Pairing, crystallization and string correlations of mass-imbalanced atomic mixtures in one-dimensional optical lattices

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Abstract – We numerically determine the very rich phase diagram of mass-imbalanced binary mixtures of hardcore bosons (or equivalently — fermions, or hardcore Bose/Fermi mixtures) loaded in one-dimensional optical lattices. Focusing on commensurate fillings away from half-filling, we find a strong asymmetry between attractive and repulsive interactions. Attraction is found to always lead to pairing, associated with a spin gap, and to pair crystallization for very strong mass imbalance. In the repulsive case the two atomic components remain instead fully gapless over a large parameter range; only a very strong mass imbalance leadsto the opening of a spin gap. The spin-gap phase is the precursor of a crystalline phase occurring for an even stronger mass imbalance. The fundamental asymmetry of the phase diagram is at odds with recent theoretical predictions, and can be tested directly via time-of-flight experiments on trapped cold atoms.

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Introduction. – One-dimensional quantum liquids occupy a special place in the context of quantum many-body systems: indeed interactions of any strength lead to quantum fluctuations as strong as to discard Bose condensation for bosons and the Fermi liquid picture for fermions down to zero temperature. For sufficiently weak interactions a new unifying paradigm of the so-called Tomonaga-Luttinger liquids (TLL) emerges [1], characterized by the fact that all elementary excitations are gapless, and both diagonal and off-diagonal correlations decay algebraically with the distance. Recent advances in the trapping of ultracold atoms in optical lattices allow to realize one-dimensional quantum liquids in a highly flexible way, with the possibility of fully controlling the statistics and the interaction strength [2]. A series of recent experiments has demonstrated the physics of one-dimensional Bose gases with strong interactions up to the hardcore (or Tonks-Girardeau) limit [3]. A special role in the context of one-dimensional systems is played by binary mixtures, either bosonic, fermionic, or Bose-Fermi ones, for which TLL theory predicts the separation of spin and charge modes [1]. In the case of particles with equal masses and repulsive short-range interactions, both charge and spin sectors can be gapless, and one recovers an effective picture of two decoupled TLLs. Such a picture can be made unstable via several mechanisms: via Mott localization in the presence of an underlying lattice and for integer total filling; via localization into a true (long-range–ordered) crystal (TC) in the presence of a strong off-site repulsion; via phase separation; or via the formation of bound states (e.g., Cooper pairs for attractive interactions) leading to the appearance of a spin gap.

Here we show that the TLL picture undergoes a complex series of instabilities in binary mixtures with mass imbalance between the two species.

Model Hamiltonian. – We focus here on quantum particles on a lattice with intraspecies hardcore repulsion and on-site interspecies interactions, describing at the same time spin-1/2 fermions, spin-1/2 hardcore bosons, and mixtures of hardcore bosons and spinless fermions.
Our main findings are the following: 1) in the attractive regime, the latter figure refers to the case in which the system displays a PSF phase, characterized by quasi-condensation of bound a-b pairs, giving rise to an algebraic decay of the pairing correlation function \[ G_{ab}(r) = \langle a_i^\dagger b_{i+a+r} \rangle \sim r^{-1/K_p}; \] density-density correlations are also decaying algebraically as
\[ C_{\rho}(r) = \langle n_i n_{i+r} \rangle - \langle n_i \rangle \langle n_{i+r} \rangle \approx -K_p \pi^2 r^2 \cos(2\pi n r) / r K_p + K_p; \] here, \( n_i = n_{i+a} + n_{i+b} \), and \( K_p \) is the charge TLL parameter.

