

Crystalline phase for one-dimensional ultra-cold atomic bosons

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Abstract. We study cold atomic gases with a contact interaction and confined into one-dimension. Crossing the confinement induced resonance the correlation between the bosons increases, and introduces an effective range for the interaction potential. Using the mapping onto the sine-Gordon model and a Hubbard model in the strongly interacting regime allows us to derive the phase diagram in the presence of an optical lattice. We find the appearance of a phase transition from a Luttinger liquid with algebraic correlations into a crystalline phase with a particle on every second lattice site.

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Cold atomic gases confined into one-dimension exhibit remarkable properties as the interplay between interactions and reduced dimensions strongly enhances quantum fluctuations. The most prominent example is the appearance of a Tonks-Girardeau gas for bosonic particles [2, 1], and the possibility to pin the bosons into a Mott insulating phase for arbitrary weak optical lattices [3, 4]. Most remarkably, it has recently been proposed [5] and experimentally observed [6], that it is possible to access a regime, where the bosonic many body system exhibits even stronger correlations. This opens the question, whether it is possible to enhance the correlations to a point, where the bosonic systems forms a crystalline ground state. In this letter, we demonstrate that indeed in the presence of an optical lattice a solid phase appears.

The transverse confinement for cold atomic gases is experimentally efficiently achieved using optical lattices [2, 7] or atomic chips [8]. Within this one-dimensional regime with the kinetic energy of the particles much lower than the transverse trapping frequency, the interaction between the particles is described by the one-dimensional scattering length a_{1D} [9]. Remarkably, the system can undergo a confinement induced resonance, where the scattering length crosses zero. For $a_{1D} < 0$, the properties of the system have been studied in terms of the exactly solvable Lieb-Liniger model [10, 11], while at $a_{1D} = 0$ the system is denoted as Tonks-Girardeau gas. Crossing the confinement induced resonance with $a_{1D} > 0$ the mathematical model describing the system admits a two-particle bound state. Then, the physical state smoothly connected to the Tonks-Girardeau gas corresponds to an highly excited state of the mathematical model; a regime denoted as Super-Tonks-Girardeau gas [12].

In this letter, we analyze the phase diagram within this regime and demonstrate the appearance of a solid phase in the presence of an optical lattice with a bosonic particle on every second lattice site. A simplified picture of this transition is that the particles behave as hard spheres with a range $\sim a_{1D}$ [12]. Then, it is natural to expect the appearance of a solid phase for a density comparable to the range of the interaction. The rigorous derivation of the phase diagram follows in two steps: First, we analyze whether an arbitrary weak optical lattice allows to pin the solid structure. Using the mapping to the sine-Gordon model, we find, that a finite strength of the optical lattice is required. Therefore, we focus on deep optical lattices in a second step, and provide the derivation of a Hubbard model using the duality mapping between bosons and fermions [13, 14]. The combination of the two methods allows us to identify an accessible region, where a solid phase can be expected, see Fig. 1. It is important to note, that throughout our calculations we restrict the analysis to a setup with very strong transverse confinement, such that the system behaves one-dimensional with the scattering described by a_{1D} .

We start with the many-body theory describing bosonic particles confined into one-dimension. Introducing the bosonic field operators $\psi^\dagger(x)$ and $\psi(x)$, the Hamiltonian takes the form

$$H_B = \int_{-\infty}^{\infty} dx \psi^\dagger(x) \left[-\frac{\hbar^2}{2m} \Delta + V(x) \right] \psi(x) \quad (1)$$

