Expansion after a geometric quench of an atomic polarized attractive Fermi gas in one dimension

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Abstract. The expansion of an ultracold lattice gas of fermions in a one-dimensional optical lattice after a geometric quench in which the atoms are released from a box (or parabolic) trap is studied numerically using the time-dependent density matrix renormalization group method. It is found that the momentum distributions of the two atomic species present in the simulations quickly converge toward stationary values dictated by the integrals of motion of the lattice gas at the expansion onset. An account of the central results and some of the technical details is given along with explicit examples.

1. Introduction

Developments in atomic laser cooling and trapping allow researchers to capture clouds of atomic gases and reach the limit of quantum degeneracy. The combined use of these techniques and Feshbach resonances, can be tailored to produce systems in which both the confining potentials and the interactions are controllable and yield interesting quantum behaviors like, for instance, exotic superfluid phases. Recent experimental efforts on systems of trapped cold atomic Fermi gases were aimed at studying the effects of polarization on superfluid pairing in low-dimensional systems [1]. The findings for atomic gases confined by a strong 2D optical lattice to move preferentially in one direction were consistent with the predictions for 1D systems of dilute polarized attractive gases [2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12, 13, 14]. The measurements are in quantitative agreement with theoretical calculations (using a wide array of numerical and analytical techniques) in which a partially polarized region is found to be the 1D analogue of the so called Fulde-Ferrell [15] or Larkin-Ovchinikov [16] states (1D-FFLO), —which are superfluid states produced by the condensation of Cooper pairs with non-zero center-of-mass momentum. This unusual paired states are not found in standard metals, but are thought to be present in
certain organic conductors [17] or heavy fermions [18], and even in nuclear and quark matter [19].
To go beyond the recent round of experiments, it is arguable that modifying the trapping or the optical-lattice strength could yield practical ways to better characterize and understand this system (for a recent review, discussing these and other ideas, see [20]). In this proceeding article, we will focus on the expansion dynamics after a sudden quench and make predictions for possible such experiments.

For 1D gases, interaction effects in the presence of a lattice cannot be neglected and they modify the expansion dynamics [21, 22, 23]. We use time-dependent density-matrix renormalization group (t-DMRG) [24, 25] to study the expansion process and we interpret our findings by referring to analytical (Bethe-Ansatz) results. We show that a process similar to the so called quantum distillation effect [26] takes place and the momentum distribution functions (MDFs) of majority and minority atoms become stationary after a relatively short expansion time, while the 1D-FFLO typifying characteristics are lost during the expansion.

2. Modeling
We shall model the system using the standard Hubbard model (see [27]), which with the usual second-quantized notation is given by:

\[ H = -J \sum_{\sigma=\uparrow,\downarrow} \sum_{\ell=1}^{L-1} (c_{\ell+1,\sigma}^\dagger c_{\ell,\sigma} + \text{H.c.}) + U \sum_{\ell=1}^{L} n_{\ell\uparrow} n_{\ell\downarrow}. \]  

As the initial pre-quench state, we take the ground state of a trapped system (here we focus on the case of a centered box-trap of size \( L_0 \) for which results can be more easily interpreted in terms of Bethe-Ansatz rapidities). We consider lattices with \( L \) sites and \( N = N_\uparrow + N_\downarrow \) particles distributed with a global polarization given by \( p = (N_\uparrow - N_\downarrow)/N \); positions are given in units of the lattice spacing and momenta in inverse units of the lattice spacing (we use the convention that \( \hbar = 1 \)). The type of quench we shall consider consists of the sudden turning off of the confining potential, this will be described in the next sections.

3. Computational Results
Before proceeding further in the description of the process and into considerations of analytical nature, we first show some representative results for the expansion of a polarized attractive gas obtained by direct calculation using t-DMRG.

3.1. Density Distributions
We prepare the system in the ground state of an infinitely-tall-box trap of size \( L_0 \) and, at time \( t = 0 \), we perform a geometric quench (i.e. a sudden change of boundary conditions which does not modify the strength of the interactions or other parameters that define the system) consisting of turning off the box-trap potential and letting the atoms expand in a larger Hubbard chain with \( L \) sites. \( L \gg L_0 \) is chosen large enough that during the maximum expansion times considered none of the atoms reach the outer edges of the larger chain. In the initial ground state, all the minority atoms are paired up and it is thus natural to study the expansion of the pairs as well as that of the excess majority atoms that remain unpaired (the latter identified with the spin density). These two time-dependent density distributions are displayed in Fig. 1 for typical values in the range of parameters we considered.

