Fermi super-Tonks-Girardeau state for attractive Fermi gases in an optical lattice

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Abstract. We demonstrate that a kind of highly excited state of strongly attractive Hubbard model, named of Fermi super-Tonks-Girardeau state, can be realized in the spin-1/2 Fermi optical lattice system by a sudden switch of interaction from the strongly repulsive regime to the strongly attractive regime. In contrast to the ground state of the attractive Hubbard model, such a state is the lowest scattering state with no pairing between attractive fermions. With the aid of Bethe-ansatz method, we calculate energies of both the Fermi Tonks-Girardeau gas and the Fermi super-Tonks-Girardeau state of spin-1/2 ultracold fermions and show that both energies approach to the same limit as the strength of the interaction goes to infinity. By exactly solving the quench dynamics of the Hubbard model, we demonstrate that the Fermi super-Tonks-Girardeau state can be transferred from the initial repulsive ground state very efficiently. This allows the experimental study of properties of Fermi super-Tonks-Girardeau gas in optical lattices.

1 Introduction

Ultracold atomic gases trapped in one-dimensional (1D) waveguides have become one of the most active research field of cold atom physics in recent years [1]. Due to their good tunability, the 1D atomic gases have provided an ideal platform for studying and testing the theory of low-dimensional many-body systems [2,3]. Tuning the effective interaction strength between atoms via Feshbach resonance has led to the experimental realization of Tonks-Girardeau (TG) gases [2,3], which describes the Bose gas in the strongly repulsive limit and exhibits the feature of fermionization. By switching the interaction between atoms of an initial TG gas from strongly repulsive to strongly attractive, the experimental observation of a 1D super Tonks-Girardeau (STG) gas [4] of bosonic cesium atoms was reported very recently [5]. In contrast with the strongly repulsive interacting TG gas, bosons in STG state interact via strongly attractive interaction. A surprising feature of this many-body state is its good stability under strongly attractive interaction instead of decaying into the lower atomic bound states [6–8]. The stability of the STG gas could be well understood from the quench dynamics of the 1D integrable Bose gas [9].

The experimental realization of stable excited quantum gas phase opens a new area for searching exotic quantum phases in ultra-cold systems [9–19]. So far, most of the theoretical works on the STG gases have focused on the bosonic gases in continuum systems. In this work, we study the possible realization of the Fermi super-Tonks-Girardeau (FSTG) gas for a Fermi gas loaded into a deep 1D optical lattice, which is described by the Fermi Hubbard model [22]. The FSTG state for a 1D Fermi continuum gas was studied in references [13,14], however it is not clear whether the FSTG gas could be also realized in the lattice systems. In comparison with the continuum Yang-Gaudin model [23,24], the Hubbard model exhibits some new features due to the existence of the band structure for the lattice model. One of the new features is the existence of repulsive bound pairs in the high bands which is absent in the continuum model. The other one is the existence of the Mott insulating phase in the half-filling case. Although the Hubbard model is one of the fundamental model in condensed matter physics, most of previous theoretical works focused on its ground state and thermodynamical properties. Our study shall shed lights on properties of some highly excited states which can be accessible in current experimental conditions.

Stimulated by the experiment of the bosonic STG gas, we suppose that the ultracold Fermi gas is initially in the strongly repulsive regime, and then the interaction is suddenly switched to the strongly attractive regime. Through this way, we can reach a stable highly excited phase which is the lowest scattering state of the attractive Fermi gas. To understand properties of the STG state of the attractive Hubbard model, we shall analyze the spectrum structure of the Hubbard model for both the...
repulsive and attractive cases. By calculating the energy of the FSTG state analytically based on the Bethe-ansatz (BA) method, we show that the energy of FSTG gas state in the strongly attractive limit approaches the same limit of the ground state energy of 1D strongly repulsive Fermi Hubbard model. This implies that the FSTG state can be accessible from the the ground state of the strongly repulsive Fermi gas by a sudden switch of interactions, which is also confirmed by the exact calculation of the quench dynamics of the 1D Fermi gas on the optical lattice by using numerical exact diagonalization method.

