Gap solitons of a super-Tonks–Girardeau gas in a one-dimensional periodic potential

T F Xu\textsuperscript{1}, X L Jing\textsuperscript{1}, H-G Luo\textsuperscript{2,3}, W C Wu\textsuperscript{4} and C S Liu\textsuperscript{1,4}

\textsuperscript{1} Department of Physics, Yanshan University, Qinhuangdao 066004, People’s Republic of China
\textsuperscript{2} Center for Interdisciplinary Studies and Key Laboratory for Magnetism and Magnetic Materials of the MoE, Lanzhou University, Lanzhou 730000, People’s Republic of China
\textsuperscript{3} Beijing Computational Science Research Center, Beijing 100084, People’s Republic of China
\textsuperscript{4} Department of Physics, National Taiwan Normal University, Taipei 11677, Taiwan

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Abstract
Motivated by the recent experimental realization of a super-Tonks–Girardeau (STG) gas (Haller et al 2009 Science 325 1224), we study in detail the existence and stability of gap solitons of the STG gas in a one-dimensional optical lattice. In particular, we explore the composition relationship of various gap solitons and nonlinear Bloch waves, taking into account the interplay between the periodic potential and the nonlinear interaction. The analysis of the linear stability indicates that unstable gap solitons can become stable by increasing the amplitude of the periodic potential or decreasing the nonlinear interaction. Moreover, it is found that due to the weak contribution of the interaction, gap solitons in a higher band gap (higher family) can easily form near the bottom of the linear Bloch band gaps in comparison with their counterparts in a lower band gap (lower family). Numerical calculations verify the validity of the composition relationship between various gap solitons and nonlinear Bloch waves in the STG phase. The results predicted for an STG gas confined by an optical lattice should be experimentally observable.

1. Introduction

Recent developments in the Feshbach resonance techniques have enabled the experimental realization of the one-dimensional (1D) stable excited state, called a super-Tonks–Girardeau (STG) gas, by sudden quenching of the effective 1D interaction from a strongly repulsive to a strongly attractive interaction regime [1–3]. The STG gas-like state describes the lowest lying gas-like phase of the attractive Bose gas which corresponds to a highly metastable excited state [4–6]. The existence of these metastable gas-like states is due to the existence of the Fermi-pressure-like kinetic energy inherited from the strongly repulsive interaction [7–10, 5]. However, the metastability, dynamics and statistical signature of this kind of novel quantum state are still far from well understood.

In general, the atomic matter waves form stable bright solitons when the linear spreading due to kinetic energy is compensated by the attractive interaction between atoms. While stable dark solitons can only form in the repulsive case, a Bose gas with attractive interaction can form bright solitons [11–13]. Bright matter wave solitons with a repulsive atom–atom interaction can also form inside a weak periodic potential [14, 15]. In particular, a class of gap solitons called ‘fundamental gap solitons’ may exhibit a single peak localized within a unit cell (one period of the potential) [16]. Gap solitons with two peaks of opposite signs within a unit cell are called ‘sub-fundamental gap solitons’ [17]. Similar to a TG gas in an optical lattice [18], it is interesting and important to investigate whether various gap solitons can exist in an STG gas confined in a 1D optical lattice.

Due to the interplay between periodicity and nonlinearity, a typical feature that arises is a nonlinear Bloch wave which...
is extensive and can spread over the whole space [19]. It has been pointed out that a certain relationship in the composition can exist between various gap solitons and nonlinear Bloch waves in the TG phase [18]. The question is thus whether this relationship remains valid in the STG phase, and how would the solitons and waves behave when the interaction changes suddenly from repulsive to attractive?

As is well known, due to strong quantum fluctuations, the mean-field theory typically does not work well for a 1D system, except in a weakly interacting regime [20–24]. In the absence of an external potential, the Bethe ansatz method has been used to extract the energy density and chemical potential for a Bose gas in the STG phase in the thermodynamic limit [7]. This gives us an opportunity to derive a modified nonlinear Schrödinger equation for the STG phase based on the local-density approximation (LDA). This modified equation can then be used to investigate the dynamical properties of the Bose gas in a strongly interacting regime.

