonian experimentally is even harder than to obtain the state itself. A technique to decide without a doubt whether entanglement is contained in a given system should hence not rely on knowing the Hamiltonian; it should, in fact, not rely on any kind of knowledge about the system other than measured data, but be able to quantify entanglement by just relying on measured observables.

Here we present a scheme to quantify entanglement in condensed matter systems that fulfils all the above requirements and relies only on measurements that are already available: Neutron scattering from spin systems and time-of-flight imaging of cold atoms. Hence, we show that it is possible to directly—without any assumptions—measure entanglement in many-body systems. To this end we exploit the substantial body of work concerning the characterization (which states are entangled), quantification (how much of it do we have), and verification (on the basis of simple measurements we need to answer the previous questions) of entanglement (see [3] for a tutorial review and [4] for an advanced and very comprehensive review) that have been established in quantum information science. More precisely, we combine methods for determining the presence of entanglement in quantum many-body systems [5,6] with proposals for the quantification of entanglement in

many-body quantum systems [2,7–10] to achieve an experimentally accessible method for measuring entanglement.

Spin systems.—One of the standard tools to analyze condensed matter samples is neutron scattering; see, e.g., Ref. [11]. The deflected neutrons carry information about the structural and magnetic properties of the sample, which can be read off the differential scattering cross section [12]. The Fourier transform of the magnetic cross section gives access to spin correlations in reciprocal space such as the positive Hermitian observable $\hat{S}(\mathbf{q}) = \sum_{\alpha=x,y,z} \hat{S}_{\alpha}(\mathbf{q})$, where

$$\hat{S}_{\alpha}(\mathbf{q}) = \frac{1}{M} \sum_{i,j} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \hat{\sigma}_i^{\alpha} \hat{\sigma}_j^{\alpha}, \quad (1)$$

$\hat{\sigma}_i^x$, $\hat{\sigma}_i^y$, $\hat{\sigma}_i^z$ are Pauli spin matrices acting on lattice site i located at \mathbf{r}_i , and M is the total number of spins, so the number of lattice sites.

In the following we will show how a measurement of observables of the type in Eq. (1) alone is sufficient to quantify the entanglement contained in the sample. We will consider systems comprised of spin-1/2 particles on a lattice and set out to derive a lower bound to the entanglement that is consistent with the measurement data. It will turn out that it is possible to find a lower bound that is a simple function of the static structure factor $\langle \hat{S}(\mathbf{q}) \rangle$. Hence, for this, no assumptions about the state are necessary; in particular, no knowledge about the Hamiltonian is required.

In the following we present definitions and a derivation that will lead to the central result in Eq. (3), which provides a lower bound on the entanglement of any spin state under investigation that can be used directly on experimental data. Several entanglement measures may be expressed in the form [3,13]

$$\mathcal{E}_{\mathcal{C}}(\hat{\rho}) = \max\{0, -\min_{\hat{W} \in \mathcal{W} \cap \mathcal{C}} \text{tr}[\hat{W} \hat{\rho}]\}, \quad (2)$$