2 Model and FSTG state

We consider a 1D ultracold Fermi gas composed of \( N = N_1 + N_1 \) spin-1/2 fermionic atoms in a deep optical lattice, which can be well described by the well-known Hubbard model (HM),

\[
\hat{H} = -t \sum_{i,\sigma} (\hat{c}_{i,\sigma}^\dagger \hat{c}_{i+1,\sigma} + \hat{c}_{i+1,\sigma}^\dagger \hat{c}_{i,\sigma}) + U \sum_i \hat{n}_{i\uparrow} \hat{n}_{i\downarrow},
\]

where \( \hat{c}_{i,\sigma} \) with \( \sigma = \uparrow, \downarrow \) is the creation (annihilation) operator of fermions at the \( i \)th site, and \( U \) denote the hopping amplitude and the on-site interaction strength, respectively. For the repulsive interaction with \( U > 0 \), both the solutions of \( k_j \) and \( A_n \) for the ground state (GS) and low excited states are real numbers. The ground state solution corresponds to \( J_j = (N + 1)/2 - j \) and \( A_n = (M + 1)/2 - \alpha \). In the strongly repulsive interaction limit \( U/t \to \infty \), the ground state energy is identical to that of a polarized N-fermion system [25]. On the other hand, if the on-site interaction between fermions with different spin is attractive, i.e. \( U < 0 \), the ground state is then composed of \( N \) real \( k \)s and \( 2M \) complex ones. In the strongly attractive interaction limit \( U/t \ll 1 \), the complex solutions take the 2-string form [26]:

\[
\sin k_n \approx A_n / i(U/4t),
\]

where \( k_n \) is the ordering of the rest fermions, \( y_1, y_2, \ldots, y_M \) are the coordinates of down spins in the lattice with length \( L \), and

\[
\psi(y_1, y_2, \ldots, y_M; P) = \sum_R \epsilon(R) \prod_{j < l} (A_{pj} - A_{jl} - iU/2t) \times \prod_{i=1}^N \left[ \prod_{s=1}^{y_i-1} (\sin k_{Ps} - A_{Pi} + iU/4t) \times \prod_{t=y_i+1}^N (\sin k_{Pt} - A_{Pi} - iU/4t) \right].
\]

The parameters \( k_j \)s and \( A_n \)s are determined by the Bethe-ansatz equations (BAEs) [22]:

\[
k_j L = 2\pi I_j - 2 \sum_{\beta=1}^M \tan^{-1} \left( \frac{\sin k_j - A_\beta}{U/4t} \right),
\]

\[
\sum_{j=1}^N 2 \tan^{-1} \left( \frac{A_j - \sin k_j}{U/4t} \right) = 2\pi J_\alpha + 2 \sum_{\beta=1}^M \tan^{-1} \left( \frac{A_\beta - A_0}{U/2t} \right),
\]

where \( L \) is the size of the optical lattice. The eigenvalues are given by \( E = -2t \sum_{j=1}^N \cos k_j \). The structure of the solution of BAEs of Hubbard model is relevant to the filling factor of \( N/L \). In the following, we shall consider the case with \( N/L < 1 \).

The BAEs (3) and (4) hold true for both the repulsive and attractive \( U \), however the structure of the solutions is quite different for \( U > 0 \) or \( U < 0 \). For the repulsive interaction with \( U > 0 \), both the solutions of \( k_j \) and \( A_n \) for the ground state (GS) and low excited states are real numbers. The ground state solution corresponds to \( J_j = (N + 1)/2 - j \) and \( A_n = (M + 1)/2 - \alpha \). In the strongly repulsive interaction limit \( U/t \to \infty \), the ground state energy is identical to that of a polarized N-fermion system [25]. On the other hand, if the on-site interaction between fermions with different spin is attractive, i.e. \( U < 0 \), the ground state is then composed of \( N \) real \( k \)s and \( 2M \) complex ones. In the strongly attractive interaction limit \( U/t \ll 1 \), the complex solutions take the 2-string form [26]:

\[
\sin k_n \approx A_n / i(U/4t),
\]

and \( \sin k_{M+n} \approx A_n - i(U/4t) \). Besides the complex solutions, the BAEs also have real solutions for \( U < 0 \), which describe the scattering states of attractive fermions. The Fermi super-Tonks-Girardeau (FSTG) gas state corresponds to the lowest real solutions of the BAEs (3) and (4) with \( U < 0 \). These scattering states are gas-like excited states of the attractive spin-1/2 ultracold fermions which are above states including at least one paired bound state, while the ground state of the system is composed of \( M \) tightly bound fermion pairs.