For equal masses, \( K_p > 1 \) for all \( u < 0 \), so that the dominant correlations are the pairing ones. Moreover, \( K_p = 0 \) due to the presence of the spin gap (see below). We extract the Luttinger exponent from the slope of the density structure factor at \( q \to 0 \), \( S_p(q) = \sum_\mathbf{K} \exp(\mathrm{i} q \mathbf{r}) C_p(r) \approx K_p / q / \pi \), and we find that mass imbalance leads to a reduction of \( K_p \), consistently with what observed for other fillings in ref. [10]. For large mass imbalance, \( K_p \) becomes smaller than unity (fig. 2); this corresponds to the loss of quasi-condensation, in favor of a quasi-solid phase (or charge density wave, CDW), with dominant density correlations. This phase is the precursor of a quantum phase transition.
to a TC of pairs —phase TC2 of fig. 1— with the onset of long-range density order at wave vector \( Q = \pm 2\pi n \). We determine the extent of the TC phase via QMC by determining the mass imbalance at which \( S_\rho(\Omega) \) starts diverging linearly with system size; and by DMRG detecting the onset of the exponential decrease of \( G_{ab} \) and \( C_\rho \), marking the opening of a charge gap (fig. 2). The TC instability is well understood coming from the Falicov-Kimball (FK) limit, \( J_b = 0 \). In this limit, which reduces to a 1D lattice gas in a static potential, we find that the ground state corresponds to the TC of pairs for all values \( u < 0 \). The gap \( \Delta_k \) to the formation of kink-antikink pairs in the TC is found to be a non-monotonic function of \( |u| \), displaying an intermediate maximum. We observe that, for small \( |u| \), the boundary of the crystalline region follows closely the locus at which the gap \( \Delta_k \) equals \( J_b \), and it has a re-entrant shape mimicking the non-monotonic behavior of the gap as a function of \( u \). This suggests that the quantum melting transition corresponds to a condensation of kink-antikink pairs in the ground state.

Repulsive regime. — The repulsive side of the phase diagram is more complex. Combining bosonization with renormalization group calculations up to two loops, refs. [5,6] conclude that a spin gap should open for any infinitesimal mass imbalance as \( \Delta_s \approx \Lambda \exp(-A'/|J_a - J_b|) \) for \( J_b \lesssim J_a, J_b \). On the contrary, ref. [7], also based upon bosonization, concludes that the spin gap is absent in the repulsive case. All our numerical findings point toward the persistence of a fully gapless TLL behavior for both the charge and spin sector over a dominant portion of the repulsive phase diagram. Our conclusion is based on a number of crossed evidences. First of all, we observe that the one-body correlation functions \( G_{\sigma}(r) = \langle a_{i}^\dagger a_{i+r} \rangle \) and \( G_{\rho}(r) = \langle \tilde{b}_{i}^\dagger \tilde{b}_{i+r} \rangle \) can be very well fitted with the simple power-law form \( G_{\sigma}(r) = A_{\sigma}(d)|r/L|^{-1/(2K_{\eta}(\sigma))} \), where \( d(r) = L|\sin(\pi r/L)|/\pi \) is the conformal distance (see fig. 3(a)). In particular we find that, for weak and moderate repulsions, \( K_{\eta}(\rho) > 0.5 \) which implies that the momentum distribution \( n_{\rho}(b) = \sum_{r} \exp(iqr)G_{\rho}(b)(r) \) displays a quasi-condensation divergent peak at \( q = 0 \), to be detected in time-of-flight experiments (see below). Moreover we exploit the fact that an explicit counting of the number of gapless degrees of freedom in the system comes from the central charge \( c \) of the conformal field theory corresponding to our model of interest. This quantity can be directly extracted via DMRG, using the fundamental result that the entanglement entropy (EE) of a boundary block of the system grows with the size \( l \) of the block [18] as

\[
S_l = -\text{Tr}(\rho_l \log_2 \rho_l) \approx \frac{c}{6} \log_2[d(l/L)] + C(1/l) + \text{const},
\]

where \( \rho_l \) is the reduced density matrix of the boundary block, and open boundary conditions are employed. Figure 3(b) shows that the scaling of the EE is fully consistent with \( c = 2 \) in the repulsive regime, providing further evidence for the fact that the TLL has two gapless components even for a significant mass imbalance.

