Entanglement entropy, single-particle occupation probabilities, and short-range correlations

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For quantum many-body systems with short-range correlations (SRCs), the intimate relationship between their magnitude, the behavior of the single-particle occupation probabilities at momenta larger than the Fermi momentum, and the entanglement entropy is a new qualitative aspect not studied and exploited yet. A large body of recent condensed matter studies indicate that the time evolution of the entanglement entropy describes the non-equilibrium dynamics of isolated and strongly interacting many-body systems, in a manner similar to the Boltzmann entropy, which is strictly defined for dilute and weakly interacting many-body systems. Both theoretical and experimental studies in nuclei and cold atomic gases have shown that the fermion momentum distribution has a generic behavior $n(k) = C/k^4$ at momenta larger than the Fermi momentum, due to the presence of SRCs, with approximately 20% of the particles having momenta larger than the Fermi momentum. The presence of the long momentum tails in the presence of SRCs changes the textbook relation between the single-particle kinetic energy and occupation probabilities, $n_{mf}(k) = 1/[1 + \exp(\beta(\epsilon(k) - \mu))]$ for momenta very different from the Fermi momentum, particularly for dynamics processes. SRCs induced high-momentum tails of the single-particle occupation probabilities increase the entanglement entropy of fermionic systems, which in its turn affects the dynamics of many nuclear reactions, such as heavy-ion collisions and nuclear fission.

Short-range correlations (SRCs) are defined as correlations between the constituents of a quantum many-body system at interparticle separations smaller than the average separation between its constituents, which is of order $1/\sqrt{n(r)}$, where $n(r)$ is the number density. Such interparticle separations correspond to particle momenta larger than the local Fermi momentum $hk_F(r) = h\sqrt{2\pi^2n(r)}$, when the particle motion is essentially unperturbed by the mean field. A great example was discussed by Landau [1], when he discussed the dispersion relation between the (quasi)particle kinetic energy and its momentum $\epsilon(p)$ in superfluid helium II, where he identified three branches of this spectrum: the phonon branch, the roton branch, and at higher momenta essentially the atom free motion. If the SRCs are strong, their role should appear at relatively small momenta, close to the Fermi momentum $hk_F$ and the fraction of the quasiparticles with such momenta can be significant. In particular, the single particle occupation probability for Landau quasiparticles is given by the textbook formula [2], apart from the trivial energy shift due the presence of the mean field,

$$n_{mf}(k) = \frac{1}{1 + \exp(\beta(\epsilon(k) - \mu))},$$

where $\beta = 1/T$ is the inverse temperature, $\mu$ is the chemical potential, and $\epsilon(k) = h^2k^2/2m$ is the kinetic energy. This formula is valid only in a relatively small energy interval around the Fermi level, strictly speaking only for systems in (quasi)equilibrium and it is in agreement with kinetic theory in the long time limit and quasi-locally for dilute and weekly interacting systems. Its range of validity and accuracy are however not established. Decades long studies of fermion momentum distribution in nuclei and cold atomic gases, where SRCs are important, require a more sophisticated approach. The relation between the SRCs and the entanglement entropy were discussed recently in Refs. [3–6].