Next we explore the scattering solution of the Bethe-ansatz equations in the strongly interacting limit. As \( U/t \to \infty \), the solution of \( A_n \) is proportional to \( U \), whereas \( \sin k_j \) is always finite with \( |\sin k_j| \leq 1 \). Therefore the quasimomenta can be given approximately

\[
k_j L = 2\pi I_j + A_0 - A_1 \left( \sin k_j \right)/U \to \frac{A_0}{U} - \frac{A_1}{U^2} + O(U^{-3})
\]

where

\[
\begin{align*}
A_0 &= 2 \sum_{\alpha=1}^M \tan^{-1} \left( \frac{A_\alpha}{U} \right) \\
A_1 &= 2 \sum_{\alpha=1}^M \frac{1}{(A_\alpha/U)^2 + 1} \\
A_2 &= 2 \sum_{\alpha=1}^M \frac{A_\alpha}{|(A_\alpha/U)^2 + 1|}
\end{align*}
\]

with \( U = U/4t \). Here we consider the case with \( N_1 = N_1 \). Under this condition, the values of \( A_\alpha \)s are symmetric.
about zero. It follows that \( A_0 = A_2 = 0 \) and correspondingly equation (5) is simplified as

\[
k_j L = 2 \pi I_j - A_1 |\varphi_i^{\prime}| + O(U^{t-3}), \tag{6}
\]

i.e.,

\[
\begin{align*}
  k_j L &= 2 \pi I_j - \varphi_i^{\prime} |\varphi_i^{\prime}| + O \left( U^{t-3} \right) & U > 0 \\
  k_j L &= 2 \pi I_j + \varphi_i^{\prime} |\varphi_i^{\prime}| + O \left( U^{t-3} \right) & U < 0
\end{align*}
\]

where \( \varphi = A_1 \). In general, \( A_1(U) \neq A_1(-U) \) since the solution \( A_0 \) of equation (4) are not symmetric for \( U \) and \(-U\). However, in the strongly interacting limit, up to the order of \( U^{-1} \) equation (4) becomes \( 2 \tan^{-1} \left( \frac{U}{2t} \right) = \frac{1}{2} 2 \pi I_j + \frac{1}{2} \sum_{i=1}^{N} 2 \tan^{-1} \left( \frac{U_i}{2t} \right) \), which has the same form as BAE of the Heisenberg spin chain and is invariant under the operation \( P : U^{t} \rightarrow U, A_0^{t} \rightarrow -A_0^{t} \). Therefore, we have \( A_1(U) = A_1(-U) \) up to the order of \( U^{-2} \). It follows that the ground state energy of the Fermi Tonks-Girardeau (FTG) gas in the strongly repulsive limit and the energy of FSTG state in the strongly attractive limit are given by

\[
E_{FTG} = -2t \sum_{i=1}^{N} \cos \left( \frac{2 \pi I_j}{L} \left( 1 - \frac{\varphi_i^{\prime}}{L |U|} \right) \right) + O(U^{t-3})
\]

\[
E_{FSTG} = -2t \sum_{i=1}^{N} \cos \left( \frac{2 \pi I_j}{L} \left( 1 + \frac{\varphi_i^{\prime}}{L |U|} \right) \right) + O(U^{t-3})
\]

where \( I_j = (N + 1)/2 - j \) for both the FTG and FSTG gas. Here, for convenience, we call the ground state of the spin-1/2 Fermi gas in the strongly repulsive limit as the FTG state. Obviously, in the limit of \( |U| \rightarrow \infty \), we have \( E_{FSTG} = E_{FTG} \). In Figure 1, we make a comparison between the exact solutions given by numerically solving equations (3) and (4) directly and the approximate solutions given by solving equation (6) iteratively. For an example systems with \( L = 100, N = 10 \) and \( M = 5 \), we show that for large enough values of \( U/t \), the approximate solutions agrees very well with the exact solutions.