Finally, using QMC we gain further insight into the gapless phase by investigating the spin-spin correlation function \( C_{\sigma}(\eta)(r) = \langle S_i^\sigma S_{i+r}^\sigma \rangle \approx -K_{\sigma} \exp(2\pi \eta r)/\pi \), where \( S_i^\sigma = (n_{i,a} - n_{i,b}) \), and \( K_{\sigma} \) is the spin TLL parameter; in the absence of a spin gap, \( K_{\sigma} \geq 1 \). We extract the Luttinger exponent from the low-\( q \) behavior of the spin structure factor, \( S_a(q) \approx K_{\eta}q/\pi \), giving the finite-size estimate \( K_{\eta}(L) = ([L/2]S_a(2\pi/L; L) + (L/4)S_a(4\pi/L; L))/2 \). At the SU(2) invariant point \( j = 1 \), \( K_{\eta}(L) \) is known to obey the Kosterlitz-Thouless (KT) critical scaling \( K_{\eta}(L) \approx 1 + [a \log(L/L_0)]^{-1} \), which implies that the quantity \( \kappa_{\eta}(L) = [K_{\eta}(L) - 1]^{-1} \) scales linearly with \( \log(L) \). Quite remarkably, this scaling law remains
valid over a broad range of \( j < 1 \) values, and even for strong inter-species coupling, as shown in fig. 3(c). This means that, even if the SU(2) symmetry is broken in the Hamiltonian, it appears to be restored in the means that, even if the strong inter-species coupling, as shown in fig. 3(c). This scaling of valid over a broad range of

\[
O_x(r) = - \langle S_x^z e^{i \sigma \sum_{j=i+1}^{j=i+r} S_j^z} S_{i+r}^z \rangle. \tag{5}
\]

As shown in fig. 4(c), (d), string correlations are significantly enhanced when entering the SG phase: indeed the string structure factor, \( O_{x,int} = \sum_{r} O_x(r) \), shows a more pronounced divergence with system size, which signals the slower decay of \( O_x(r) \). As shown in appendix A, in the presence of spin-charge separation the dominant decay of the string correlations is governed solely by the \( K_p \) exponent, \( O_x(r) \sim r^{-K_p} \); therefore \( K_p \) controls the divergence of \( O_{x,int} \sim L^{-K_p} \), and in fig. 4(d) we observe that the \( 1 - K_p \) exponent (extracted from the low-\( q \) behavior of \( S_\rho(q) \)) is significantly enhanced in the SG phase. Given that both the spin and charge structure factor exhibit a peak whose divergence with system size is hindered by the slow size-scaling of the divergence exponent \( 1 - K_s - K_p \), we find that the string correlations best characterize the “fluid” magnetic order of the SG phase.

The bound trimers appearing in the SG phase undergo crystallization — phase TC1 in fig. 1 — for moderate repulsion and extreme mass imbalance. The TC1 phase is analogous to the one discussed in ref. [20]. This phase is marked by a suppression of \( C_{nn,b} \) which attains its absolute minimum \( C_{nn,b} = 1 - 2n \) for \( j \to 0 \), due to the suppression of the weight of configurations with contiguous trimers. The resulting non-monotonic behavior of \( C_{nn,b} \) as a function of \( j \), shown in fig. 4(b), provides further evidence that the SG phase is a liquid of pre-formed trimers — the enhancement of \( C_{nn,b} \) in that phase is due to trimer binding, while the suppression in the TC1 phase is due to crystal ordering of the trimers.

**Discussion of the theoretical results and relevance for experiments.** — The theoretical findings discussed in this work can be compared with a series of recent theoretical results based on complementary analytical and numerical approaches in both the attractive and repulsive regimes. In the former case, the re-entrant shape of the CDW-PSF transition is in full agreement with both analytical predictions based on a combination of weak- and strong-coupling arguments [5] and DMRG calculations [10]. The crystalline instability TC2, related with the
opening of a charge gap in the spectrum, was not predicted in previous studies, since none of them focused on the commensurate case away from half-filling. Its appearance can be explained in terms of a TLL theory for a liquid of bound dimers with effective finite-range repulsion, undergoing a crystallization transition when the effective dimer hopping is overcome by the repulsion [1]; as such the TC2 phase is a generic feature for commensurate fillings.