where \mathcal{W} denotes the set of Hermitian operators that fulfil $\langle \hat{W} \rangle \geq 0$ for separable states [14] (i.e., the set of entanglement witnesses [15]) and \mathcal{C} distinguishes the quantities: For example, if \mathcal{C} is the set of operators \hat{W} fulfilling $\langle \hat{W} \rangle \leq 1$ for separable states, then $\mathcal{E}_{\mathcal{C}}$ is the robustness of entanglement [16], for $\mathcal{C} = \{\hat{W} \in \mathcal{W} | \mathbb{1} - \hat{W} \geq 0\}$, $\mathcal{E}_{\mathcal{C}}$ measures the generalized robustness of entanglement [17], and if $\mathcal{C} = \{\hat{W} \in \mathcal{W} | \mathbb{1} + \hat{W} \geq 0\}$ then $\mathcal{E}_{\mathcal{C}}$ is equal to the best separable approximation [18]. In fact, $\mathcal{E}_{\mathcal{C}_{n,m}}, \mathcal{C}_{n,m} := \{\hat{W} \in \mathcal{W} | -n\mathbb{1} \leq \hat{W} \leq m\mathbb{1}\}$, is an entanglement monotone for every $n, m \geq 0$ [13]. One can now exploit the fact that for any choice $\hat{W} \in \mathcal{W} \cap \mathcal{C}$ one obtains the lower bound $\mathcal{E}_{\mathcal{C}}(\hat{\rho}) \geq \max\{0, -\text{tr}[\hat{W} \hat{\rho}]\}$ for all $\hat{W} \in \mathcal{W} \cap \mathcal{C}$. Given this expression, it is possible to arrive at lower bounds to $\mathcal{E}_{\mathcal{C}}$ by simply constructing operators $\hat{W} \in \mathcal{W} \cap \mathcal{C}$ that are functions of observables that are within experimental reach. This works of course for any spin system and any observable.

In the following, we will focus on the best separable approximation and the observable \hat{S} . Consider the operator $\hat{W}(\mathbf{q}) = \hat{S}(\mathbf{q})/2 - \mathbb{1}$, for which we now show that

$\hat{W} \in \mathcal{W} \cap \mathcal{C}$. We find $\hat{W}(\mathbf{q}) + \mathbb{1} \geq 0$, and for a product state $\hat{\rho} = \otimes_i \hat{\rho}_i$, we have

$$\langle \hat{W}(\mathbf{q}) \rangle = \sum_{i,\alpha} \frac{1 - \langle \hat{\sigma}_i^{\alpha} \rangle^2}{2M} - 1 + \frac{1}{2M} \sum_{\alpha} \left| \sum_i e^{i\mathbf{q}\cdot\mathbf{r}_i} \langle \hat{\sigma}_i^{\alpha} \rangle \right|^2,$$

which is non-negative as the last term is and the first term may be bounded by using the uncertainty relation $\sum_{\alpha} (1 - \langle \hat{\sigma}_i^{\alpha} \rangle^2) \geq 2$. Hence, $\hat{W} \in \mathcal{W} \cap \mathcal{C}$, i.e., for every state $\hat{\rho}$ and every \mathbf{q} , the quantity

$$E(\mathbf{q}) = \max\left\{0, 1 - \frac{1}{2M} \sum_{i,j,\alpha} e^{i\mathbf{q}\cdot(\mathbf{r}_i - \mathbf{r}_j)} \langle \hat{\sigma}_i^{\alpha} \hat{\sigma}_j^{\alpha} \rangle\right\} \quad (3)$$

provides a lower bound to the M -partite entanglement (as measured in terms of the best separable approximation) contained in $\hat{\rho}$. Similar bounds may be derived for all entanglement measures that fall into the general framework of Eq. (2).

At this point, we would like to emphasize again that $E(\mathbf{q})$ gives a lower bound to the entanglement for any state on the lattice—irrespective of how it has been prepared, what the temperature is, or what the Hamiltonian might be.

As an example, we consider thermal states of the antiferromagnetic Heisenberg model

$$\hat{H} = J \sum_{\alpha=x,y,z} \sum_{\langle i,j \rangle} \hat{\sigma}_i^{\alpha} \hat{\sigma}_j^{\alpha} \quad (4)$$