While it appears that only recently it was realized that quantum entanglement and superposition are equivalent concepts [7], with a little bit of effort one can easily convince oneself that the second century old two-slit experiment due to Thomas Young, where superposition and coherence (thus entanglement) was crucial, the EPR paradox [8], the entanglement introduced by Schrödinger discussed many times by other authors [9–11], and short-range correlations (SRCs) in quantum systems where they are present, are intimately related phenomena. Two particles in a many-body system, interacting with forces with a range much shorter than the average particle separation, become naturally entangled as in the situation discussed by Einstein et al. [8], when two particles are practically isolated from the rest of the Universe and retain the memory of the moment of “creation” of their initial state, a long time after they are fully spatially separated. Many-body systems with SRCs accordingly become entangled at all energies, irrespectively of whether the system is in equilibrium or not, and the measure of entanglement needs to be quantified. The system entanglement entropy directly affects the particle momentum distribution and its non-equilibrium dynamics [3, 4]. Isolated quantum systems in a pure state for which either von Neumann or Shannon entropy vanishes, but not necessarily in an equilibrium state, will evolve and its entanglement entropy will naturally in the long run describe their equilibration [12–32], similarly to the Boltzmann entropy for weakly interacting and dilute systems as discussed by Boltzmann [33], Nordheim [34], and Uehling and Uhlenbeck [35]. Entanglement thus becomes a measure of both mean field and short-range correlations as well [4].
The single-particle momentum distribution can be extracted from the one-body density matrix 
\[ n(\xi) = \langle \Psi | \psi^\dagger(\xi) \psi(\xi) | \Phi \rangle, \]  
(2)
where \(| \Phi \rangle\) is in general a time-dependent many-body wave function and \(\xi = (r, \sigma, \tau)\), \(\zeta = (r', \sigma', \tau')\) stand for the spatial, spin, and isospin coordinates. Since the emphasis will be on the spatial properties, the spin and isospin degrees of freedom will be suppressed in ensuing equations. In many-body systems the density matrix typically is characterized by different spatial scales in the coordinates \(R = (r + r')/2\) and \(s = r - r'\). The momentum distribution, obviously related to the Wigner distribution [36], is defined [37] using Eq. (2) for any many-body wave function 
\[ n(k) = \sum_{\sigma, \tau} \int d^3r d^3r' n(r, \sigma, \tau | r', \sigma, \tau) e^{-i k \cdot (r-r')}, \]  
(3)
where \(\int d^3r d^3r' n(k) = A\) and \(A = N + Z\) is the atomic number. The properties of the nucleon momentum distribution have been investigated for decades [37–69]. Sar-tor and Mahaux [40] have shown in 1980 that the momentum distribution of a dilute Fermi system is characterized by the presence of very long momentum tails \(n(k) \propto 1/k^4\) at large momenta. Shina Tan [62–64] later proved that in the momentum interval \(1/|a| < k < 1/r_0\), where \(a\) and \(r_0\) are the \(s\)-scattering length and effective range respectively, the momentum distribution has the behavior \(n(k) \propto C/k^4\). George Bertsch pointed in 1999 that dilute neutron matter [56, 70] is exactly such a system. Subsequent both theoretical and experimental studies for nuclear systems [41, 42, 46–49, 52–55] and for cold fermionic atom systems [56–61, 71] confirmed these predictions, even in cases where the interaction has a complex character, as in the case of a nuclear tensor interaction. The important conclusion of this study was that approximately 20% of the spectral strength is found for momenta \(k > k_F\). As was mentioned by many “A crucial feature of the Tan relations is the fact that they apply to any state of the system, e.g., both to a (normal) Fermi-liquid or to a superfluid state, at zero or at finite temperature and also in a few-body situation.” [56, 57, 59, 62–64]. While nuclear studies were performed for understandable reasons only for the ground states of the systems, the experimental and theoretical results for cold fermionic atoms were obtained both at zero and finite temperatures, confirming Shina Tan’s [62–64] prediction that the \(n(k) = C/k^4\) behavior is in fact generic for strongly interacting many-fermion systems, and thus a feature of such systems in both equilibrium and out of equilibrium. In Refs. [3, 4] this aspect is illustrated for the case of highly excited fission fragments, with temperatures well above the critical temperature, where superfluid correlations are absent.

Typically one discusses the angle averaged momentum distribution \(n(k) = \int d\Omega_k n(k)\), which can be evaluated by constructing the eigenvalues and eigenfunctions 
\[ \int d\xi n(\xi) \phi_\alpha(\xi) = n_\alpha \phi_\alpha(\xi), \quad n(\xi) = \sum_\alpha \phi_\alpha(\xi) n_\alpha \phi_\alpha^*(\xi) \]  
(4)
known as the canonical basis in the case of the mean field Hartree-Fock-Bogoliubov approximation [72] or natural orbitals [73, 74] in general and evaluating 
\[ \epsilon(k) = \left( \phi_\alpha \left| \frac{\hbar^2 \Delta}{2m} \right| \phi_\alpha \right) = \frac{\hbar^2 k^2}{2m} \]  
(5)
and thus relating the occupation probability \(n_\alpha = n(k) = n(\epsilon(k))\) with \(\epsilon(k)\). (N.B. Obviously, the spectrum of Eq. (4) does not depend on the specific representation, either coordinate, momentum, etc.) In saturating systems, such as nuclei, the magnitude of the wave vector \(k\) is relatively well defined, up to corrections arising from surface effects [75], and the semiclassical approximation reproduces with very good accuracy single-particle energies and shell structure, an approximation going back to Bohr’s model of the hydrogen atom. For superfluid systems, if the pairing potential is local, then there is always a range of the wave vectors \(k\) in which \(n(k) = C/k^4\) [4], see Fig. 1. The presence of the high momentum tails \(n(k) = C/k^4\) is clearly incompatible with Eq. (1), which decays exponentially when \(k \to \infty\). Note that 
\[ n(k) = \sum_{\alpha, \sigma, \tau} n_\alpha |\phi_\alpha(k, \sigma, \tau)|^2, \]  
(6)
\[ \phi_\alpha(k, \sigma, \tau) = \int d^3r e^{-i k \cdot r} \phi_\alpha(r, \sigma, \tau). \]  
(7)

