Long-Time Behavior of the Momentum Distribution During the Sudden Expansion of a Spin-Imbalanced Fermi Gas in One Dimension

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Long-time behavior of the momentum distribution during the sudden expansion of a spin-imbalanced Fermi gas in one dimension

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We study the sudden expansion of spin-imbalanced ultracold lattice fermions with attractive interactions in one dimension after turning off the longitudinal confining potential. We show that the momentum distribution functions of majority and minority fermions quickly approach stationary values due to a quantum distillation mechanism that results in a spatial separation of pairs and majority fermions. As a consequence, Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) correlations are lost during the expansion. Furthermore, we argue that the shape of the stationary momentum distribution functions can be understood by relating them to the integrals of motion in this integrable quantum system. We discuss our results in the context of proposals to observe FFLO correlations, related to recent experiments by Liao *et al.*, Nature **467**, 567 (2010).

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The combination of strong correlations and quantum fluctuations makes one-dimensional (1D) systems the host of exotic phases and physical phenomena [1, 2]. Those phases and phenomena, in many occasions first predicted theoretically, have been observed in condensed matter experiments and have begun to be studied with ultracold atomic gases [2]. A system of particular interest in recent years has been the spin imbalanced 1D Fermi gas. Following theoretical predictions [3–9], its grand canonical phase diagram has recently been investigated experimentally [10]. The major interest in this model comes from the fact that its entire partially polarized phase has been theoretically shown [5, 6, 11–15] (for a review, see [16]) to be the 1D-analogue of the Fulde-Ferrell-Larkin-Ovchinnikov (FFLO) state [17, 18]. The FFLO phase was introduced to describe a possible equilibrium state in which magnetism and superconductivity coexist thanks to the formation of pairs with finite center-of-mass momentum leading to a spatially oscillating order parameter. The existence of such a phase has remained controversial in dimensions higher than one in theoretical studies [19–21], while experiments have found no evidence of the FFLO phase in three-dimensional systems [22, 23].

An important challenge in ultracold fermion experiments, which may have already realized the FFLO state [10], is to confirm the existence of FFLO correlations (for recent proposals see, *e.g.*, [24–27]). A direct measurement of the pair momentum distribution function (MDF) in the partially polarized state [5, 6, 14] has been suggested to provide such evidence [28]. However, this remains very difficult because after turning off all confining potentials, the transverse expansion (in the directions of very tight confinement) dominates over the longitudinal one [29]. Another interesting possibility is to let the gas expand in the 1D lattice after turning off the longitudinal confining potential, and then measure the density profiles or the MDFs of the independent species and/or pairs after some expansion time. Some aspects of such an expansion experiment have already been successfully carried out in 1D tubes [30, 31] as well as in 2D and 3D optical lattices [32], namely the independent control over lattice and the trapping potential and the measurement of the density profiles after the expansion. For 1D gases, interaction effects during the expansion cannot in general be neglected, leading to fundamentally different behavior of observables before and after the gas has expanded. For example, the expansion of the Tonks-Girardeau gas in 1D results in a bosonic gas with a fermionic MDF [33–35], and initially incoherent (insulating) states of bosons [36, 37] and fermions [38] can develop quasi-long range correlations during the expansion.

The question we are set to address is the fate of the MDFs of fermions and pairs during an expansion in one dimension, as described by the attractive Hubbard model. We use a combination of numerical simulations, based on the time-dependent density matrix renormalization group approach (t-DMRG) [39, 40], and analytical (Bethe-Ansatz) results. We first show that the MDFs of majority and minority fermions become stationary after a relatively short expansion time, $t \sim L_0/J$, where L_0 is the initial size of the cloud and J is the hopping amplitude. For strong interactions, we explain this behavior in terms of a quantum distillation process [41], as a consequence of which FFLO correlations are destroyed during the expansion. Finally, we discuss how these stationary MDFs can be theoretically understood within the framework of the Bethe-Ansatz. Our results suggest that the final form of the MDFs of minority and majority fermions are related to the distributions of Bethe-Ansatz rapidities (a full set of conserved quantities) of this integrable lattice system.