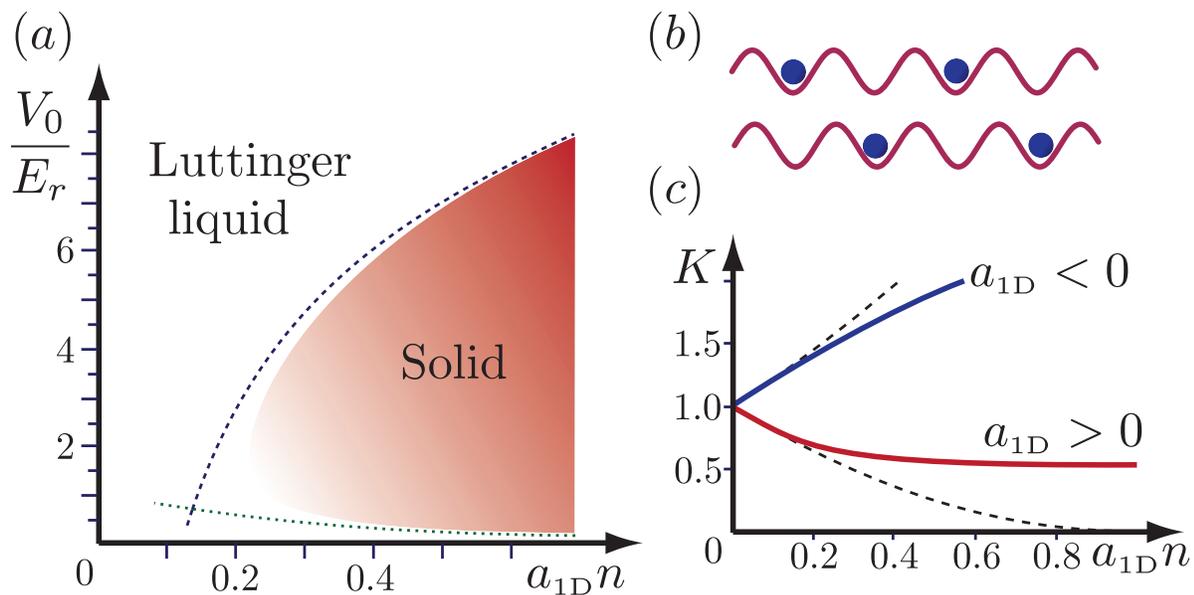


Figure 1. (a) Phase diagram: The solid phase appears at intermediate strength of the optical lattice for $a_{1D}n \gtrsim 0.2$. The blue (dashed) line derives from the transition within the Hubbard model, while the green (dotted) line denotes the estimation of the transition line from the sine-Gordon model. (b) Illustration for the two degenerate ground states with an atom on every second lattice site. (c) Luttinger parameter derived from the exact Bethe ansatz equation. The dashed line denotes the asymptotic behavior $K = (1 - na_{1D})^2$.

$$+ \frac{1}{2} \int_{-\infty}^{\infty} dx dy U_B(x-y) \psi^\dagger(x) \psi^\dagger(y) \psi(y) \psi(x).$$

Here, $V(x) = V_0 \cos^2(xk)$ accounts for the optical lattice along the tubes. The interaction potential between the bosons confined into the lowest state of the transverse trapping potential reduces to $U_B(x) = g_B \delta(x)$ with the coupling strength $g_B = -2\hbar^2/(ma_{1D})$ [9]. Here, the one-dimensional scattering length $a_{1D} = -a_\perp^2/a_s(1 - Ca_s/a_\perp)$ is related to the three-dimensional s -wave scattering length a_s and the transverse confining length a_\perp with $C \approx 1.46$ [9]. The system exhibits a confinement induced resonance at $a_s = a_\perp/C$, where the coupling strength diverges and eventually changes its character from repulsive to attractive.

A physical interpretation of the confinement induced resonances is provided by the following property: The 1D scattering length a_{1D} describes the distance, where the scattering wave function for two particle crosses zero. While for $a_{1D} < 0$, the zero appears in the unphysical region $|x| < 0$, the scattering wave function exhibits a node for $a_{1D} > 0$. This behavior is achieved by an attractive interaction potential $U_B(x)$ giving rise to a bound state. Then, the scattering wave function is orthogonal to the bound state and consequently exhibits a node. However, it is important to note, that the sudden appearance of a bound state is an artifact of the mathematical model Eq. (1), which is valid in low energy sector with the relevant momenta q satisfying the condition $qa_\perp \ll 1$. In the physical system a bound state is always present and its position across

the confinement induced resonance has been studied in detail [15]. As a consequence, the atomic system is for all values of a_{1D} a highly excited metastable state, and losses via three-body recombination reduce the life time of the atomic gas. This indicates that the transition from the regime with repulsive interaction into the Super-Tonks-Girardeau gas is described by a smooth cross-over. Indeed, the Super-Tonks-Girardeau gas exhibits a positive compressibility giving rise a linear sound mode accounting for the low energy excitations of this excited state; the compressibility has recently been determined via Bethe ansatz solutions [16, 17], and quantum Monte Carlo simulations [5], and is in agreement with DMRG calculations [18] and experimental observation [6]. The influence of the states with negative energy is well accounted for by a finite life-time of the system via three-body recombination; these rates have recently been determined for Super-Tonks-Girardeau gas [19].