In this paper, we investigate the gap soliton and nonlinear Bloch wave of an STG gas in a 1D optical lattice by numerically solving the modified nonlinear Schrödinger equation. In particular, we are interested in the existence and the stability of the gap solitons. It is found that the amplitude of the periodic potential and the strength of the nonlinear interaction are two important factors for the stability of the gap solitons. The linear stability analysis indicates that a stable gap soliton can easily form near the bottom of the linear Bloch band gaps, and moreover, the composition relationship remains valid in the STG phase.

The rest of the paper is organized as follows. In section 2, we introduce the model equation for studying the 1D periodic Bose system in the STG phase. To understand the properties of this system, we introduce the Gaussian-like Bose density profile ρ(x) within a unit cell and the chemical potential for different interaction constants. In section 3, a theoretical analysis and numerical simulations are given to investigate the stability of various gap solitons upon the change of the strength of the interaction and the amplitude of the periodic potential. In section 4, it is shown that the composition relationship between the nonlinear Bloch waves and the gap solitons remains valid in the STG case. A generalized composition relation between the high-order solitons and the multiple periodic waves also exists. In section 5, we present a brief summary.

2. Model equation

We consider a quasi-1D system of N interacting bosons tightly confined in an elongated trap. As a simple but fundamental integrable interacting boson model, it can be exactly solved by the Bethe ansatz method. In the case of an attractive Bose gas, the Bethe ansatz solutions can be real, corresponding to some highly excited states. In the thermodynamic limit with N, L → ∞ but ρ = N/L finite, the energy density can be expressed as $e(\gamma) = \frac{\hbar^2}{2m} \gamma^2 e(\gamma)$ [7], where $\gamma \equiv c/\rho$ with $c \equiv mg/\hbar^2$ (g being the interaction strength). The function $e(\gamma)$ can be accurately fitted from the Bethe ansatz solutions in the attractive STG phase. This leads to

$$e(\gamma) = \frac{4\pi^2}{3} \left( 1 + p_1 |\gamma| + p_2 |\gamma|^2 + p_3 |\gamma|^3 /4 \right)$$

where $p_1 = 0.075$, $p_2 = 0.013$, $q_1 = 0.227$, $q_2 = 0.034$ and $p = 0.004$ are the best fitting parameters.

To deduce the bulk properties of an inhomogeneous system, we have to combine the analytical solution of the homogeneous system with the LDA calculation, in which it is assumed that the system is in equilibrium for the local position $x$ with an external periodic potential $V_{ext}(x) = v \cos(\frac{2\pi}{\Lambda} x)$. Here, $\Lambda$ is the lattice constant and $v$ is the potential strength.

For convenience, we define $\Phi \equiv \sqrt{p}$ and the normalization condition $N = \int dx |\Phi(x)|^2$. The energy functional $\mathcal{E}$ is then represented as

$$\mathcal{E} = \int dx \left[ \frac{\hbar^2}{2m} \left| \frac{d}{dx} \Phi(x) \right|^2 + V_{ext}(x) \rho + \rho e(\rho) \right].$$

The first (gradient) term represents an additional kinetic energy quantity associated with the inhomogeneity of the gas that is not considered in the LDA [25]. In fact, the LDA is only applicable when $N \gg 1$. It may become ineffective with the decreasing particle number $N$ when the tunnelling of the density profile beyond the Thomas–Fermi radius becomes relatively more important [26, 27]. In this case, we may need to use a method beyond the LDA, such as the microscopic density-functional theory.

We now consider the free-energy functional $\mathcal{F} = \mathcal{E} - \mu N$ [28], where the chemical potential $\mu$ is introduced as a Lagrange multiplier. By minimizing $\mathcal{F}$ corresponding to the lowest lying state $\Phi$, we obtain the following time-independent ‘modified’ nonlinear Schrödinger equation [28]:

$$\left[ -\frac{\hbar^2}{2m} \frac{d^2}{dx^2} + V_{ext}(x) + \tilde{F}(\rho) \right] \Phi(x) = \mu \Phi(x),$$

where $\tilde{F}(\rho) = \frac{\partial}{\partial \rho}[\rho e(\rho)] = \frac{\hbar^2}{2m} [3e(\gamma) - \gamma \partial_\gamma e(\gamma)]$ corresponds to the interaction energy. A similar method has been used to discuss two-component Bose gases in 1D harmonic traps [29]. Equation (2) can also be obtained by reformulating the corresponding hydrodynamic equations for the density and atomic velocity [30].