The Hubbard model (in standard notation [42]) reads:

$$H_0 = -J\sum_{\ell=1}^{L-1}(c^\dagger_{\ell+1,\sigma}c_{\ell,\sigma} + \text{H.c.}) + U\sum_{\ell=1}^{L} n_{\ell\uparrow}n_{\ell\downarrow}\,. \quad (1)$$

As the initial state, we always take the ground state of a trapped system. In the main text, we focus on a box trap, *i.e.*, particles confined into a region of length L_0 while we present results for the expansion from a harmonic trap in the supplementary material [43]. We study lattices with L sites, N particles, and a global polarization of $p = (N_\uparrow - N_\downarrow)/N$, where $N_\sigma = \sum_\ell \langle n_{\ell\sigma}\rangle$. All positions are given in units of the lattice spacing and momenta in inverse units of the lattice spacing ($\hbar = 1$).

The expansion is triggered by suddenly turning off the confining potential, thus allowing particles to expand in the lattice. We then follow the time-evolution using the numerically exact *t*-DMRG algorithm [39, 40]. We use a Krylov-space based time-evolution method and enforce discarded weights of 10^{-4} or smaller with a time-step of $\delta t = 0.25/J$. Our main focus is on the time-evolution of the three MDFs: the ones for majority ($\sigma=\uparrow$) and minority fermions ($\sigma=\downarrow$), denoted by $n_{k,\sigma}$ and the pair MDF, $n_{k,\mathrm{p}}$. These functions are computed from the corresponding one-particle ($\lambda=\uparrow,\downarrow$) or one-pair ($\lambda = p$) density matrices via a Fourier transform

$$n_{k,\lambda} = \frac{1}{L}\sum_{\ell,m} e^{\mathrm{i}(\ell-m)k}\langle\psi^\dagger_{\ell,\lambda}\psi_{m,\lambda}\rangle \quad (2)$$

where $\psi^\dagger_{\ell,\sigma} = c^\dagger_{\ell,\sigma}$, $\psi^\dagger_{\ell,p} = c^\dagger_{\ell,\uparrow}c^\dagger_{\ell,\downarrow}$ and λ stands for $\uparrow,\downarrow,p$. We normalize the MDFs so that $\sum_k n_{k,\lambda} = N_\lambda$ (note that $N_p = \sum_\ell \langle n_{\ell\uparrow}n_{\ell\downarrow}\rangle$, *i.e.*, it is equal to the total double occupancy in the system).

For the expansion from a box, we concentrate on an initial density fixed to $n = N/L_0 = 0.8$. In our *t*-DMRG simulations, which were carried out for $N = 8$ and $N = 16$ ($L_0 = 10$ and 20, respectively) and various values of U, we were able to reach times of order $t_{\max} \sim 80/J$ for large U and $t_{\max} \sim 40/J$ for intermediate values of $U \sim 4J$. $t_{\max}$ also depends on p, with small values of p being more demanding.

Typical results for the three MDFs of interest are presented in Fig. 1 for $U = -10J$ and $p = 0.5$ (corresponding to $N_\uparrow = 6$ and $N_\downarrow = 2$; see the supplementary material for more data [43]). During the time evolution, they are all seen to quickly approach time-independent forms. In Fig. 1(a), it is apparent that the MDF of the majority fermions becomes narrower and develops small oscillations in the vicinity of $k = 0$ as time passes. We find that those oscillations become smaller in amplitude and get restricted to smaller values of k after long expansion times, *i.e.*, they seem to be a transient feature not present in the asymptotic distributions. The momentum distribution of the minority fermions [Fig. 1(b)], on the other hand, becomes broader during the time evolution.

The time evolution of the MDF of the pairs, depicted in Fig. 1(c), yields information on the fate of FFLO correlations in the expanding cloud. In the FFLO state, $n_{k,p}$ has maxima at $Q = \pm(k_{F\uparrow} - k_{F\downarrow})$ [5]. These are visible in the $t = 0$ curve (dashed line), where $\pm Q$ are marked by vertical lines. As the comparison of $n_{k,p}(t > 0)$ with the initial $n_{k,p}(t = 0)$ shows, the peaks at $\pm Q$ rapidly disappear, and $n_{k,p}(t)$ becomes narrower. In addition, new and shallower peaks form at $k < Q$. Since we do not find those peaks at the same values of k for other values of N when N/L_0 and p are the same, and we do not find them for all values of U, N/L_0, and p studied, they appear to be related to finite-size effects. Hence, the double peak structure in $n_{k,p}(t = 0)$, which makes evident the presence of FFLO correlations in the initial state, is found to disappear during the expansion. Even though the FFLO correlations are lost during the expansion, the integral over the pair MDF, which equals the total double occupancy, does not vanish. This implies that not all interaction energy is converted into kinetic energy and that some fraction of the original pairs remains by the time the MDFs have become stationary, which in experiments could be probed by measuring the double occupancy.