The SRCs, which modify in a qualitative manner the behavior the dependence of the occupation probabilities as a function of their kinetic energy, lead to significant changes of the entropy. This aspect can be appreciated in a much more “down-to-earth” language. In practice, when increasing the spatial resolution, and thus opening new channels and allowing higher momenta to actively participate in the dynamics, the system will always take advantage of new “open roads” and the the wave functions will spread naturally over a larger part of the Hilbert space. The entropy is simply a measure of the available and allowed states into which the system can dynamically evolve. As mentioned in introduction, for isolated quantum many-body system the entanglement entropy describes the non-equilibrium dynamics [12–32, similarly to the Boltzmann entropy [33–35]. As recently discussed, the entanglement entropy is also a natural measure of the complexity of the many-body wave function [4]. The complexity of a many-body wave function \(|\Phi\rangle\) [4] can be quantified by evaluating the orbital entanglement or quantum Boltzmann one-body entropy [3, 34, 35, 77–83] 
\[ S = -g \sum_\alpha \left[ n_\alpha \ln n_\alpha + (1 - n_\alpha) \ln(1 - n_\alpha) \right], \]  
(8)
where the Boltzmann constant is \(k_B = 1\) when the temperature is measured in energy units, and \(g\) is spin-isospin degeneracy factor. The set of occupation numbers
Three different amplitudes of the pairing field were considered here $\Delta_0 = 1, 5$, and $15$ MeV [4], the last one comparable to the strength of the pairing field in the unitary limit [56]. For $\epsilon(k) > 75$ MeV the momentum occupation probabilities have the behavior $n(k) = C/k^4 \approx 1/[(\epsilon(k))^2]$. The UV-cutoff is determined by $\epsilon(k)$ of the highest canonical state with a wave function located inside the system. The states with $\epsilon(k)$ beyond the UV-cutoff are not expected to be physically relevant [4], as their corresponding canonical occupation probabilities vanish in the continuum limit. In the inset, the occupation probabilities $n(k)$, shown in a linear scale, have an expected Bardeen-Cooper-Schrieffer [76].

The momentum distribution $n(k)$, for a thermal mean field distribution, see Eq. (10) and where the temperature $\beta = 1/T$, increases from the lowest to the highest curve.

The dependence of the dimensionless “contact” $C(k_0)/k_F^7$ on the choice of momentum scale $k_0$ extracted by imposing the normalization condition Eq. (12) on the occupation probability $n(k)$, for a thermal mean field distribution, see Eq. (10) and where the temperature $\beta = 1/T$, increases from the lowest to the highest curve.
Assuming that $\Lambda = \infty$ and
\[
n_0 = g \int \frac{d^3k}{(2\pi)^3} n_{\text{mf}}(k),
\]
a lower limit for $\eta(k_0)$ can be obtained in the case of a free Fermi gas at zero temperature by choosing $k_0 = k_F$. One can now evaluate the fraction of the particles with momenta greater than $k_0$, see Fig. 4,
\[
n(k > k_0) = \frac{3 \eta n_{\text{mf}}(k_0) k_0^3}{k_F^3} \frac{3C(k_0)}{k_0 k_F^3},
\]
which can reach quite large values. It is not my goal here to select the best choice for the mean field momentum probability distribution, as that should be decided in accurate microscopic calculation, specific for various systems [47–49, 51, 52, 55–57, 59–61, 88, 89].