It is interesting to notice in Fig. 1(b) that the pair density is seen to first focus in during the initial stages of the expansion (for \( t \leq 5/J \)) before it starts growing in size. This is the period during which the pairs are drawn to the center of the trap as the unpaired fermions that were initially distributed throughout move to the outer edges of the atom cloud and expand faster.
Figure 1. Typical contour plots of the excess-fermion (or spin) density $\langle S_i^z(t) \rangle$ and the pair density $\langle N_{p,i}(t) \rangle$, panels (a) and (b) respectively, during the expansion starting from the ground state of a polarized attractive Fermi gas ($|U| = 10J$, $N = 8$, $p = 1/2$ and $L_0 = 10$). In here, $N_{p,i}$ is defined as the site double occupancy ($n_{i\uparrow}n_{i\downarrow}$), which is only an approximate proxy for the local pair density but has the advantages of being experimentally accessible and constituting an appropriate measure to illustrate the quantum distillation process. The slanted enveloping contours indicate the different maximum speeds at which the excess fermions and pairs, respectively, propagate during the expansion.
Figure 2. Contour plots for the momentum distribution function of the excess (unpaired) fermions defined as the spin-sector of the time-dependent Fourier transforms of the single-particle density matrices, \( \delta n_k(t) = n_{k,\uparrow}(t) - n_{k,\downarrow}(t) \) (cf. Ref. [28]). The parameters are the same as in Fig. 1 above (i.e., \(|U| = 10J, N = 8, p = 1/2\) and \(L_0 = 10\)). Contour lines becoming vertical indicate the convergence of that part of the distribution to its asymptotic large-time limit.

This mechanism is possible thanks to a quantum-distillation-like process that takes place driven by the dynamics of the interacting system (for more details and further results see [28]). It is during this initial stage that the 1D-FFLO characteristic spatial coexistence of pairs and unpaired atoms is lost and ulterior direct probing of the modulated superfluid order is no longer possible.

3.2. Momentum Distributions

After reaching a steady expansion regime, the real-space densities can be scaled into fixed-in-time distributions that correspond to asymptotic momenta. Numerically, we can see this more clearly by going into reciprocal space and studying the expansion of the MDFs. This procedure clearly shows that the distributions quickly converge towards an asymptotic limit as illustrated by Fig. 2. After an initial complicated transient regime, we find that the outer shape of the MDF of the excess fermions becomes stationary for \( t \geq 10/J \) and, slowly, that convergence moves towards the center of the Brillouin zone. This is because the faster particles quickly order themselves according to their relative speeds and effectively stop interacting, while for pairs and unpaired atoms with smaller momentum this process takes longer.

4. Analytical Results

We turn now to analytical considerations and exploit our choice of model (a Hubbard chain) by making use of its integrability. We consider the case of \( N \) fermions in a lattice with open boundary conditions (OBCs) and label their rapidities as \( \{\kappa_j\}_{j=1}^N \). These charge rapidities (augmented by a second set of spin rapidities, \( \{\lambda_m\}_{m=1}^M \) with \( M = N/2 \)); which turn out to
play only an auxiliary role in the ground state of the attractive case) constitute the integrals of motion that fully characterize any eigenstate of the system. To determine them, it is possible to write down a set of $N + M$ coupled algebraic equations known as the Bethe-Ansatz Equations (BAEs). These equations for the case of the Hubbard model are “trigonometric” and can be conveniently written in terms of the phase parameters $z_j = e^{i\kappa_j}$. For the case of OBCs, the equations are (cf. Ref. [29, 30, 31]):

$$z_j^{2L+2} = \prod_n \left( \frac{z_j^2 - 1}{z_j^2 - 1} + z_j (i\lambda_n - c) \frac{z_j^2 - 1}{z_j^2 - 1} - z_j (i\lambda_n + c) \right)$$

$$\prod_{m \neq n} \frac{\lambda_n + \lambda_m + 2ic \lambda_n - \lambda_m + 2ic}{\lambda_n + \lambda_m - 2ic \lambda_n - \lambda_m - 2ic} = \prod_j \frac{(i\lambda_n - c) z_j + \left( \frac{z_j^2 - 1}{z_j^2 - 1} \right) (i\lambda_n - c) z_j - \left( \frac{z_j^2 - 1}{z_j^2 - 1} \right)}{(i\lambda_n + c) z_j + \left( \frac{z_j^2 - 1}{z_j^2 - 1} \right) (i\lambda_n + c) z_j - \left( \frac{z_j^2 - 1}{z_j^2 - 1} \right)}$$

which can be seen to have a $z \to 1/z$ and $\lambda \to -\lambda$ symmetry (and the solutions need to be restricted accordingly to avoid double counting). Starting from this form of the BAEs, one can readily multiply out by the denominators and get high-order polynomial equations, which are more suitable for practical numerical solution using computer-algebra methods, provided that $N$ and $L$ are not too large. A direct solution confirms (as expected by continuity with the $L \to \infty$ thermodynamic limit) that the charge rapidities for the ground state appear as two sets: (i) $N - 2M$ real rapidities corresponding to the unpaired fermions, and (ii) $M$ pairs of complex rapidities corresponding to the paired fermions. An example of these rapidities for the same values of the parameters as those used in the figures above is given in Table 1.