on a square lattice. This model has been analyzed in great detail in the literature (see Ref. [19] for a review) using several analytical and numerical techniques. In Ref. [20] the two-dimensional Heisenberg antiferromagnet copper deuterioformate tetradeurate has been analyzed experimentally using extensive neutron scattering measurements, and it has been suggested—under the assumption that the system is indeed described by \hat{H} with known coupling constants and by a comparison of a classical to a quantum description—that entanglement is present in this system. Using $E(\mathbf{q})$, the presence of entanglement cannot only be confirmed but, as it is a lower bound to the best separable approximation, also quantified. In Fig. 1, we show $E(\mathbf{q})$ for a thermal state at different values of $J\beta$ as obtained from a quantum Monte Carlo computation (QMC) [21]. The plot shows that entanglement is present up to fairly high temperatures; i.e., measuring entanglement is well within experimental reach (in [20], e.g., the sample was at a temperature of 1.5 K and the data well fitted by $J = 6.19$ meV, i.e., $k_B T/J = 0.02$). In addition, the plot exemplifies the quality of our bound: The best separable approximation is upper bounded by unity and at low temperatures $E(\mathbf{0}) \approx 1$. $E(\mathbf{q})$ also scales properly with the system size: For the ground state of \hat{H} it is known that $S(\mathbf{q}) \sim |\mathbf{q}|$ for small $|\mathbf{q}|$ [19], i.e., $E(\mathbf{q}) - 1 \sim |\mathbf{q}|$; see also Ref. [22].

Bosons in optical lattices.—A standard measurement in the context of ultracold atoms is the following: One switches off all potentials, allows the atom cloud to expand freely, and then takes an absorption image of the atoms,

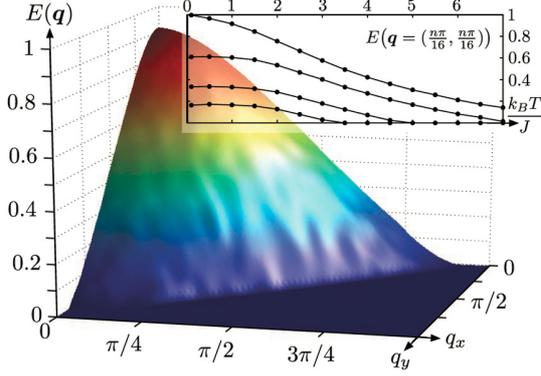


FIG. 1 (color online). Lower bound E on the entanglement—as measured in terms of the best separable approximation (BSA)—for a thermal state $\hat{\rho} = \exp(-\beta\hat{H})/Z$, $\beta J = J/k_B T = 1$, of the Heisenberg model in Eq. (4). For every \mathbf{q} , $E(\mathbf{q})$ provides a lower bound to the BSA. The square lattice with open boundary conditions and lattice constant $a = 1$ has 30×30 lattice sites, and $\langle \hat{S}(\mathbf{q}) \rangle$ was obtained using the generalized directed loop QMC algorithm [29] of the ALPS package [21]. Inset shows $E(\frac{n\pi}{16}, \frac{n\pi}{16})$, $n = 0, 4, 6, 7$ (top to bottom), as a function of the temperature. Lines are a guide to the eye. Note that the BSA is upper bounded by unity, a bound that $E(\mathbf{q})$ saturates at low temperatures and $\mathbf{q} = \mathbf{0}$.

which reveals the velocity, quasimomentum, or time-of-flight distribution of the atoms before the expansion. This technique was used to demonstrate the Mott insulator-superfluid transition of bosons in optical lattices [23] and to observe Fermi surfaces of fermions in optical lattices [24] to name just a few. We focus on the situation in which bosons of mass m are kept in an optical lattice with lattice constant a . After a time of flight t , the density of the atoms reads (see, e.g., Refs. [25,26])

$$n(\mathbf{r}) = \sum_{i,j} f_{i,j} \left(\mathbf{k} = \frac{m\mathbf{r}}{\hbar t} \right) \langle \hat{b}_i^\dagger \hat{b}_j \rangle, \quad (5)$$

where

$$f_{i,j}(\mathbf{k}) = \left(\frac{m}{\hbar t} \right)^3 |w(\mathbf{k})|^2 e^{i[\mathbf{k}(r_i - r_j) + (m/2\hbar t)(r_i^2 - r_j^2)]}, \quad (6)$$

