Quantum degenerate Bose-Fermi mixtures on 1-D optical lattices

Pinaki Sengupta\(^1\) and Leonid P. Pryadko\(^2\)

\(^1\)Department of Physics & Astronomy, University of Southern California, Los Angeles, California, 90089, USA
\(^2\)Department of Physics, University of California, Riverside, California 92521, USA

(Dated: March 23, 2022)

We combine model mapping, exact spectral bounds, and a quantum Monte Carlo method to study the ground state phases of a mixture of ultracold bosons and spin-polarized fermions in a one-dimensional optical lattice. The exact boundary of the boson-demixing transition is obtained from the Bethe Ansatz solution of the standard Hubbard model. We prove that along a symmetry plane in the parameter space, the boson-fermion mixed phase is stable at all densities. This phase is a two-component Luttinger liquid for weak couplings or for incommensurate total density, otherwise it has a charge gap but retains a gapless mode of mixture composition fluctuations. The static density correlations are studied in these two limits and shown to have markedly different features.

Recent advances in experiments with cold atoms in magneto-optical traps have led to a series of exciting results. One area of emerging interest is the study of degenerate mixtures of bosons and fermions in various trap and lattice geometries. While the original motivation for such studies was the sympathetic cooling of the fermions via interactions with bosons, such systems provide a unique opportunity to study experimentally quantum phases and associated transitions in a system of mixed quantum statistics, which are rare in condensed matter systems. The absence of defects and impurities as well as the ability to tune the interactions between the particles will enable the exploration of various quantum many-body phenomena. Stable boson-fermion mixtures have been realized with \(^6\)Li-\(^7\)Li, \(^23\)Na-\(^6\)Li, \(^87\)Rb-\(^40\)K and \(^6\)Li-\(^87\)Rb. On the theoretical front, the ground state properties of boson-fermion mixtures – in the continuum and on a lattice – have been investigated using mean field theories and bosonization, Bethe ansatz (BA) and numerical simulation of small systems.

In this work we study the nature of the ground state of a boson-fermion mixture on a 1D optical lattice, concentrating specifically on the special case of equal hopping coefficients for bosons and fermions, \(t_B = t_F\) in Eq. (1). We construct mappings to several known models in appropriate limits and use known analytic results from these to supplement our numerical results. In addition to exploring the unique quantum demixing transitions, we have investigated the nature of the ground state in the homogeneous (mixed) phase at different interaction strengths and densities. Our results are summarized in Fig. 1. At large \(\mu_B\) (\(\mu_F\)), the ground state is purely fermionic (bosonic) with \(n_B(n_F) = 0\), whereas a thermodynamically stable mixed phase (B-F) with \(n_B, n_F > 0\) exists over a finite range of parameters around \(\mu_B \approx \mu_F\). The exact analytic boundary between the pure fermion F-F and B-F phases obtained from the solution of Eqs. (2) and (3) is also shown. The agreement between the two approaches is excellent in the weak coupling limit, whereas the B-F phase is overestimated in the numerical data at strong coupling. The extent of the mixed phase gets smaller at low densities, especially at large \(U\) and \(V\). For the case \(U = V\), we show that even at very strong coupling, there is no direct transition between pure bosonic and fermionic phases. A mixed phase is always stable, contrary to the mean field results. At weak couplings, the mixed phase is dominant and one needs large differences in the chemical potentials for the two components to observe demixing, consistent with the bosonization results.

A mixture of interacting bosons and spinless fermions in an optical lattice is well described by the one-band Bose-Fermi Hubbard model (BFHM),

\[
H = \sum_{i=1}^{N} \left[ -t_B (b_{i+1}^\dagger b_i + h.c.) - t_F (f_{i+1}^\dagger f_i + h.c.) - U \sum_{\alpha=B,F} n_{i\alpha}^B (n_{i\alpha}^B - 1) + V n_{i\alpha}^B n_{i\alpha}^F - \sum_{\alpha=B,F} \mu_{\alpha} n_{i\alpha}^\alpha \right]. \tag{1}
\]
Here, $U$ and $V$ parametrize the on-site boson-boson and boson-fermion interactions; we assume $U, V > 0$. The chemical potentials $\mu_B$ and $\mu_F$ couple to the densities of the individual components, $n_B$ and $n_F$. In the experiments, there is also a trapping potential that confines the particles to a certain region of the lattice. As a simplification, we have ignored such a confining potential. The present description is applicable in the central part of a system with a shallow trapping potential. In the discussion of the numerical results, we assume $t_B = t_F = t = 1$ which sets the energy scale. All other parameters are (implicitly) expressed in terms of $t$.