In Figure 1a, one can see that the quasimomentum distributions for the ground state of the repulsive Fermi gas and the FSTG state of the attractive Fermi gas. Here, for convenience, we call the ground state of

\[
\begin{align*}
  \left( |\varphi_i^{\prime}| \right) \text{ vs. } U. \text{ Dots in the figure denote the approximate solutions via expansion in strongly interacting limit. For large enough } |U|, \text{ they agree very well with the exact solutions.}
\end{align*}
\]

\[
\begin{align*}
  \text{Fig. 1. (Color online) Comparison between exact solutions (denoted by C) and approximate solutions (denoted by +) of BAEs. (a) Quasi-momentum distributions for the ground state of the repulsive Fermi gas and the FSTG state of the attractive Fermi gas. Here, for convenience, we call the ground state of}
\end{align*}
\]

3 Preparation of FSTG state

The FSTG state can be realized in a 1D deep optical lattice by a sudden switch of interaction similar to the experimental realization of bosonic STG gas in reference [5]. Suppose that the initial state \( |\varphi_i^{ini}(t = 0)\rangle = |\varphi_0(U_0)\rangle \) is prepared at the ground state in the strongly repulsive regime with \( U_0/|t| \gg 1 \), after a sudden switch to the opposite regime with interaction strength \( U/|t| \ll 1 \), the wave-function \( |\psi(t)\rangle = e^{-iH(U)t} |\varphi_i^{ini}(U_0)\rangle \) can be calculated via

\[
|\psi(t)\rangle = \sum \left. e^{-iE_n t} c_n |\varphi_n(U)\rangle \right).
\]

where \( c_n = \langle \varphi_n(U) | \varphi_0(U_0) \rangle \) with \( |\varphi_n(U)\rangle \) representing the \( n \)th eigenstate of the Hubbard model with on-site interaction \( U \). It is straightforward that \( |c_n|^2 \) is the transition probability from the initial state to the \( n \)th eigenstate of \( H(U) \).

To give a concrete example which may help us get an intuitive understanding of the properties of the FSTG state of the attractive Hubbard model, we display the full energy-momentum spectra of the Hubbard model with \( L = 30, N = 4, M = 2, \) and \( U = \pm 15 \) in 3. As shown, the spectra is split into a series of separated bands. For
the repulsive case, the lowest band is a scattering continuum of $N$ (here $N = 4$) unpaired fermions. The middle band is a scattering continuum formed by one tightly bound fermion pair and two unpaired fermions, whereas the top band is a scattering continuum of two tightly bound fermion pairs. The spectra for the attractive case is similar but in reverse order. The gap between centers of neighboring bands equals approximately to the binding energy $|U|$ of a fermion pair. These separated bands are no longer distinguishable as the interaction strength is comparable to the bandwidth. The zero-momentum lowest scattering state of $N$ unpaired fermions denoted by a red star in Figure 3a is just the ground state of the repulsive Fermi gas, whereas the red star in Figure 3b indicates the Fermi super-Tonks-Girardeau gas state.

Starting from the ground state of the HM with a repulsive interaction and then suddenly switching the interaction to the attractive side, we evaluate the transition probabilities from the initial repulsively GS to each eigenstate of the attractive Hubbard model by the method of the exact diagonalization. As shown in Figure 4a, we find that the transition probability to the lowest state (FSTG) of a given $S$ in the top scattering band is very close to 1, when both the repulsive interaction of the initial state and the attractive interaction of the final state are strong enough. As the transition probability to the lowest scattering phase is almost 1 in the strongly interacting regime, the transition probability to the lower paired states is almost completely suppressed, thus we expect that such a highly excited gas-like state of the strong attractive Fermi gas in optical lattice can be experimentally realized. Actually, the stable excited scattering state prepared in this way can be viewed as a Fermi generalization of the STG gas in the optical lattice. If the system enters to the weakly interacting regime, the transition probability to the FSTG state decreases quickly, whereas the transition probability to the ground state increases. The FSTG state is more stable when the interaction strength is closer to the Feshbach resonance point. When the interaction strength is weak, the FSTG state is not expected to be stable.