It is convenient to rescale and make equation (2) a dimensionless form. The coordinate $x$ is scaled in units of $\Lambda/(2\pi)$, while the periodic potential $V_{ext}(x)$, the interaction energy $\tilde{F}(\rho)$ and the chemical potential $\mu$ are all scaled in units of $8E_r$ with $E_r = \hbar^2 \pi^2/2m\Lambda^2$ being the recoil energy. As a consequence, equation (2) is reduced to

$$\left[ -\frac{1}{2} \frac{d^2}{dx^2} + v_0 \cos(x) + F(\rho) \right] \Phi(x) = \mu \Phi(x),$$

where $v_0 = v/8E_r$, $F(\rho) = \frac{\partial}{\partial \rho}[\rho e(\rho)] = \frac{\hbar^2}{8} [3e(\gamma) - \gamma \partial_\gamma e(\gamma)]$ and the reduced $\rho = 2\pi N/\Lambda \Lambda$. Equation (3) is the starting point of this study.

For an intuitive understanding of equation (3), we first numerically study the density profile and the corresponding
chemical potential $\mu$ of the attractive STG gases and compare the results with those of the repulsive TG gases (see figure 1). We use the finite-element method along with the periodic boundary condition [31], and then evolve several hundreds of steps in imaginary time until the lowest chemical potential $\mu$ is reached. (The wavefunctions obtained are called the nonlinear Bloch waves.) In addition, we consider overall ten lattice sites ($x$ ranging from $-10\pi$ to $10\pi$), the periodic potential strength $v_0 = 10$ and the particle number $N = 50$ (an average of five particles per unit cell).

As shown in figure 1(a), when $c < 0$ and $|c|$ increases from the weak-coupling regime (may not yet be in the STG phase) to the strong-coupling regime (STG phase), the Gaussian-like density profile increases at the centre and decreases at the edges. Note that the weak (strong) coupling result corresponds to point A (B) marked in figure 1(b). It indicates that the STG Bose gas behaves effectively more repulsively in the weak-coupling regime than in the strong-coupling regime. On the other hand, for STG gases, the chemical potential $\mu$ is seen to decrease with increasing $|c|$, which is in great contrast to the result of the TG case with $c > 0$ (see cases C and D in figure 1). In the extremely strong-coupling regime ($|c| \rightarrow \infty$), chemical potentials of both STG and TG gases merge, as shown in figure 1(b). This is consistent with the observation that the density profiles of cases B and C are closest to the Fermi case (blue line; obtained by the Bose–Fermi mapping method), apart from the artificial five peaks (see figure 1(a)). In the extremely strong limit, regardless of an STG or TG gas, the system behaves like a noninteracting Fermi gas. In contrast, STG gases behave in a very different way from TG gases [1, 7].

**Figure 1.** (a) The Gaussian-like Bose density profile $\rho(x)$ within a unit cell for different interaction constants $|c|$. For the attractive cases ($c < 0$, red lines), the interaction energy $F(\rho) = \frac{\hbar^2}{2m}(3\epsilon(\gamma) - \gamma \partial_\gamma \epsilon(\gamma))$ is used with $\epsilon(\gamma)$ given in equation (1) and the parameters therefrom, while for the repulsive cases ($c > 0$, black lines), the same $F(\rho)$ is used with $\epsilon(\gamma) = \frac{1}{2}[\epsilon(\gamma) + \epsilon_{\text{K}}]$ and $p = -5.048947$ and $g = -20.8604983$ [29]. For comparison, the density profile labelled by ‘Fermi’ is for a noninteracting Fermi gas, obtained by the Bose–Fermi mapping method [18]. (b) The dependence of the chemical potential $\mu$ on the interaction constant $|c|$. The cases of A, B, C and D in (a) and (b) are obtained with the same parameters. Other parameters: $N = 50$ and $v_0 = 10$.