An insight into the model \cite{1} can be gained by studying the limiting cases. For $V = 0$, the boson and fermion sectors are decoupled. The fermions are non-interacting; they fill a band with momenta $|k| < k_F = \pi n_F$. The fermion sector has a commensurate density and an associated band gap for $|\mu_F| > 2t_F$; otherwise it is gapless. The boson sector is described by the Bose-Hubbard model\cite{15}. At incommensurate densities $n_B$, the ground state is a gapless superfluid (SF) for any $U > 0$; at commensurate densities, there is an SF to Mott insulator transition at $U \approx 3.5t_B$\cite{16}. Finally, the boson sector is trivially an insulator at zero density, $n_B = 0$, at $\mu_B < -2t_B$.

In the hard-core limit $U \to \infty$, the bosons can be mapped to a second “flavor” of fermions. Then, for $t_B = t_F$, the resulting model can be rewritten as the usual Hubbard model, where the fermion flavor serves as the (pseudo)spin index. The effective external magnetic field is $\tilde{h} = \mu_F - \mu_B$, the Hubbard coupling constant is $\tilde{U} \equiv U$, the hopping $\tilde{t} = t_B$, and the chemical potential $\tilde{\mu} = (\mu_B + \mu_F)/2$ couples to the density $n = n_B + n_F$. This model is exactly solvable\cite{18}. Most importantly, there is no charge or spin gap away from the commensurate density, $0 < n < 1$. Given the density $n$, the Hubbard fermions reach full spin polarization at the field\cite{19}

$$\tilde{h}_c(n, \tilde{U}) = \frac{\tilde{U}}{\pi} \int_0^{\pi n} dk \frac{\cos k - \cos \pi n}{(\tilde{U}/4\tilde{t})^2 + \sin^2 k}. \quad (2)$$

At this point one of the Luttinger components disappears, we are left with only one kind of the fermions. The corresponding value of the chemical potentials

$$\mu_F = -2\tilde{t}\cos \pi n, \quad \tilde{\mu} = \mu_F + \tilde{h}_c(n, \tilde{U})/2. \quad (3)$$

The system acquires a gap at the commensurate density, $n = 0.1$. The corresponding values of the critical magnetic field are $\tilde{h}(0, \tilde{U}) = 0$, $\tilde{h}(1, \tilde{U}) = (\tilde{U}^2 + 16\tilde{t}^2)^{1/2} - \tilde{U}$.

For the original BFHM (1), the field $\tilde{h} = \mp \tilde{h}_c(n, V)$ would correspond to the demixing transition, where the density of either fermions or bosons turns to zero. We also note that in the latter case, $n_B = 0$, the boson repulsion constant $U$ is irrelevant. Therefore, as long as the transition is continuous (as expected for $V \lesssim 2U$), the boson demixing transition, $n_B = 0$, is expected at $\mu_B = \mu_F - \tilde{h}_c(n, V)$. The corresponding curve on the $\mu_F$-$\mu_B$ diagram \cite{3} is given parametrically in terms of $n = n_F$ by Eqs. (2), (3).

To understand the fermion demixing transition at $n_F = 0$, notice that in the “symmetric” case, $t_B = t_F$, $U = V$, and $\mu_B = \mu_F$, the Hamiltonian (1) commutes with the superoperator, $Q = \sum f_i^\dagger b_i$, and its conjugate, $Q^\dagger$. A ground state wavefunction (WF) with $N$ bosons and no fermions, $\Psi_B^{(0)}$ can be mapped to an eigenstate with $N - 1$ bosons and $N_F = 1$, $\Psi_B^{(1)} \equiv N^{-1/2} Q \Psi_B^{(0)}$. The normalization was found using the anticommutator, $\{Q, Q^\dagger\} = \tilde{N}_B + \tilde{N}_F$. While $\Psi_B^{(1)}$ may not be the ground state, the degeneracy implies that adding fermions is definitely favorable for $\mu_F > \mu_B$. Combined with the local instability of the fermion phase at the line Eqs. (2), (3), this gives a proof of thermodynamical stability of the mixed phase just above the symmetry line.