In the following, we first focus on the limit of a very weak optical lattice $V_0 \ll E_r$. The strongly interacting bosonic system exhibits also in the Super-Tonks Girardeau a regime with positive compressibility [16, 17]. Then, the low energy properties are well described within the hydrodynamics description [20] with the bosonic field operator $\psi(x) \sim \sqrt{n + \partial_x \theta} / \pi$ expressed in terms of the long-wavelength density and phase fields $\theta(x)$ and $\phi(x)$. The fields satisfy the standard commutation relation $[\partial_x \theta(x), \phi(y)] = i\pi \delta(x - y)$. The effective Hamiltonian in absence of an optical lattice reduces to

$$H_0 = \frac{\hbar v_s}{\pi} \int_{-\infty}^{\infty} dx \left[\frac{K}{2} (\partial_x \phi)^2 + \frac{1}{2K} (\partial_x \theta)^2 \right]. \quad (2)$$

The dimensionless Luttinger parameter in the strongly interacting regime $\gamma_B \equiv g_B m / n \hbar^2 \gg 1$ reduces to $K = (1 - na_{1D})^2$ [10]. This expression remains valid in the strongly repulsive situation with $a_s < 0$, as well as in the attractive case $a_s > 0$ for $|na_{1D}| \ll 1$ [16, 17]. In the latter case, the dimensionless parameter $K < 1$ reduces below the non-interacting Fermi limit ($K = 1$). Usually this regime can only be reached for bosonic particles through an interaction potential with a finite range. Here, such a finite range is achieved from the potential $U_B(x)$ by the presence of a bound state and the associated node in the two-particle scattering wave function. The behavior of the Luttinger parameter K for larger 1D scattering lengths can be derived from the exact Bethe Ansatz equation [17] and approaches 1/2 for $na_s \rightarrow \infty$, see Fig. 1.

Within this hydrodynamic description the weak optical lattice is a relevant perturbation at commensurate fillings. Here, we are interested in densities $n = 1/(sa)$ with $a = \pi/k$ the lattice spacing and $s \in \mathbf{N}$ an integer. Then the Hamiltonian accounting for the optical lattice $V_0 \cos(kx)$ takes the form [20, 4]

$$H_{\text{lattice}} = u \int dx \cos(2s\theta) \quad (3)$$

with $u = KV_0/E_r(\tilde{a}/2a)^2$ and \tilde{a} a short distance cut-off (the cut-off is in the range of the interparticle distance $\tilde{a} \approx 1/n$). The low energy description of the interacting bosonic system $H_{\text{eff}} = H_0 + H_{\text{lattice}}$ reduces to the quantum sine-Gordon model. This model is exactly solvable and exhibits a quantum phase transition from a gapless phase with

algebraic decay in the superfluid correlation function $\langle \psi^\dagger(x)\psi(0) \rangle \sim x^{-1/2\tilde{K}}$ as well as in the solid correlation $\langle n(x)n(0) \rangle \sim \cos(2\pi nx)/x^{2\tilde{K}}$, to a gapped and incompressible insulator with long range order $\langle n(x)n(0) \rangle - n^2 \sim \cos(2\pi nx)$. Below the critical value $K < K_s = 2/s^2$, the transition appears for arbitrary strength of the lattice potential, while for a fixed value of u , the transition appears at the universal value $\tilde{K} = 2/s^2$. Here, \tilde{K} denotes the renormalized Luttinger parameter due to the optical lattice; for weak optical lattices it is related to the microscopic value K via the Kosterlitz-Thouless renormalization group flow (see [21] for a review). For a bosonic density equal to the lattice spacing, i.e., $n = k/\pi$ with $s = 1$, the phase transition takes place from the superfluid to the Mott insulating phase and has been previously discussed [4].

In the regime with a positive 1D scattering length $a_{1D} > 0$, it is now possible to access values $K < 1$. This opens the question, whether it is possible to reach the second instability with $s = 2$ and particle density $n = k/2\pi$, i.e., on average there is one bosonic particle distributed over two lattice sites. Then, the phase transition takes place from a Luttinger liquid with algebraic correlations to a crystalline phase. In addition to an excitation gap and the incompressibility, the crystalline phase is characterized by a long range order with a bosonic particle localized in every second lattice site. The ground state breaks the discrete translation invariance of the system and is two-fold degenerate. This property distinguishes the solid phase from the Mott insulator at integer fillings.