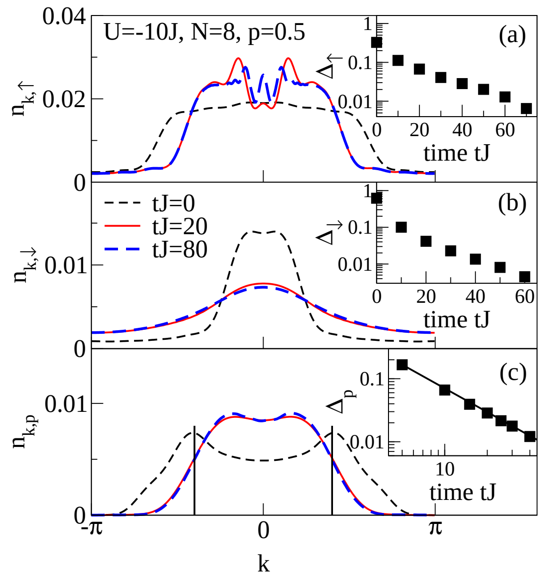

FIG. 1: (Color online) MDF for the expansion from a box trap ($U = -10J$, $N = 8$, $p = 0.5$, $L_0 = 10$): (a) $n_{k,\uparrow}$, (b) $n_{k,\downarrow}$, and (c) $n_{k,p}$. The insets show the difference Δ_λ ($\lambda =\uparrow,\downarrow,p$, see text) between the MDF at a time t compared to the one at the largest time reached in the simulation. The vertical lines in the main panel in (c) mark the position of the FFLO wave-vector $Q = \pm\pi np$.

In order to quantify how the three MDFs above approach stationary forms, in the insets in Fig. 1, we plot $\Delta_\lambda(t) = \sum_k |n_{k,\lambda}(t) - n_{k,\lambda}(t_{\max})|/\sum_k n_{k,\lambda}(t_{\max})$ vs t. These results make apparent that the approach is close to exponential for $n_{k,\uparrow}$ and $n_{k,\downarrow}$ [insets in Fig. 1(a) and 1(b)], while it is power law for $n_{k,p}$ [inset in Fig. 1(c)] [44]. Remarkably, for the parameters of Fig. 1, already at $tJ \sim 10$, all Δ_λ are $\lesssim 10\%$. This means that the stationary MDFs obtained in this work should be achievable in current optical lattice setups [32]. A comparison between expansions from different box

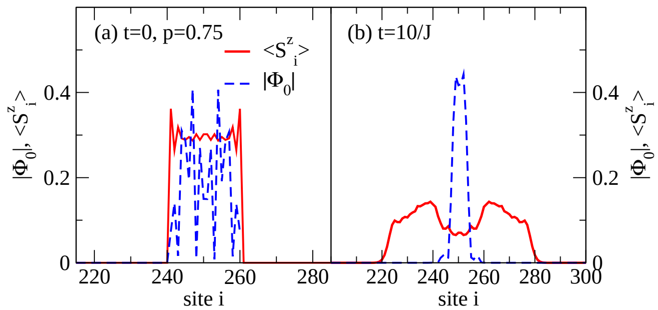

FIG. 2: (Color online) Natural orbital $|\Phi_0|$ corresponding to the largest eigenvalue of the pair-pair correlator $P(\ell, j)$ (dashed lines) and spin density $\langle S_i^z \rangle$ (solid lines). (a) $t = 0$, (b) $tJ = 10$. These results are for $U = -10J$, $L_0 = 20$, $N = 16$ and $p = 0.75$, corresponding to $N_\uparrow = 14$ and $N_\downarrow = 2$.

sizes suggests that the emerging time scale in the observables with exponential relaxation is proportional to L_0. The origin of that time scale will be discussed below.

While we are focusing the discussion on the case of the expansion from a box trap, we stress that the results for the MDFs in an expansion from a harmonic trap are quite similar (for an example, see the supplementary material [43]). Namely, we observe a comparably fast convergence of the MDFs to a stationary form and the disappearance of the peaks at $\pm Q$ in $n_{k,p}$. The latter indicates the disappearance of FFLO correlations.