The same argument could also work the other way, as long as the ground state with $N_F = 1$ fermion, $\Psi_B^{(0)}$, contains a fully symmetrical component, so that the corresponding bosonic WF $Q\Psi_B^{(0)}$ is not. This happens at strong coupling (certainly at $n = 1$ discussed below), as well as at small densities, as can be seen by analyzing the energy of the continuum BA solution\cite{12}(a). In these two cases, the fermion demixing transition is indeed located precisely at the line $\mu_F = \mu_B$ (solid diagonal in Fig. 1).

Finally, for strong but non-infinite couplings, $U, V \gg t_B, t_F$, the low-energy physics of the system is described by the effective Hamiltonian which at $t_B = t_F$ is analogous to the anisotropic $t$-$J$-$V$ or extended Hubbard model in external magnetic field\cite{20, 21}. The model has an easy-axis anisotropy for $V > 2U$, which implies a spin gap disappears via a first-order “spin-flop” transition (the discontinuous demixing transition is accompanied by phase separation). At the commensurate total filling, $\alpha = 1$, the system acquires a charge gap and is further reduced to the exactly-solvable XXX spin-chain with the parameters $J^z = 2(t_B^2 + t_F^2)/V - t_B^2/U$, $J^z = -2t_B t_F/V$, in an additional magnetic field so that $n_B = 1$ at the symmetry line discussed above. The operator $Q$ under this mapping becomes a zero-$k$ spin-wave creation operator. Again, there is no spin gap for $|J^z| > J^z$ (the BF mixture is a single-component Luttinger liquid), while for $|J^z| < J^z$ the system is fully gapped and the corresponding fermion demixing transition is first-order.

We have used the Stochastic Series expansion (SSE) quantum Monte Carlo (QMC) method\cite{22} to simulate the BFHM in the grand-canonical ensemble on chains of length $L = 8 - 128$. Ground state results are obtained by taking large enough values of the inverse temperature, $\beta$, where $\beta = 2L$ was sufficient. To characterize different phases, we have studied the charge (superfluid) stiffness of the fermions (bosons), $\rho_F^\alpha = \langle W_F^\alpha \rangle/2\beta L\tilde{t}$, $\alpha = F, B$, and the static susceptibility for the density correlations,

$$\chi^\alpha(q) = \frac{1}{L} \sum e^{i q \cdot (r_j - r_i)} \int_0^\beta d\tau \langle n^\alpha_j(\tau) n^\alpha_i(0) \rangle. \quad (4)$$
We start the discussion of the numerical results by identifying the range of parameters which result in a thermodynamically stable homogeneous mixed phase. We consider fixed (and equal) values of $U$ and $V$ and vary $\mu_F$ and $\mu_B$. We have analyzed two cases in detail—one in the weak coupling regime ($U = V = 2$), and the other in the strong coupling regime ($U = V = 10$). Since SSE is formulated in the grand canonical ensemble, one never observes a ground state with spatially separated domains. Instead, depending on the parameters of the Hamiltonian, the ground state will be in one of three phases discussed above—B-B, F-F, or B-F. Results for $L = 32-128$ are shown in Fig. 2, where the bosonic and fermionic densities are plotted as a function of varying $\mu_F$ at a fixed value of $\mu_B$. The upper(lower) panel shows the results for the weak(strong) coupling regime. With increasing $\mu_F$ (at fixed $\mu_B$), the ground state evolves continuously from B-B to B-F and finally to F-F phase. The data (along with those for other values of $\mu_B$) are combined to obtain the phase diagram Fig. 1. Experimentally, the transitions can be observed in a large system with fixed particle numbers if the trapping potentials seen by the two species of particles vary differently. For example, one can have a shallow trapping potential for the bosons and a faster varying one for the fermions. In that case, there will be purely fermionic domains at the edges and a uniform mixture at the center of the trap. Our data show the transitions to be continuous, in contrast to the mean field results, where the B-F to F-F transition is found to be discontinuous.