The UV-momentum cutoff $\Lambda$ of the momentum distribution $n(k)$ is effective field theory in nature and is determined by the internal structure of the nucleons. In the limit $k_0 \to \infty$ the “contact” $C$ naturally vanishes. The specific value of the “contact” $C$ is defined by the temperature $T$, the specific system under consideration, and the system specific momentum scale $k_0$ [40–42, 46–49, 51–53, 55, 58, 60–64, 88–92].

The momentum distribution $n(k)$ has thus two components, the mean field and the SRCs components, which can be clearly identified experimentally [53, 55, 58] by identifying the regime $k_0 < k < \Lambda$ where $n(k) \approx C(k_0)/k^4$ is valid. Below $k < k_0$ the $n(k)$ can be then identified with a mean field contribution, up to the overall renormalization constant $\eta(k_0) \leq 1$. The constant $\eta(k_0)$ is uniquely determined by the normalization condition Eq. (12) and the mean field component $n_{\text{mf}}(k)$, which is determined in a typical mean field or Density Functional Theory (DFT) [93, 94]. The momentum distribution $n(k)$ depends on a single parameter $k_0 > k_F$, that can be determined either experimentally or from DFT with a sufficiently large UV-momentum cutoff or from another accurate many-body calculation, when pairing correlations are also taken into account [3, 95].

In the classic monograph [2] there is a somewhat hard to interpret sentence, stating that the dependence of the occupation probabilities on the quasiparticle energies $\epsilon$ is a very complicated implicit definition of $n(\epsilon)$ (see Eq. (2.6) in Ref. [2] and the corresponding explanations), whereas $n(\epsilon)$ is clearly a well defined function of $\epsilon$, see Eq. (1). In Fig. 5 I show the dependence of the canonical occupation probabilities $n_\alpha = n(\epsilon(k))$ in case of induced fission $^{235}\text{U}(n,f)$, extracted from the time-dependent DFT (TDDFT) approach extended to superfluid systems and applied to this non-equilibrium process [96–100]. These results show the momentum distribution of two hot emerging fission fragments, with a separation in space $\approx 30$ fm, and at temperatures larger than the critical temperature $T_c \approx 0.5$ MeV for which the pairing gaps vanish, and which demonstrate the clear presence of proton-proton and neutron-neutron SRCs [3].

In the dynamics of isolated systems the time evolution of the entanglement entropy plays the role of thermodynamic entropy for local observables [12–14], is shown in the lower inset of Fig. 5. Note that at the initial time the nucleus is at zero temperature, but the entanglement entropy does not vanish. For more details see Ref. [4]. In these calculations nucleon momentum up to $p_{\text{cut}} = h\pi/dx \approx 600$ MeV/c (where the spatial resolution is $dx = 1$ fm) are present. According to the prevalent interpretation of time-dependent mean field treatment of many fermion systems, only long-range correlations should be present, which obviously is not the case in TDDFT extended to superfluid systems [3, 4, 96, 97]. This dependence of $n(k)$ on $\epsilon(k)$, where the long-momentum tails are present, is indeed a complicated implicit definition of the canonical occupation probabilities. The canonical basis set is the unique (gauge invariant) and at the same the minimal set...
of single-particle states to represent a many-body wave function [4, 73, 74, 85, 101]. This clarifies perhaps for the first time the meaning of the sentence quoted above and an equivalent of which I could not find in literature. The presence of the infrared (IR) knee at $\epsilon_n \approx 40$ MeV is unequivocally a qualitative new feature, absent from the textbook definition [2] of a quasi-equilibrium distribution $n(\epsilon)$.

![Graph showing final proton and neutron canonical occupation probabilities](image)

**FIG. 5.** The final proton and neutron canonical occupation probabilities $n_\alpha = n(k)$ extracted from the TDDFT extended to superfluid systems treatment of induced fission reaction $^{235}$U(n,f) as a function of $\epsilon_\alpha = \epsilon(k)$. The upper inset shows a small energy interval near the Fermi level. Above $\epsilon_n \approx 50$ MeV one can see a clear power law behavior compatible with theory prediction $n(k) \approx 1/\epsilon(k)^2$. The initial state was the compound nucleus close to the top of the outer fission barrier at $t = 0$ fm/c and in the final state the fission fragments are spatially separated by $\approx 30$ fm at $t = 1,700$ fm/c [4]. The non-equilibrium time-evolution of the orbital entanglement entropy $S(t)$ is shown in the lower inset, with solid and dashed lines corresponding to no nucleon number projections and with nucleon number projections respectively [4].