| Rapidity Type | Order | Numerical Value |
|---------------|-------|-----------------|
| Real          | $\kappa_1$ | 0.325953 |
|               | $\kappa_2$ | 0.646688 |
|               | $\kappa_3$ | 0.958605 |
|               | $\kappa_4$ | 1.260180 |
| Complex       | $\kappa_{5,6}$ | 0.347184 ± i1.70459 |
|               | $\kappa_{7,8}$ | 0.351801 ± i1.70616 |

The ground state wave function for an $L_0$-size chain when the box trap is present, has to be projected into the Bethe-Ansatz basis for an $L$-size chain after the geometric quench takes place. In the limit of large $L$, this produces a continuous distribution that is in one-to-one correspondence with the asymptotic momentum distribution of the system. As time progresses during the expansion that follows the quench, the MDFs of the paired and unpaired atoms gradually approach the limiting value given by these two rapidity distributions (for the case of the complex valued rapidities, one focuses on the real parts). These rapidity distributions encode the expectation values of $N$ integrals of motion of the system and are thus constrained by the quantum dynamics to remain invariant after the quench (since the Hamiltonian is constant and commutes with them). Given the structure of the Bethe-Ansatz wave function, they thus constitute the necessary asymptotic limit for the MDFs in the steady-expansion regime during
Figure 3. Comparison of the MDF of the excess-fermion gas $\delta n_k$ (blue solid line) and the predicted asymptotic limit obtained from modeling the geometric quench (red dashed line). The MDF is obtained after a long-time expansion ($t \approx 80/J$) starting from a box-trap potential of size $L_0 = 10$ that was turned off at $t = 0$ and the system was allowed to expand and modeled using $t$-DMRG. The rapidity distribution after the geometric quench was calculated starting from the Bethe-Ansatz data of Table 1 indicated in the figure by the vertical lines (black dot-dashed lines) and using a convolution formula with no fitting parameters (see [28] for more details). The system parameters are the same as in the previous figures (i.e., $|U| = 10J$, $N = 8$ and $p = 1/2$).

which boundary conditions play no role (formally corresponding to $L \to \infty$). A direct detailed comparison of these computational and analytic results is given below, while a demonstration of the rapid convergence of the former to the latter was already presented elsewhere [28].

4.1. Comparison with the Computational Results

To illustrate the convergence of the MDFs to the distributions of Bethe-Ansatz rapidities obtained after the quench, we show in Fig. 3 results for the excess-fermion distribution obtained as a single time slice of Fig. 2 for a sufficiently large time and the projected rapidity distribution using the $\{\kappa_j\}_{j=1}^{4}$ values from Table 1. The convergence can be convincingly observed in the tails of the distributions, but is not yet present at the center of the Brillouin zone. We point out, however, that the agreement improves systematically with increasing time, as expected from the analytic considerations given above.

An analytic calculation of the effect of the geometric quench in smearing the distribution of rapidities in the initial ground state inside the box trap proceeds via a single-particle approximation. We observe that the overlap between the post-quench state and the pre-quench eigenstate has a maximum amplitude for components of the former with the same set of rapidities as the latter (cf. [32]). We proceed to identify the distribution of real-valued charge rapidities obtained from the BAEs with that of unpaired fermions ($\delta n_k$) and model the quench by convolving the pre-quench rapidities with the (periodized) kernel $L_0\text{sinc}^2(kL_0/2)$. This procedure is motivated by the exact result for the release of a single particle from a box.
and is expected to work better the larger the polarization of the system is. An exact calculation is also possible, in principle, by using the exact Bethe-Ansatz states, but a comparison with the asymptotic MDFs going beyond the present level of detail would require the simulation of much larger times (going beyond the current state of the art in t-dmrg). The convergence of momentum distributions into rapidity distributions during an expansion has also been seen for infinitely repulsive bosons [21, 22, 23], for which it is possible to calculate much longer expansion times (due to the availability of a mapping to free fermions).

5. Conclusions
To summarize, we have studied the expansion dynamics of attractive spin-imbalanced ultracold atomic clouds of fermions in 1D geometries. We have shown that while the signatures of the 1D-FFLO state are quickly lost during the expansion, the integrals of motion are respected and emerge as asymptotic momentum distributions. Since one finds that the MDFs of paired and unpaired atoms rapidly take a stationary form (specially so for the case of the excess unpaired atoms), they should be accessible on typical experimental time scales. Since these integrals of motion fully characterize the state of the 1D Hubbard model, they constitute an indirect probe of the character of the ground state of the system before the quench.

Here we concentrated on geometric quenches which are easier to handle in the Bethe Ansatz because the information about the boundary conditions enters only through the rapidities. Other types of quenches are also calculable, but are more involved. One would like to consider, for instance, interaction quenches. In particular, it would be interesting to study the effects of turning off the interactions (or even switching their sign). This could be combined with a simultaneous release of the system to study its expansion in the absence of interactions. The challenge would be to identify a protocol that would best lend itself for the probing of the 1D-FFLO state (see Refs. [33, 34] for examples of such earlier attempts). The resulting synergy between experiments and theory is likely to bring in new insights into the properties of polarized superfluid matter, that could in turn be applicable in many different contexts.

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