Next, we investigate the properties of the mixed phase in detail across the parameter range explored in Fig. 2. We start with the charge (phase) stiffness of the fermions (bosons)—a finite value implies a gapless spectrum for, and consequently, a Luttinger liquid character of, the fermionic (bosonic) sector. The results are shown in Fig. 3. At weak couplings, $\rho_B^S$ ($\rho_F^S$) is finite for any non-zero $n_B$ ($n_F$) (except $\rho_F^S = 0$ for $n_F = 1$ as the fermions form a filled band). In particular both $\rho_B^S$ and $\rho_F^S$ are finite in the mixed phase—al low as well as high densities (or equivalently, bare chemical potentials). Hence the mixed phase in the weak coupling limit is described by a two-component Luttinger liquid at all densities.

In the strong coupling limit, the behavior is markedly different at low and high densities. At low densities ($n_F + n_B < 1$) the stiffnesses are finite in the mixed phase, implying a Luttinger liquid character of the ground state. At large $\mu_B/F$, the system is always at the commensurate filling, $n_F + n_B = 1$. In the pure phases, the stiffnesses $\rho_B^S$ and $\rho_F^S$ vanish with the corresponding densities, $n_B$ and $n_F$. Also, $\rho_B^S$ vanishes in the B-B phase in the thermodynamic limit since the bosons are in the Mott insulating phase at this $U$. In the mixed phase, the individual stiffnesses have small, but finite, values. This suggests the existence of a gapless mode, in contrast to previous studies. The stiffness data and density correlations (shown below) support the mapping to an equivalent XXZ chain, which at $U = V$ further reduces to the gapless XY chain. The gapless mode consists of the $k = 0$ spin-wave created by the superoperator $Q$ and corresponds to the “pairing superfluidity” in the BFHM explored in detail in Ref. [17].

To further characterize the nature of the mixed phase, we have studied the static charge susceptibility [Fig. 4] for the two components. Once again we find the results to be markedly different in the strong and weak coupling regimes. Fig. 4(a) shows the results of increasing inter-species interaction on the static charge susceptibility in the weak coupling regime. In the absence of boson-fermion interaction, $\chi_F(q)$ shows the familiar peak at twice the Fermi momentum ($2k_F$). As the inter-species repulsion is increased, the peak at $2k_F$ decreases and
develops a peak at twice the bosonic "fermi momentum", metrically opposite. The boson density correlation de-

commensurate filling, $n$. (b) The susceptibilities in the strong coupling limit at $V$ completely destroyed for $n_F = n_B = 1$. Numerical data suggest a gapless mode for the ground state and strong coupling mapping to the XXZ model predict that at $U = V$ this gapless mode consists of a $k = 0$ spin-wave. In the BFHM, this corresponds to fluctuations of the mixture composition $17$. We have also explored the effects of boson-fermion interaction on the density correlations of the two components and find that the results are dramatically different in the weak and strong coupling limits. These signatures should be readily observable in experiments, and, if confirmed, would indicate the emergence of novel many-body phases in these systems.

We are grateful to L. Pollet, M. Troyer, and C. Varma for useful discussions and for sharing their results before publication (LP and MT). PS was supported by the DOE under grant DE-FG02-05ER46240. Simulations were carried out in part at the HPC Center at USC.

FIG. 4: (a) The static charge susceptibility for the fermions, $\chi_F(q)$, and bosons, $\chi_B(q)$, with varying inter-species interaction strength, $V$. The peak at the Fermi wave vector is almost completely destroyed for $V = 4$. The densities of the two species are $n_B \approx 0.17$ and $n_F \approx 0.24$. The open (filled) symbols and dashed (solid) lines represent the bosonic (fermionic) data. (b) The susceptibilities in the strong coupling limit at commensurate filling, $n_B \approx 0.67$ and $n_F \approx 0.33$.

more weight is transferred to lower momenta. Finally at large values of $V$, the peak at the Fermi momentum is almost completely washed out implying that in this regime the fermions no longer retain an independent character. On the other hand, in the strong coupling limit, at commensurate filling ($n_B + n_F = 1$), the results are diametrically opposite. The boson density correlation develops a peak at twice the bosonic “fermi momentum”, $2k_B = 2\pi n_B$. In this limit of large $U$, the bosons behave effectively as hard-core bosons whose diagonal correlations are identical to those of spinless fermions.