3. Gap solitons and their stability

3.1. General features of gap solitons

We first examine the linear band structures by setting the interaction energy $F(\rho) = 0$ in equation (3). In this case, the corresponding linear Schrödinger equation can be exactly solved by the finite-element method. A large amplitude of the periodic potential, $v_0 = 50$, is used in the current case, which is essential for the strongly interacting STG Bose gas to be studied later. As a consequence, the Bloch bands are reduced to a series of narrow bands. The lowest four linear bands (the vertical ‘lines’) are shown in figure 2. We next consider the solutions for finite $F(\rho)$, where the chemical potential $\mu$ is within a linear band gap. After discretizing equation (3) on a grid, the differential equation can be transformed into a set of coupled algebraic equations. The gap solitons and nonlinear Bloch waves are then solved based on the Newton relaxation method [17]. In figure 2, the particle number $N$ of the gap solitons as a function of the chemical potential $\mu$ is shown. In addition, the gap soliton waves are shown in figure 3. Since the reduced $\rho$ is less than 1, $|\gamma| = |c/\rho|$ is larger than 10,000 when the interaction constant $c = -10,000$. Moreover, it has been shown in [7] that the transition probability from a TG phase to an STG phase is larger than 90% when $|\gamma| > 20$. This gives strong support to our model and shows that it is appropriate for describing a Bose gas in the STG phase.

The nonlinear Bloch band developed from the first linear band gap is commonly called the first-order nonlinear Bloch band. We see in figure 2 that it is lifted as $N$ increases. The lifting is simply due to the fact that a larger $N$ results in larger nonlinearity and hence a larger corresponding $\mu$. Higher order nonlinear Bloch bands developed from higher linear Bloch band gaps also lift when $N$ is increased.
two nodes. In summary, solitons developing from the third linear band gap will have and belong to the second family. Similarly, the third-family gap number. All of them have one node in the corresponding waves enter the higher linear band gap by increasing the particle begins developing from the second linear band gap and can

Thus, it is reasonable to conjecture that the nonlinear Bloch

gas has already been shown in figure 1(b). Perhaps this drastic difference between an STG and a TG

For those gap solitons whose chemical potentials are located within the same nonlinear Bloch band, all their waves should have the same number of nodes and are said to belong to the same family. For example, the lowest family or the first-family gap solitons are those matching the first nonlinear band [32, 16, 18]. This family of gap solitons will have Gaussian-like waves which are nodeless. The second class of gap solitons begins developing from the second linear band gap and can enter the higher linear band gap by increasing the particle number. All of them have one node in the corresponding waves and belong to the second family. Similarly, the third-family gap solitons developing from the third linear band gap will have two nodes. In summary, \( n \) classes (families) of gap solitons can exist within the \( nth \) linear band gap in which the maximum number of nodes is \( n - 1 \) for the \( nth \) family.

As an example, figure 3 shows the gap solitons in different families with a chemical potential within the fourth linear band gap (see also figure 2). The gap soliton waves in figures 3(a) and (b) belong to the first family with no node. The difference between the nonlinear Bloch waves in figures 3(a) and (b) is that in the latter case one has a \( \pi \)-phase shift between adjacent wells. The gap soliton waves in figures 3(c) and (d) belong to the second family of one node. More nodes exist in the higher family gap soliton waves (see figures 3(e)–(h)).

3.2. Stability of gap solitons

A basic condition for these gap solitons to be observed experimentally is the stability. Here, we shall perform a linear stability analysis of the various gap solitons studied above. It is well known that bright solitons in atomic matter waves can form only when the kinetic energy is compensated by the attractive interaction between atoms. Similarly, in the TG gases, gap solitons can form when the linear spreading and repulsive atom–atom interaction are compensated by the confinement of the periodic potential. However, in the present STG gases, gap solitons are found to exist when the kinetic energy is compensated by the attractive interaction between the atoms and the periodic potential. It is important to examine the stability of these STG gap solitons.