The critical value of the Luttinger parameter, where an arbitrary weak optical lattice allows to pin the bosonic crystalline structure reduces to $K_2 = 1/2$. As discussed above, this regime can not be accessed. However, the optical lattice increases the correlations between the bosonic particles. Using the Kosterlitz-Thouless renormalization group flow to lowest order in u for the transition line, i.e., $K = (1+u)/2$, we can expect the phase transition into the solid phase for a finite strength of the optical lattice, see Fig. 1. For values of the optical lattice $V_0 \sim E_r$, the effective low energy theory Eq. (2) is no longer valid, and different approach is required for analyzing the appearance of the solid phase.

In the regime of strong optical lattice $V_0 > E_r$, the suitable approach is to map the system to a Hubbard model. In the strongly correlated regime with $\gamma_B \gg 1$ the conventional derivation of the Hubbard model fails. However, in the following we use the well known Fermi-Bose duality in one dimension [13, 14, 18]: this transformation maps the strongly interacting bosonic system onto a weakly interacting Fermi gas. This transformation remains valid in the presence of an optical lattice, and allows us to derive a Hubbard model for the system.

The duality transformation of the strongly interacting bosons onto weakly interacting fermions has been pioneered in the past [13, 14]. On the two particle level, it requires that the scattering wave function $\psi_B(x)$ between two bosons with the interaction potential U_B , is described by the a fermionic scattering wave function $\psi_F(x)$ with a novel interaction potential U_F via $\psi_B(x) = \text{sgn}(x)\psi_F(x)$ (here, x denotes the relative

coordinate). This property is uniquely determined by the pseudo-potential

$$\langle \psi | U_F | \phi \rangle = \lim_{\epsilon \rightarrow 0^+} \frac{g_F}{4} [\psi'(\epsilon) + \psi'(-\epsilon)]^* [\phi'(\epsilon) + \phi'(-\epsilon)] \quad (4)$$

with $g_F = 2\hbar^2 a_{1D}/m$ the coupling strength and $\psi' = \partial_x \psi$ ($\phi' = \partial_x \phi$) the derivatives of the wave function. It is important to note that the role of the 1D scattering length a_{1D} is reversed in fermionic pseudo-potential U_F as compared to the bosonic one U_B . As a consequence, this mapping allows us to transform a strongly interacting bosonic model onto a weakly interacting Fermi system. Note, that the $\lim_{\epsilon \rightarrow 0^+}$ is required in order to avoid a ultraviolet divergence when applying the interaction potential on the Greens function. This behavior is in analogy to the well known regularization of the pseudo-potential for 3D s -wave scattering.

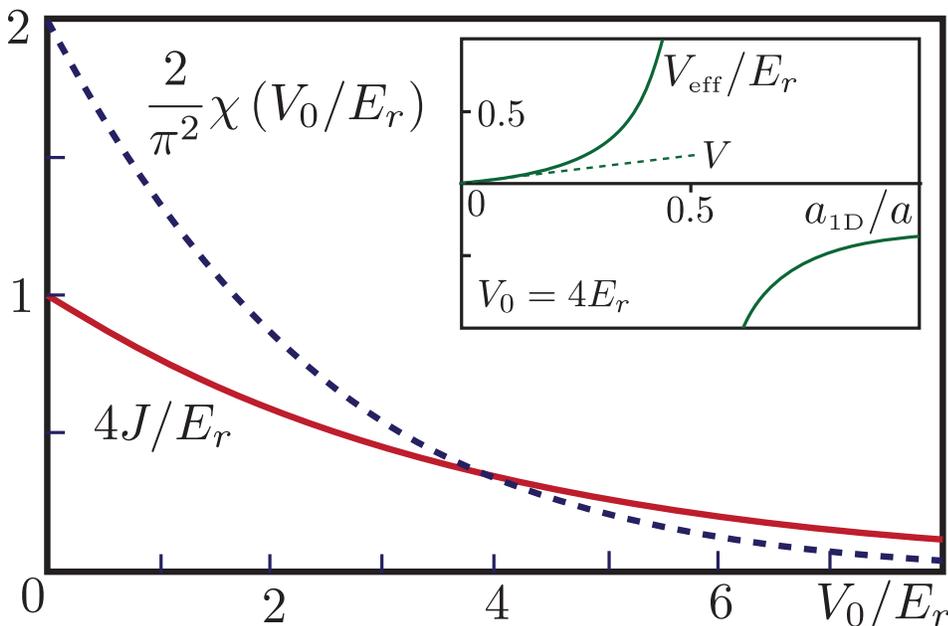


Figure 2. Tunneling amplitude $4J$ (red) and the Wannier function overlap χ (blue) for different strengths of the optical lattice. The inset shows the renormalization of the nearest-neighbor interaction V_{eff} for large 1D scattering lengths accounting for the influence of higher bands and the proper treatment of pseudo-potential U_F the at $V_0 = 4E_r$.