$w(\mathbf{k})$ is the Fourier transform of the Wannier function centered at zero, and \hat{b}_i annihilates a boson at site i located at \mathbf{r}_i . The resulting absorption image is then the integral along the optical axis, say, the z direction, of this density, i.e.,

$$n(x, y) = \sum_{i,j} f_{i,j}(x, y) \langle \hat{b}_i^\dagger \hat{b}_j \rangle =: \langle \hat{n}(x, y) \rangle, \quad (7)$$

where $f_{i,j}(x, y) = \int dz f_{i,j}(\frac{\hbar t}{m})$, $f_{i,i}(x, y) =: f(x, y)$. We now set out to show that

$$E(x, y) = \max \left\{ 0, \langle \hat{N} \rangle - \frac{n(x, y)}{f(x, y)} \right\} \quad (8)$$

provides a lower bound to the entanglement in the state in the laboratory—the main result of this section.

As we are concerned with massive particles, we will, in the following, restrict the state space to states $\hat{\rho}$ that have a finite mean number of particles, $\text{tr}[\hat{\rho}\hat{N}] < \infty$, and commute with the particle-number operator \hat{N} . In other

words, we are concerned with states respecting the particle-number superselection rule (SSR)—the only physical states allowed in this setting of indistinguishable massive particles [27]. These states are of the form $\hat{\rho} = \sum_{N=0}^{\infty} \hat{P}_N \hat{\rho} \hat{P}_N =: \bigoplus_{N=0}^{\infty} \hat{\rho}_N$, where \hat{P}_N projects on the sector with constant particle number N . The SSR also restricts the allowed physical operations to operations commuting with \hat{N} [27]. Consider now

$$\mathcal{E}(\hat{\rho}) = \max \left\{ 0, - \sum_{N=0}^{\infty} \min_{\hat{W} \in \mathcal{C}_N} \text{tr}[\hat{\rho}_N \hat{W}] \right\}, \quad (9)$$

where \mathcal{C}_N is the set of Hermitian operators \hat{W} acting on the subspace of constant particle number N that fulfil $cN \pm \hat{W} \geq 0$ for some constant $c > 0$ independent of N and $\text{tr}[\hat{\rho}_N \hat{W}] \geq 0$ for separable $\hat{\rho}_N$. Using similar methods as in Ref. [13], it can be shown that [28] \mathcal{E} is an entanglement monotone under local operations and classical communication (LOCC) operations that preserve the total number of particles, i.e., that commute with \hat{N} (and hence it is also an entanglement monotone under SSR-LOCC operations—LOCC operations that preserve the local particle number; for a discussion of entanglement under SSR see Ref. [27]).

We now show that $\hat{W}_N = \hat{P}_N[\hat{n}/f(x, y) - \hat{N}]\hat{P}_N \in \mathcal{C}_N$. To this end let $|\psi\rangle$ be a state vector on the subspace of constant particle number N . Then, with M being the number of lattices sites, we find

$$\frac{\langle \psi | \hat{n} | \psi \rangle}{f(x, y)} \leq \sum_{i,j} \sqrt{\langle \psi | \hat{b}_i^\dagger \hat{b}_i | \psi \rangle} \sqrt{\langle \psi | \hat{b}_j^\dagger \hat{b}_j | \psi \rangle} \leq NM, \quad (10)$$

i.e., $MN \pm \hat{W}_N \geq 0$. Furthermore, for separable $\hat{\rho}_N$, we find for $i \neq j$ that $\text{tr}[\hat{\rho}_N \hat{b}_i^\dagger \hat{b}_j] = 0$, and hence

$$\text{tr}[\hat{\rho}_N \hat{n}] = f(x, y) \sum_i \text{tr}[\hat{\rho}_N \hat{b}_i^\dagger \hat{b}_i] = f(x, y)N, \quad (11)$$

i.e., $\text{tr}[\hat{\rho}_N \hat{W}_N] \geq 0$. Hence, $\hat{W}_N \in \mathcal{C}_N$, which implies that

$$- \min_{\hat{W} \in \mathcal{C}_N} \text{tr}[\hat{\rho}_N \hat{W}] \geq \text{tr}\{\hat{\rho}_N [N - \hat{n}/f(x, y)]\}, \quad (12)$$

and thus, for all x, y , the quantity in Eq. (8) provides a lower bound to the M -partite entanglement available in the system. Here, $n(x, y) = \langle \hat{n}(x, y) \rangle$ is obtained in standard time-of-flight measurements and E is a lower bound for any state on the lattice.