Due to the existence of band structure, there exist states of repulsively bound pairs above the lowest continuum band for the repulsive Hubbard model. Such kind of repulsively pairing state is absent in the continuum Yang-Gaudin system [14]. Particularly, the top band of the strongly attractive Hubbard model is completely composed of repulsively bound pairs, which is very similar to the ground state of attractive Hubbard model composed of attractively bound pairs. Next we show that the highest excited state composed of repulsive bound pairs can be realized from the ground state of strongly attractive Hubbard model by a sudden switch of interaction from $U < 0$ to $U > 0$. To see it clearly, we calculate the transition probability from the ground state of attractive Hubbard model (marked by the symbol of cross in Fig. 3b) to the highest state in the top band of the repulsive Hubbard model (marked by the symbol of cross in Fig. 3a). As shown in Figure 4b, when both the attractive interaction of the initial state and the repulsive interaction of the final state are strong enough, the transition probability is very close to 1. By this way, we can realize the repulsively paired state for the repulsive Hubbard model. We note that such a repulsively paired state is a very highly excited state with zero total momentum, which is different from the $\eta$-pairing state discussed in references [21,27].

Next we calculate the number of doubly occupied sites $N_d = \sum_i \langle \hat{n}_i^\dagger \hat{n}_i \rangle$ for the FSTG state by exact diagonalization, which can be obtained by differentiation of the energy. As shown in Figure 5a, $N_d$ decreases monotonically with increasing $|U|$ and tends to zero for $U \to -\infty$. This indicates that there is no pairing for the FSTG state even in the strongly attractive limit. As a comparison, we also calculate $N_d$ for the ground state of the attractive Fermi gas in Figure 5b. Instead, $N_d$ for the ground state of the attractive Fermi gas monotonically increases to $N/2$.
as the ground state is composed of \( N/2 \) pairs of fermions with the binding energy proportional to \( U \). For a bosonic STG gas, it is known that the STG state has even stronger local correlation than the repulsive TG gas \([4,9]\). To see whether FSTG state in the optical lattice has similar properties, we also calculate the local correlation function for the repulsive ground state. Here we note that the local correlation function \( \sum_i \langle \hat{n}_i^\uparrow \hat{n}_i^\downarrow \rangle \) is noting else but \( N_d \) defined above. As shown in in Figure 5a, \( N_d \) for the ground state of repulsive Fermi gas also monotonically decreases to zero with the increase in the repulsion strength \( U \). Nevertheless, the local correlation functions shown in Figure 5a indicate that the FSTG state has stronger local correlation than the corresponding repulsive ground state, which is similar to its bosonic correspondence.

In contrast to the spinless Bose system, the ground state of a spin-1/2 Hubbard model is highly degenerate in the limit of \( U \to \infty \) due to the existence of the spin degree \([28–30]\). Nevertheless, the degeneracy is broken for a large but finite interaction strength and the true ground state of the repulsive fermions is the state with the lowest \( S \) \([31]\). In Figure 6, we show the ground state energy of repulsive Fermi gases and the lowest energy of the FSTG state for systems with a fixed \( N = 10 \) but various \( S \). It is clear that \( E(S_1) < E(S_2) \) for \( S_1 < S_2 \) on the repulsive side. The energy difference between different spin states vanishes as \( U \to \infty \). On the other hand, for the FSTG state, the state with the larger \( S \) has lower energy, i.e., \( E(S_1) > E(S_2) \) for \( S_1 < S_2 \) on the attractive side, as shown in Figure 6. This implies that the ferromagnetic state with maximum \( S = N/2 \) has lowest energies for the FSTG states with large but finite interaction strength. Nevertheless, energies for states with different total spins approach the same limit of the polarized state as \( |U| \to \infty \).