Following the standard procedure as given in [18], we have obtained linear eigen-equations for the perturbation. Amongst all the eigenvalues, if there exists a finite imaginary part, the solution of \( \Phi(x) \) would be unstable; otherwise, the solution of \( \Phi(x) \) is stable.

The stability of gap solitons is studied and presented in figure 4 for different amplitudes of the potential: (a) \( v_0 = 10 \) and (b) \( v_0 = 50 \). It is shown that gap solitons in the first family are stable when their chemical potentials \( \mu \) are located near the bottom of the first linear Bloch band gap. They will become unstable when \( \mu \) increases towards the top of the first linear band gap (with increasing \( N \)) and enters further into the second and the third band gaps (not shown in figure 4). The same feature is also found for the second and higher family gap solitons.

When gap solitons are developed from the bottom of each linear band gap, the number of particles contained in the gap solitons is small (see figure 2). In this case, the particles behave as a non-interacting system within a single potential well, and the gap solitons are, in fact, the stationary states in discrete energy levels. They are hence stable. In the present model, the interaction energy \( F(\rho) \) actually contains information about both the kinetic energy and the attractive interaction of the STG Bose gas, and the resulting effect is repulsive. As a matter of fact, the interaction effect will increase as the particle number increases. When the interaction energy is increased and cannot be compensated by the confinement potential, the gap solitons will become unstable.

It is interesting to note that gap solitons in the first family are stable only in a narrow regime when their energies are near the bottom of the first linear band gap. The stable regime
becomes wider for higher family gap solitons. This is because gap solitons of high-order families have nodes and thus have larger kinetic energies compared to those of low-order families. This gives us a rough idea when the stability of different-family gap solitons is compared.

In what follows, we quantitatively study the stability of the gap solitons of different families by looking into the competition between the kinetic energy $E_K \equiv \int dx \left| \frac{\partial \phi}{\partial x} \right|^2$ and the interaction energy $E_I \equiv \int dx F(\rho) \rho$. We then introduce a quantity $\eta(\mu) \equiv E_I/(E_K + E_I)$, which serves as a direct measure of the effective repulsion between atoms. The values of $\eta(\mu)$ are shown in figure 5, where the chemical potentials $\mu$ are taken to be 0.3 and 0.6 times the band gap width, respectively. In view of figure 5, the effective repulsive interaction is relatively weaker (relative to its kinetic energy) for higher family gap solitons. As discussed before, by ignoring the atom interactions, the stable gap wave is just the stationary state, and the stable gap solitons can become unstable due to the increasing nonlinearity. In the present case, the nonlinearity of higher family gap solitons is actually weaker than that of the lower order families. Consequently, for the same particle number, higher order family gap solitons are more stable than those of lower order families.

Based on the linear stability analysis given in figures 4(a) and (b), when $v_0 = 10$ the fourth-family gap solitons will be unstable only in a narrow regime near the top of the band gap (see figure 4(a)), while when $v_0 = 50$, they are stable for the entire regime (see figure 4(b)). With the increasing amplitude of the periodic potential $v_0$, the unstable gap solitons can become stable. This is because increasing the confinement potential is physically equivalent to decreasing the atom interactions. When the confinement potential is strong enough to compensate for the effective repulsive interaction, unstable gap solitons can become stable.

We have also studied the linear stability of gap solitons for different values of the interaction constant $c$. To see this effect in a more obvious way, we have chosen $c = -1$ for an extremely weak case in which the Bose gas may not yet be in the STG phase. However, the choice of this low limit will not affect the main results reported here. As shown in figure 4(a), the stable regime increases with the increase of the attractive interaction constant $c$. This is because the effective (or equivalent) repulsive interaction decreases with the increase of the interaction constant $c$ (also shown in figure 1(b)). As emphasized before, this is in great contrast to the case of a TG Bose gas of repulsive interactions. In the latter case, the effective repulsive interaction increases with the increase of interaction constant $c$. Typical results are shown in figure 4(c).