Extending this two-particle analysis to the many-body system, therefore maps the bosonic Hamiltonian in Eq.(1) onto a fermionic model

$$H_F = \int_{-\infty}^{\infty} dx \psi_F^\dagger(x) \left[-\frac{\hbar^2}{2m} \Delta + V(x) \right] \psi_F(x) + \frac{1}{2} \int_{-\infty}^{\infty} dx dy U_F(x-y) \psi_F^\dagger(x) \psi_F^\dagger(y) \psi_F(y) \psi_F(x) \quad (5)$$

with the fermionic field operators ψ_F^\dagger and $\psi_F(x)$. The parameter γ_F characterizing the strength of the interaction in the fermionic model is given by the ratio between the kinetic energy $E_{\text{kin}} = \hbar^2 n^2/m$ and the interaction energy $E_{\text{int}} = n^3 g_F$, i.e. $\gamma_F =$

$E_{\text{int}}/E_{\text{kin}} = 2na_{\text{1D}} = -1/\gamma_{\text{B}}$. The ground state wave function $|g_{\text{F}}\rangle$ of the fermionic problem is related to the ground state of the bosonic problem $|g_{\text{B}}\rangle$,

$$\langle x_1, \dots, x_N | g_{\text{B}} \rangle = A(x_1, \dots, x_N) \langle x_1, \dots, x_N | g_{\text{F}} \rangle \quad (6)$$

with the total asymmetric factor $A(x_1, \dots, x_N)$. For bosons with $a_{\text{1D}} = 0$, this mapping reduces to the well known relationship between impenetrable bosons and fermions in 1D [1].

In the interesting regime with strong interactions between the bosons $|\gamma_{\text{B}}| = |1/\gamma_{\text{F}}| \gg 1$, the fermionic system is weakly interacting and the conventional approach to derive the Hubbard model is valid [22]. For $V_0 > E_r$, we obtain the Hubbard model for spinless fermions

$$H_{\text{HM}} = -J \sum_{\langle ij \rangle} c_i^\dagger c_j + \frac{V}{2} \sum_{\langle ij \rangle} c_i^\dagger c_j^\dagger c_j c_i, \quad (7)$$

with the fermionic creation (annihilation) operator c^\dagger (c_i). In addition, the hopping amplitude J accounts for the single particle band structure $\epsilon_k = -2J \cos ka$, while the fermionic pseudo-potential U_{F} gives rise to a dominant nearest-neighbor interaction

$$V = \frac{2}{\pi^2} E_r \frac{a_{\text{1D}}}{a} \chi \left(\frac{V_0}{E_r} \right). \quad (8)$$

Here, χ is determined by the overlap between the Wannier functions $w(x)$ on neighboring lattice sites,

$$\chi \left(\frac{V}{E_r} \right) = a^3 \int dx |\partial_x w(x)w(x-a) - w(x)\partial_x w(x-a)|^2.$$

The hopping amplitude J as well as the dimensionless overlap χ can be efficiently determined numerically for different strengths of the optical lattice, see Fig. 2. Note, that additional interaction terms are strongly suppressed due to the fast decay of the wannier functions.

At half filling with one particle on every second lattice site, the Hubbard model Eq. (7) exhibits a quantum phase transition from a phase with algebraic correlations between the fermions for $J \gg V$ to a charge density wave with an excitation gap for $V \gg J$. The latter phase corresponds to the interesting crystalline phase. The critical point for the phase transition is determined by the special point at $J = V/2$, where the system becomes $SU(2)$ invariant and maps to the spin-1/2 Heisenberg model. It is this enhanced symmetry, which fixes the transition point to $J = V/2$ even in the one-dimensional situation.