In the $U > 0$ regime, the picture is more intricate. While the PS phase boundary is in perfect agreement with the stability analysis performed in ref. [22] and perturbation theory results [10], a consistent portion of the phase diagram contrasts with previous analytical findings. In particular, the SG phase was not predicted in ref. [7], whereas in refs. [5,6] the SG-2TLL phase transition was located exactly on the $j = 1$ line, making an infinitesimal mass imbalance sufficient to open a gap. Our results, based on non-perturbative, numerically exact methods and complemented with finite-size scaling, indicate that the SG phase emerges in the repulsive domain only for relatively large mass imbalances $j \lesssim 0.3$. While a very small gap may indeed be numerically hard to figure out, the complementary study of various observables such as entanglement properties and the spin TLL parameter strongly point towards an extended, gapless region close to $j = 1$. Future works, combining more sophisticated renormalization group approaches which allow to go beyond the one-loop $g$-ology employed in refs. [5,6] such as, e.g., functional renormalization group, may indeed shed further light on this issue. Finally, the occurrence of a second crystalline instability, TC1, and the enhancement of string correlations in the SG phase represent new, experimentally relevant results, as discussed below.

In the context of many-body physics in ultracold gases, our aforementioned theoretical findings have immediate consequences for current experiments on one-dimensional mixtures of mass-imbalanced cold atoms. Such experiments can probe both attractive and repulsive interactions, within the same experimental conditions, via the use of Feshbach resonances [14]. Our phase diagram reveals a fundamental asymmetry between the attractive and the repulsive case for weak and moderate mass imbalance, with the formation of bound pairs on the attractive side and the absence of spin gap on the repulsive one. This asymmetry is very well seen in time-of-flight experiments probing the momentum distributions $n_{\alpha}(k)$, $n_{\nu}(k)$, which are very broad on the attractive side, while they exhibit sharp quasi-condensation peaks on the repulsive side—as shown in fig. 5. This asymmetry can be used as strong evidence of pairing on the attractive side. A partial symmetry is recovered only for strong mass imbalance, with the opening of a spin gap in the repulsive case, and the occurrence of a crystalline phase for both signs of the interaction. This is also well captured by the momentum distributions, showing this time a suppression of the quasi-condensation peaks on the repulsive side due to the appearance of the SG phase and of the crystalline phase. Finally the availability of high-resolution in situ imaging [23] sensitive to the spin [24] allows to detect the formation of bound trimers and the enhancement of string correlations characterizing the SG phase.

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### Appendix A: decay of string correlations from bosonization

In the following, we will study the dependence on the TLL parameters of the generalized string correlation function:

\[ O_{\beta}^r(r) = \left\langle \tilde{S}_i^z \exp \sum_{r<\ell<r} \tilde{S}_k^z \tilde{S}_{\ell+r}^z \right\rangle \tag{A.1} \]

where we have defined $\tilde{S}_i^z = n_{a-b}^{\alpha} - n_{b-a}^{\beta}$. After applying standard bosonization identities to $a, b$ operators by introducing the bosonic $\phi, \phi_0$ fields [1], one can define effective spin and charge fields as $\phi_{\sigma, \rho} = (\phi_{a} \pm \phi_{b})/\sqrt{2}$ such that

\[ \tilde{S}_i^z = \frac{\partial_{\tau} \phi_{\sigma}(r)}{\sqrt{\pi}} + \gamma V^\pm_{\sigma}(r) V^\pm_{\rho}(r) + \ldots \tag{A.2} \]

where $V^\pm_{\sigma, \rho}(r) = e^{\pm i\alpha \phi_{\sigma, \rho}(r)}$ are vertex operators related to the charge and spin fields and $\gamma$ is a constant; additional contributions with higher scaling dimension play no significant role in the remaining, and can thus be neglected. The non-local contribution in eq. (A.1) can be
we observe that these quantities grow more slowly than $\log(L)$ over the entire SG phase for all the system sizes we considered (up to $L = 96$ —see fig. 6). To observe their divergence with the system size, one might need exceedingly big system sizes, both for simulations and for experiments. Therefore, string correlations stand as a unique tool to characterize the correlations in the SG phase.

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