To conclude, we have studied the ground state phases of the BFHM on a 1D optical lattice. The analytical expressions (2), (3) for the boson-demixing boundary, constructed assuming a continuous transition, are in an excellent agreement with the numerical results. For the symmetrical interactions, $t_B = t_F$, $U_B = U_F$, the F-F phase becomes locally unstable at $\mu_F = \mu_B + \hbar c(n, V) > \mu_B$ [Eq. (3)], any phase along the diagonal $\mu_B = \mu_F$ is gapless to boson-fermion conversion, while the fermion demixing transition happens strictly for $\mu_B \geq \mu_F$. This establishes the stability of the mixed phase at all densities and couplings. For strongly interacting bosons and fermions, the extent of the mixed phase gets progressively narrower at low densities. On the other hand, for weakly interacting particles, the homogeneous phase is stabilized over a wide range of chemical potentials. Investigation of the properties of the B-F phase at $U = V$ reveals that at weak interactions, the mixed phase is a two-component Luttinger liquid at all densities. For strong interactions, this statement is valid at low densities, but breaks down at the commensurate total density, $n_F + n_B = 1$. Numerical data suggest a gapless mode for the ground state and strong coupling mapping to the XXZ model predict that at $U = V$ this gapless mode consists of a $k = 0$ spin-wave. In the BFHM, this corresponds to fluctuations of the mixture composition $17$. We have also explored the effects of boson-fermion interaction on the density correlations of the two components and find that the results are dramatically different in the weak and strong coupling limits. These signatures should be readily observable in experiments, and, if confirmed, would indicate the emergence of novel many-body phases in these systems.

We are grateful to L. Pollet, M. Troyer, and C. Varma for useful discussions and for sharing their results before publication (LP and MT). PS was supported by the DOE under grant DE-FG02-05ER46240. Simulations were carried out in part at the HPC Center at USC.

1. A. G. Truscott et.al., Science 291, 2570 (2001).
2. Z. Hadzibabic et.al., Phys. Rev. Lett. 91, 040403 (2003).
3. G. Roati, F. Riboli, G. Modugno, and M. Inguscio, Phys. Rev. Lett. 89, 150403 (2002).
4. C. Sibler et.al., cond-mat/0506217.
5. K. Mölmer, Phys. Rev. Lett. 80, 1804 (1998); L. Viverit, and S. Giorgini, Phys. Rev. A 66, 063604 (2002).
6. A. Albus, F. Illuminati, and J. Eisert, Phys. Rev. A 68, 023606 (2003).
7. K. K. Das, Phys. Rev. Lett. 90, 170403 (2003).
8. M. Lewenstein, L. Santos, M. A. Baranov, and H. Fehrmann, Phys. Rev. Lett. 92, 050401 (2004).
9. T. Miyakawa, H. Yabu, and T. Suzuki, Phys. Rev. A 70, 013612 (2004).
10. Z. Akdeniz, P. Vignolo, and M. P. Tosi, cond-mat/0505412.
11. M. A. Cazalilla, and A. F. Ho, Phys. Rev. Lett. 91, 150403 (2003).
12. A. Imamabekov, and E. Demler, cond-mat/0505632 and cond-mat/0510801; M. T. Batchelor, M. Bortz, X. W. Guan, and N. Oelkers, cond-mat/0506478.
13. R. Roth, Phys. Rev. A 66, 013614 (2002); R. Roth, and K. Burnett, Phys. Rev. A 69, 021601 (2004).
14. Y. Takeyuchi, and H. Mori, cond-mat/0508247, cond-mat/0509068.
15. D. Jaksch et.al., Phys. Rev. Lett. 81, 3108 (1998).
16. T. D. Kühner, and H. Monien, Phys. Rev. B 58, R14741 (1998), and references therein.
17. L. Pollet, M. Troyer, K. Van Houcke, and S. M. A. Rom-bouts, unpublished (2005).
18. E. H. Lieb and F. Y. Wu, Phys. Rev. Lett. 20, 1445 (1968).
19. H. Frahm and V. E. Korepin, Phys. Rev. B 42, 10553 (1990).
20. R. Z. Bariev, J. Phys. A: Math. Gen. 27, 3381 (1994).
[21] A. Kitazawa, J. Phys.: Cond. Matt. 15, 2587 (2003).
[22] A. W. Sandvik, Phys. Rev. B 59, R14157 (1999).
[23] E. L. Pollock, and D. M. Ceperley, Phys. Rev. B 36, 8343 (1987).

[24] Due to exponential increase in autocorrelation times, simulations for Fig. 4(d) had to be limited to small systems, $L \leq 16$. We thank L. Pollet for pointing this out.