Finally, we discuss the half-filling case, for which the ground state is a Mott state for any finite repulsion \([22]\). Similar to the low-density case, we display the full energy-momentum spectra of the the half-filling Hubbard model with \( L = 10, N = 10, N_\uparrow = N_\downarrow = 5 \), and \( U = \pm 15 \) in Figure 7. Similarly, the spectra is split into a series of separated bands. For the repulsive case, the lowest band corresponds to the Mott states with each site occupied by a single fermion. Above the Mott band, the separated middle bands correspond to the scattering continuum composed of paired fermions and unpaired fermions, whereas the top band is the scattering continuum of \( N/2 \) paired fermions. In contrast to Figure 3, the lowest Mott band is obviously very narrow as the hopping process of a single fermion to its neighboring sites is suppressed. In the large \( U \) limit with \( U/t \gg 1 \), the double occupied states have much large energy than the states with no double occupancy, and the effective Hamiltonian is given by \([32,33]\)

\[
H_{\text{eff}} = \frac{4t^2}{U} \sum_i \left( \hat{S}_i \hat{S}_{i+1} - \frac{1}{4} \right)
\] (8)
where $\hat{S}_x^\alpha = \frac{1}{\sqrt{2}} \sigma^\alpha_{\sigma^\prime} \hat{c}_i \sigma^\prime \hat{c}^\dagger_i \sigma$ are the usual spin operators with $\sigma^\alpha$ being the Pauli matrices. As shown in the inset of Figure 7a, the enlarged spectrum of the lowest band is consistent with the spectrum of antiferromagnetic (AFM) Heisenberg model of equation (8). For the attractive case with $U = -15$, as shown in Figure 7b, the spectrum has similar structure as the repulsive case but in a reverse order with the top band corresponding to the Mott states. By projecting the original Hamiltonian (1) into the Hilbert spaces without any double occupancy, we can also get the effective Hamiltonian given by equation (8). Although the effective Hamiltonian has the same form for both the repulsive and attractive Hubbard model, the effective coupling strength $J$ has different sign, i.e., $J = \pm \frac{U}{2}$ for $U > 0$ or $U < 0$. For $U > 0$, the effective model is an AFM Heisenberg model which describes the lowest continuum band of the original Hubbard model. On the other hand, the effective model is a ferromagnetic (FM) Heisenberg model for $U < 0$, which describes the highest continuum band of the attractive Hubbard model. Given the initial state as the ground state of half-filling repulsive Hubbard model (or effectively the ground state of AFM Heisenberg model of equation (8) labelled by the star in the inset of Fig. 7a), after a sudden switch of interaction from $U = 15$ to $U = -15$, the state is transferred to the highest state of the attractive Hubbard model (or effectively the highest excited state of the FM Heisenberg model labelled by the star in the inset of Fig. 7b). This way, we can effectively prepare the highest excited state of a FM Heisenberg model. Here we indicate the difference from the low-density case: the final state obtained by sudden switch is on the top of the top band in Figure 7b, whereas the FSTG state in Figure 3b is on the bottom of the top band. The difference can be attributed to the different structures of the energy spectra of the low-density and half-filling systems. In the half-filling case, a narrow Mott band is formed with a Mott gap separated from the excited bands. The ground state and dynamic behaviors are thus determined by the effective AFM Heisenberg Hamiltonian, which describes the physics of the narrow Mott band and displays different behaviors from the low-density case. On the other hand, if the initial state is the ground state of half-filling attractive Hubbard model, we can access the repulsively paired state in the top band of the repulsive Hubbard model by the sudden switch of the interaction to the repulsive side.

4 Summary

In summary, we study the properties of the FSTG state of the attractive Hubbard model, which is a highly excited state of the attractive Hubbard model without paired states and corresponds to the lowest real solution of the Bethe-ansatz equations with $U < 0$. Starting from the ground state of strongly repulsive spin-1/2 fermion in 1D deep optical lattices, such a state can be realized via a sudden switch of the interaction to the strongly attractive regime. By calculating the transition probabilities, we have shown that the excited FSTG state can be efficiently achieved in the strongly interacting regime and thus is possible to be realized experimentally with cold fermionic atoms in optical lattices.

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