From the behavior of V and J for different strengths of the optical lattice, we can now derive the complete phase diagram, see Fig. 1: for very deep optical lattices the nearest neighbor interaction is strongly suppressed compared to the hopping term, see Fig. 2, and consequently, the ground state is determined by a Luttinger liquid phase with algebraic correlations. Reducing the strength of the optical lattice, the nearest-neighbor interaction increases and a phase transition into the solid phase takes place for sufficiently strong interaction $a_{\text{1D}}n \gtrsim 0.2$. For even weaker optical lattices, the

mapping to the Hubbard model breaks down, and the effective theory is given by the sine-Gordon model. The sine-Gordon model requires a finite strength of the optical lattice for the appearance of the solid phase. Therefore, a second phase transition takes place for decreasing optical lattice, and the system enters again the Luttinger liquid phase, i.e., the system exhibits a remarkable reentrant feature. Consequently, we predict the existence of a solid phase for cold atomic gases at strong interactions $a_{1D}n \gtrsim 0.2$ and intermediate strengths of the optical lattices $V \approx 3E_r$.

Finally, we have to verify the validity of the Hubbard model in the interesting regime with $na_{1D} \gtrsim 0.2$. The derivation of the Hubbard model involves two approximations: (i) first, we restrict the analysis onto the lowest Bloch band, i.e., we introduce a high energy cut-off $\Lambda \gtrsim a$ determined by the lattice spacing. (ii) Second, the interaction potential U_F is treated without the proper regularization. The influence of these two-approximation has recently been studied in detail for the derivation of the Hubbard model in a three-dimensional optical lattice [23]. Here, the situation is equivalent and the main results can be directly carried over. It follows, that the Hubbard model is correct for weak interactions $a_{1D} \ll a$, while in the interesting parameter range $a_{1D}n \sim 0.2$ corrections from higher bands and the proper treatment of the interaction potential appear. The main influence is a renormalization of the nearest neighbor interaction strength, which takes the form $V_{\text{eff}} = V/(1 + \eta V/E_r)$ [24]. Here, $\eta = -E_r/2J$ derives from the duality mapping between the Bosons and Fermions: in the limit $a_{1D}/a \rightarrow \infty$ the system has to reproduce the scattering of non-interacting bosons. Therefore, we find that the influence of higher bands and the proper treatment of the interaction potential increases the strength of the nearest-neighbor interaction, see Fig. 2. Therefore, we expect that the solid phase appears even for weaker interactions than shown in Fig. 1.

Finally, it is important to note, that the behavior of losses by crossing the confinement induces resonance are not yet well understood. While the Super-Tonks Girardeau gas is exactly solvable by Bethe ansatz equation and consequently stable, one can expect that for increasing 1D scattering length, additional terms to the Hamiltonian, e.g., corrections from higher transverse states and additional non-universal three-body interactions, break the integrability of the model and provide a decay rate and eventually an instability of the Super-Tonks-Girardeau gas towards the formation of bound states; such a behavior was observed within the variational Monte Carlo simulations [5]. This implies a finite lifetime for the realization of the experiments and suggests that the search for the solid phase should be performed for intermediate interaction strengths $na_{1D} \sim 0.4$. In addition, it is important to point out, that in the presence of an optical lattice with $V \gtrsim 3$, three-body losses are suppressed as the probability to find three particles in a single well of the lattice is strongly suppressed. Furthermore, the opening of a Band structure quenches many decay channels as discussed in the context of repulsively bound pairs [25]. Consequently, one can expect that for increasing interactions the losses are increased, but in turn can again be suppressed by ramping up the optical lattice.

The experimental setup required for the observation of the solid phase can be achieved by the combination of strong transverse confining by an optical lattice with

a Feshbach resonance to tune the strength of the s -wave scattering length. Such a setup has recently been realized for the observation of correlations beyond the Tonks-Girardeau regime [6]. An additional weak optical lattice along the tubes then opens the path to the experimental search of the solid phase. However, the experimental realization avoiding losses is most conveniently achieved using a double well lattice as experimentally realized [26]. Then, the system can be prepared in a conventional Mott insulating phase for $a_{1D} < 0$ with a single particle per lattice site. For a strong optical lattice, it is possible to cross the confinement induced resonance without losses. Then, in a second step the lattice is lowered and each site split into a double well. Eventually, one ends up with an optical lattice with 1/2 of lattice spacing of the starting lattice and the required particle density with one particle shared on two lattice sites. Using such an adiabatic ramping scheme circumvents regions in the phase diagram, where strong losses are expected. It is important to note, that the solid phase is incompressible with an excitation gap. In analogy to the Mott insulating phase [22], the solid phase will extend over a large fraction of the parabolic trap, with the particle density pinned to a commensurate value.

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