To understand how the FFLO state breaks down as the gas expands, we calculate the eigenvector Φ_0 of the pair-pair correlator $P(\ell, m) = \langle \psi^\dagger_{\ell,p} \psi_{m,p} \rangle$ that corresponds to the largest eigenvalue. $|\Phi_0|$, shown in Fig. 2(a), unveils the spatial structure of the quasi-condensate in the initial state: it has an oscillatory behavior with nodes (see also Ref. [5]). In these nodes, the spin density has its maxima to accommodate the majority fermions (Fig. 2(a), see also [43]), indicative of the spin-density wave character with a modulation of $(2Q)^{-1}$ in the FFLO state. During the expansion, the nodes in $|\Phi_0|$ disappear while $|\Phi_0|$ develops a maximum at $L/2$, exceeding its initial value [see Fig. 2(b)]. The latter is a consequence of a quantum distillation mechanism, described in Ref. [41] for $U > 0$, which allows the unpaired fermions to move away from the center of the system (*i.e.*, they escape from the nodes of $|\Phi_0(t = 0)|$). Loosely speaking, during first-order processes unpaired fermions exchange their positions with the pairs (a minority fermion hops towards the center of the trap), allowing the former to expand while the pairs move towards the center of the trap. This occurs over a time scale proportional to L_0 and inversely proportional to J, which explains the time scale observed in the exponential approach of the majority and minority fermions to their stationary values. Once the unpaired fermions have spatially separated themselves from the pairs, they form a non-interacting gas whose MDF is stationary. On much longer time scales (assuming $U > 4J$), we expect the pairs to slowly expand as well. This transient dynamics of the pairs may be the reason for the power-law, as opposed to exponential, relaxation observed for $n_{k,p}(t)$ in Fig. 1(c).

In a recent work [45], extrema in the spin-density of the expanding gas were observed in numerical calculations using various approaches. By comparing with the time-dependence of the order parameter within a time-dependent Bogoliubov-deGennes approach, it was argued that they are related to FFLO correlations. Our results show that, in a lattice system, the nodal structure of the FFLO state is ultimately lost as the system expands. Note, however, that in Ref. [45] the main focus was on rather small polarizations p [3, 4, 8] leading to a wide partially polarized core before the expansion. We therefore expect the quantum distillation mechanism to take much longer to depolarize the core than what has so far been reached in numerical simulations [45], leaving this case as an open question.

We are now in a position to explain the anticorrelated behavior of $n_{k,\uparrow}$ and $n_{k,\downarrow}$ mentioned in the discussion of Fig. 1. For large values of U, N_p is essentially equal to $N_\downarrow$ and is approximately unchanged during the expansion, rendering the interaction energy almost time independent. This implies that also the kinetic energy $E_{\text{kin}} = -2J \sum_k \cos k (n_{k,\uparrow} + n_{k,\downarrow})$ is approximately conserved, which is only possible if the two MDFs behave in the opposite way during the expansion. The broadening of the minority MDF $n_{k,\downarrow}$ with respect to the initial state is a direct consequence of the spatial separation of excess fermions from the pairs, leaving the latter confined in the center of the cloud. Since in the center the local polarization decreases, the stationary form of $n_{k,\downarrow}$ is well approximated by the equilibrium one for equal populations $N_\uparrow = N_\downarrow$ instead of $N_\uparrow > N_\downarrow$ [43].

The fact that the MDFs become stationary after the expansion from a box or a harmonic trap is in itself not surprising, as in the limit of long expansion times, the cloud becomes very dilute with, for the attractive case, the typical inter-particle distance being much larger than the bound-state size. Hence, one may assume that pairs and unpaired particles are essentially noninteracting. The MDF in such an asymptotic limit should be determined by the initial conditions right after the quench. For instance, for generic models, the total energy (which is conserved during the expansion) plays a fundamental role in determining the expansion dynamics (see Ref. [46] for a related work for $U > 0$). For an integrable model, such as the (attractive) Hubbard model of Eq. (1), all integrals of motion are in principle known from the Bethe Ansatz and are conserved during the expansion [42]. We argue below how to interpret the shape of certain stationary MDFs in terms of such integrals of motion. This is closely related to the previously studied fermionization of the MDF of an expanding gas of hard-core bosons [33–35].