4. Composition relationship

As discussed above, different-family gap solitons originating from the stable bound states of a single periodic well can develop in the linear band gaps. On the other hand, the nonlinear Bloch band can be viewed as a lifted linear Bloch band by increasing the nonlinear interaction. However, the linear Bloch band can be viewed as an evolution from the discrete energy levels of an individual well. Therefore, the gap solitons and nonlinear Bloch waves should share certain common features. This is called the ‘composition relationship’. It has been shown that gap solitons and nonlinear Bloch waves belonging to the $n$th nonlinear Bloch band have $n - 1$ nodes in an individual well of the periodic potential. In particular, it has also been pointed out and proven numerically throughout the whole interaction regime that gap solitons are...
the building blocks of the nonlinear Bloch waves \cite{32, 18}. It is important to note that the gap soliton waves shown in figures 3(a) and (b) belong to the first family and hence have no node. In figures 3(c) and (d), however, the gap soliton belongs to the second family and hence has one node. Good matches are also found between the nonlinear Bloch waves and the high-order family gap solitons in figures 3(e) and (f) and in figures 3(g) and (h) where multiple peaks exist within one unit cell.

In addition to the gap solitons and nonlinear Bloch waves studied above, there are additionally two types of waves which are also common in a nonlinear system. One is called high-order gap solitons, which are gap soliton waves with multiple peaks over multiple unit cells \cite{33}. The other is called multiple periodic waves which are defined as $\Phi(x) = \exp(ikx)\psi_n(x)$, with $\psi_n(x) = \psi_0(x + 2n\pi)$ and $n$ being a positive integer \cite{34}. For the repulsive atom interaction, it has been shown that the composition relationship between the gap solitons and the nonlinear Bloch waves can be generalized to construct multiple periodic waves from the high-order gap solitons \cite{16, 18}. It is interesting to see whether the generalized composition relationship remains valid in the present STG phase.

Figure 6(a) shows the four-peak high-order gap solitons (two central peaks pointing upwards and two adjacent peaks pointing downwards). An almost perfect match is found between the high-order gap solitons and the nonlinear Bloch waves, except for their different phases in some cells. Thus, high-order gap solitons can also be viewed as truncated nonlinear Bloch waves within the whole interaction regime. In addition, we have also obtained five-peak periodic high-order gap solitons, as shown in figure 6(b). More multiple period high-order gap solitons can also be obtained, such as the six- and seven-peak periodic waves shown in figures 6(c) and (d), respectively. As an interesting and special case, we show 16-peak periodic waves in figures 6(e) and (f). The good match between gap solitons and high-order gap solitons, as well as multiple periodic waves and nonlinear Bloch waves, strongly support our premise that gap solitons are the basic entity, from which other waves can be built up.

The above conclusion is useful in deriving both the nonlinear Bloch waves and the multiple periodic waves from the nonlinear Schrödinger equation. This can first be solved to obtain gap solitons of different families, from which we then build up an initial wavefunction. If we wish to obtain $n$-period waves in an $m$-period potential well, the initial trial wavefunction can be built up from the $n$-gap solitons as a building block ($m/n$ is assumed to be an integer). To obtain nonlinear Bloch waves in an $m$-period potential well, the initial trial wavefunction can then be built from the $m$-gap solitons aligned one by one. With these initial wavefunctions, the Newton-relaxation method can again be used to solve equation (3) to obtain the gap solitons and multiple-period waves accurately. The advantage of this method is that the initial wavefunction is very close to the final wavefunction, so few iterations are needed to obtain precise results.

5. Summary

In summary, we have investigated the gap solitons of a 1D periodic Bose gas in the super-Tonks–Girardeau phase, focusing on the existence and stability of these solitons. By a linear stability analysis, it is found that the interplay between the periodic potential and the nonlinear interaction plays an important role in the stability of gap solitons. By increasing the amplitude of the potential or decreasing the nonlinear interaction, the unstable gap solitons can become stable. We have also found that the high-family gap solitons can easily form near the bottom of the linear Bloch band gaps. Our numerical calculations verify that the composition relation between various gap solitons and nonlinear Bloch waves is valid in a general sense. This provides an alternative way to obtain the nonlinear Bloch waves.

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