As an example, we consider thermal states of the Bose-Hubbard model on a three-dimensional cubic lattice,

$$\hat{H} = -J \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j + \frac{U}{2} \sum_i \hat{n}_i (\hat{n}_i - 1) - \mu \sum_i \hat{n}_i, \quad (13)$$

where $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$, the summation is over nearest neighbors, J accounts for tunneling of atoms between adjacent sites, U is the strength of the on-site repulsion of atoms, and the chemical potential μ controls the particle number. Bosons in deep optical lattices are well described by this model, which displays a quantum phase transition from a Mott

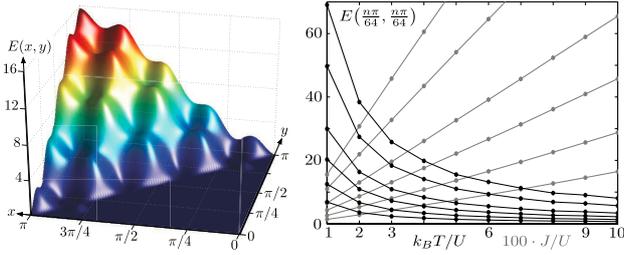


FIG. 2 (color online). Lower bound $E(x, y)$ on the entanglement for a thermal state $\hat{\rho} = \exp(-\hat{H}/k_B T)/Z$ with constant filling factor $\langle \hat{n}_i \rangle = 1$ of the Bose-Hubbard model in Eq. (13). The three-dimensional cubic lattice with periodic boundary conditions and lattice constant $a = 1$ has $10 \times 10 \times 10$ lattice sites and $\langle \hat{n}(x, y) \rangle$ was obtained using the same numerical code as for Fig. 1. Left-hand plot shows $E(x, y)$ as in Eq. (8) for $\beta U = 1/5$, $J/U = 0.01$. Right-hand plot shows $E(\frac{n\pi}{64}, \frac{n\pi}{64})$, $n = 64, 48, 44, 36, 34, 33$ (top to bottom) as a function of the temperature (black lines) and of the tunneling amplitude J/U (gray lines). Lines are guides to the eye.

insulator (small J/U) to superfluid (large J/U) that was observed in [23] via the interference pattern displayed in $\langle \hat{n}(x, y) \rangle$. In Fig. 2, we show $E(x, y)$ for a thermal state as obtained from a QMC computation [21]. We can see that $E(x, y)$ increases linearly with J/U and stays finite up to high temperatures. Hence, quantifying entanglement in these systems is already well within experimental reach. While the data in Fig. 2 suggest that in order to detect entanglement the measurement precision needs to be very high, i.e., $\langle \hat{N} \rangle$ and $n(x, y)/f(x, y)$ known to very high precision, one has to keep in mind that these data correspond to the deep Mott regime, which by its very nature exhibits only a small amount of entanglement. For the ground state on a cubic three-dimensionally translationally invariant lattice with $M = L^3$ in the deep superfluid regime ($U = 0$), one finds at $x = y = 0$ that $\langle \hat{N} \rangle = \rho L^3$ and $n(x, y)/f(x, y) = \rho L^2$, where $\rho = \langle \hat{n}_i \rangle$, which leaves sufficient room for experimental uncertainties.

Conclusion.—We have derived lower bounds to the entanglement contained in lattice systems. These lower bounds are a simple function of routinely measured observables and do not require any additional information about the system. This makes the quantification of entanglement in condensed matter samples possible. Without making any assumptions (such as the temperature, the Hamiltonian, the way the state was created), entanglement can be directly measured using only measurements that belong to the toolbox for the analysis of quantum many-body systems. The presented schemes straightforwardly generalize to other many-body systems and observables.

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