| $\epsilon_F$ | $S_{0.25}$ | $S_{1.3}$ | $S_{1.2}$ | $S_{1.1}$ | $S_{1.05}$ | $S_{1}$ |
|------------|---------|--------|--------|--------|--------|--------|
| 0.25 MeV  | 1       | 1      | 1      | 1      | 124.8  | 124.8  |
| 0.5 MeV   | 1       | 1      | 1      | 2.18   | 60     | 60     |
| 1 MeV     | 1       | 1      | 1.28   | 8.92   | 29.8   | 29.8   |
| 2 MeV     | 1       | 1.11   | 4.01   | 10.48  | 14.9   | 14.9   |
| 4 MeV     | 1.27    | 2.41   | 5.57   | 6.81   | 7.60   | 7.60   |

**TABLE I.** The values of the ratio of the entropy of the system, in the presence of SRCs, evaluated with Eq. (10), over the entropy evaluated in pure mean field approximation evaluated with Eq. (1), for different values of the momentum scale $k_0$, is shown in columns 2-6.

After a cursory analysis of Eq. (8), one is lead to the conclusion that due to the presence of the SRCs contribution this entanglement entropy likely exceeds in value the corresponding entanglement mean field entropy, see Table I. The SRCs contribution to $n(k)$ has a very long power law tail, which would lead to $n(k_0) < 1$, see Fig. 3, and thus to an expected depletion of the occupation probabilities of the low-momentum states $k < k_0$, even at very low temperatures. This occupation probability depletion of the states with $k < k_0$ alone would lead to an increase of the corresponding contribution of these states to the entropy density of the system. At the same time, the long tails of the momentum distribution for $k > k_0$ would lead to a further increase of the entropy density, when compared to the mean field value. Since $\Lambda \gg k_0$, the effect of considering the internal nucleon structure have likely a relatively small effect on the entropy, which is well converged when $n(A) \approx 10^{-7}$. Upon performing a projection on exact proton and neutron numbers the many-body wave function is an exponentially large sum of Slater determinants (a typical shell-model or configuration interaction many-body wave function), the canonical/natural orbital occupation probabilities remain largely unchanged [4, 5] and thus the particle projected many-body wave function retains a very high degree of entanglement. This many-body wave function is solution of the quantum equivalent of the semiclassical Boltzmann equation [4].

Pairing correlations alone lead to $1/k^4$ tails in the momentum distribution at all temperatures [3, 95]. Moreover, the dynamical pairing effects, namely the presence of a pairing field, but the absence of a true pairing condensate at temperatures higher than the critical temperature, lead to the occupation of high-momentum states with $k > k_0$ [3, 99, 100], even in time-dependent processes and for intrinsic excitation energies of nuclei corresponding to temperatures above the critical temperature. Since these pairing correlations in current nuclear simulations take into account only the $nn$ and $pp$ correlations [3], the effects of $np$ SRCs can be included in dynamical calculations by an extension of time-dependent DFT described in Ref. [3], are expected to be significantly larger. Since entanglement entropy and many-body level density control the dynamics of an isolated quantum system [12–14], the level density in the presence of SRCs exceeds the level density of the system in a simpler mean field approximation. The possibility that the momentum distribution may be time-dependent as well was not explicitly discussed here, only indirectly illustrated in the lower inset in Fig. 5, it was definitely observed in time-dependent microscopic quantum studies [3–5]. The highly non-equilibrium nuclear fission $^{235}$U(n,f) illustrated here and in Refs. [4, 5] in arguably the largest many-body system studied so far [15–32], with aspects related to the widely studied topics of Hilbert space and many-body localization. The presence of SRCs lead to qualitative changes of the entanglement properties, the complexity of the many-body wave functions, the single-particle occupation probabilities, and the dynamics of many-body systems [3–5, 99, 100, 102–106]. Nuclear and cold atom systems present a unique opportunity to study time-dependent non-equilibrium and entanglement properties of strongly
interacting fermions.

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