For the model studied here, we first note that the formation of a distinct minimum in the difference distribution $\delta n_k = n_{k,\uparrow} - n_{k,\downarrow}$ [see Figs. 3(a) and (b)] is reminiscent of the corresponding distribution of real-valued charge rapidities (for intermediate U) in the ground state in a box. From the point of view of the rapidity distributions, they need to be determined right after turning off the trap and the subsequent expansion does not play any role; it is the MDFs which will evolve and asymptotically approach the former as the expansion proceeds [47]. We can calculate the pre-quench values of the rapidities by numerically solving the Bethe-Ansatz equations for a system of size L_0 and open boundary conditions [48–50]. For the ground state of the attractive Hubbard model, there are two types of rapidities present: real- and complex-valued charge rapidities (κ_ν and κ_σ) which correspond to unpaired fermions and pairs, respectively ($\nu = 1, \dots, N_\uparrow - N_\downarrow$, $\sigma = 1, \dots, 2N_\downarrow$, with κ_σ and κ_σ^* appearing pairwise).

To calculate the effect of the quench of the trapping potential exactly is in principle possible but complicated in practice [51], so we will resort to some simplifications. To start, we assume that the number of pairs is conserved during the quench, and thus no pure-spin excitations are produced. Further, we use the observation that the overlap between the pre-quench eigenstate and the post-quench state has a maximum amplitude for components of the latter with the same set of rapidities [51]. We then identify, asymptotically, the distribution of real-valued charge rapidities with that of unpaired fermions (δn_k), and of the real part of complex-valued (string) charge rapidities with that of minority fermions ($n_{k,\downarrow}$) since they remain paired. Finally, we model the quench by convolving the pre-quench distributions $\rho_1 = (1/2)\sum_\nu \delta(k \pm \kappa_\nu)$ and $\rho_2 = (1/2)\sum_\sigma \delta(k \pm \mathrm{Re}\kappa_\sigma)$ with the (periodized) kernels: (i) $L_0 \,\mathrm{sinc}^2(kL_0/2)$ for the former and (ii) a simple Lorentzian for the latter. The first choice is inspired by the exact result for the release of a single particle from a box, while the second choice is done for simplicity given that the results are relatively featureless in comparison. Illustrative results are shown in Fig. 3 and the agreement is very good, specially away from the Brillouin-zone center. Note that there are no fitting parameters in the case of δn_k and a single fitting parameter, the width of the Lorentzian, in the case of $n_{k,\downarrow}$.

In conclusion, we demonstrated that the initial FFLO state is destroyed during the expansion of an attractively interacting partially polarized 1D Fermi gas, and that direct signatures of the FFLO phase in the initial pair MDF are washed out as a consequence of interactions. Nevertheless, the sudden expansion is an interesting non-equilibrium experiment that through the asymptotic form of the MDFs yields information on the initial state. Our analysis suggests that the shape of the MDFs can be related to the distribution of rapidities, which constitute a full set of integrals of motion for this integrable quantum model and fully determine the initial state. Since we showed that the MDFs of majority and minority fermions as well as the one of pairs rapidly take a stationary form, this should be accessible on typical experimental time-scales.

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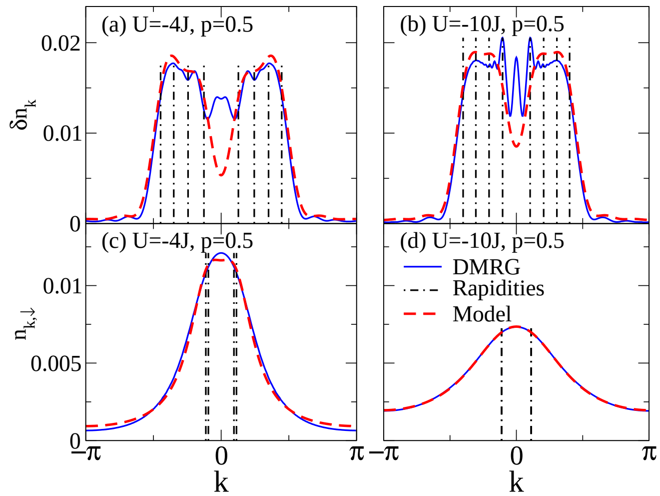

FIG. 3: (Color online) Comparison of the stationary MDFs $\delta n_k = n_{k,\uparrow} - n_{k,\downarrow}$ [(a),(b)] and $n_{k,\downarrow}$ [(c),(d)] for the expansion from a box with $N = 8$, $p = 0.5$ (corresponding to $N_\uparrow = 6$, $N_\downarrow = 2$) [(a),(c): $U = -4J$, (b),(d): $U = -10J$] to the form expected from the rapidities known from the Bethe-Ansatz: t-DMRG (solid lines), models discussed in the text (dashed lines). The vertical lines mark the positions of the rapidities.

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