Superfluid and Mott-insulator phases of one-dimensional Bose-Fermi mixtures
Zujev, A.; Baldwin, A.; Scalettar, R.T.; Rousseau, V.G.; Denteneer, P.J.H.; Rigol, M.

Citation

Version: Not Applicable (or Unknown)
License: Leiden University Non-exclusive license
Downloaded from: https://hdl.handle.net/1887/59993

Note: To cite this publication please use the final published version (if applicable).
I. INTRODUCTION

The experimental realization of strongly correlated systems with ultracold gases loaded in optical lattices [1] has generated tremendous excitement during recent years. Initially thought of as a way to simulate condensed matter model Hamiltonians, such as the Bose-Hubbard Hamiltonian [2], loading atoms on optical lattices has enabled the creation of quantum systems that are unexpected in the condensed matter context. Among these systems the realization of Bose-Fermi mixtures in optical lattices intraspecies interactions can be tuned to be attractive or repulsive [6], is a remarkable example of the scope of realizable models.

Theoretical studies of Bose-Fermi mixtures in one-dimensional lattices have been done for homogeneous [7–13,17] and trapped [14–16] systems. Several approaches have been used: Gutzwiller mean-field theory [14], strong coupling expansions [8,17], bosonization [7,9], and exact analytical [10] and numerical [11–13,16,17] studies. Recently, a mixture of bosonic atoms and molecules on a lattice was studied numerically [18]. The landscape of phases encountered is expansive, and includes Mott insulators, spin and charge density waves, a variety of superfluids, phase separation, and Wigner crystals. However, the phase diagram in the chemical potential-interaction strength plane has not yet been reported.

It is our goal in this paper to present a study of repulsive Bose-Fermi mixtures in one-dimensional lattices that generalizes previous studies, which focused on specific special densities, to more general filling. After mapping the phase diagram we will explore different sections in greater detail. Since the particular case in which the lattice is half filled with bosons and half filled with fermions has been carefully studied in Ref. [11], we will instead concentrate here on two cases: (i) when the number of bosons is commensurate with the lattice size but the number of fermions is not, and (ii) when the sum of both species is commensurate with the lattice size but the number of bosons and fermions are different. Some of the phases present in these cases have been identified by Sengupta and Pryadko in their grand canonical study in Ref. [12] and by Hébert et al. in the canonical study recently presented in Ref. [13].

The Hamiltonian of Bose-Fermi mixtures in one dimension can be written as

$$\hat{H} = -t_B \sum_l (\hat{b}^\dagger_{l} \hat{b}_{l+1} + \hat{b}^\dagger_{l+1} \hat{b}_{l}) - t_F \sum_l (\hat{f}^\dagger_{l} \hat{f}_{l+1} + \hat{f}^\dagger_{l+1} \hat{f}_{l}) + U_{BB} \sum_l n^B_l (n^B_l - 1) + U_{BF} \sum_l n^B_l n^F_l,$$

(1)

where $b^\dagger_l (b_l)$ are the boson creation (destruction) operators on site $l$ of the one-dimensional lattice with $L$ sites. Similarly, $f^\dagger_l (f_l)$ are the creation (destruction) operators on site $l$ for spinless fermions on the same lattice. For these creation and destruction operators $n^B_l$ and $n^F_l$ are the associated number operators. The bosonic and fermionic hopping parameters are denoted by $t_B$ and $t_F$, respectively, and the on-site boson-boson and boson-fermion interactions by $U_{BB}$ and $U_{BF}$. In this paper we will consider the case $t_B=t_F=1$ (i.e., when the boson and fermion hopping integrals are equal) and choose $U_B=U_F=1$ to set the scale of energy.

It is useful to begin a discussion of the phase diagram with an analysis of the zero hopping limit ($t_B=t_F=0$) similar to the one done by Fisher et al. in Ref. [19] for the purely bosonic case. Consider a particular fermion occupation of one fourth of the lattice sites, $N_F=L/4$ fixed. Bosons can be added up to $N_B=3L/4$ without sitting on a site which is already occupied by either a boson or a fermion. Therefore the associated chemical potential $\mu$ is small. What happens when $N_B$ exceeds $3L/4$ depends on the relative strength of $U_{BB}$ and $U_{BF}$.
If $U_{BB}$ is less than $2U_{RB}$ then the extra bosons sit atop of the fermions and $\mu$ jumps by $U_{BF}$. The chemical potential stays at this elevated value of $U_{BF}$ until all the sites with fermions also have a boson. At that point additional bosons start going onto sites with a boson already, and $\mu$ jumps to $2U_{RB}$. Thus, in general, there are incompressible phases where the boson chemical potential jumps both at commensurate $\rho_B=1,2,3,\ldots$ (as for the pure boson-Hubbard model) and also at $\rho_B=1-\rho_F,2-\rho_F,3-\rho_F,\ldots$. For $U_{BF}$ greater than $2U_{RB}$ and less than $6U_{RB}$ the incompressible phases still start at $\rho_B=1-\rho_F$ but the following potential jumps are shifted up by $1-\rho_F$. Turning on the hoppings $t_B$, $t_F$ introduces quantum fluctuations which will ultimately destroy these Mott plateaus and introduce new, intricate phases.

II. CANONICAL WORM ALGORITHM

We perform quantum Monte Carlo simulations (QMC) using a recently proposed canonical worm algorithm [20,21]. This approach makes use of global moves to update the configurations, samples the winding number, and gives access to the measurement of $n$-body Green functions. It also has the useful property of working in the canonical ensemble. This is particularly important for the present application since working with two species of particles leads to two different chemical potentials in the grand canonical ensemble. These prove difficult to adjust such that the precise, desired fillings are achieved. In our canonical simulations the Bose and Fermi occupations are exactly specified and the chemical potentials $\mu_B$ and $\mu_F$ are instead computed [22] via appropriate numerical derivatives of the resultant ground state energy [e.g., $\mu_B=E_0(N_B+1)-E_0(N_B)$].

The canonical worm algorithm is a variation of the Prokof’ev et al. grand-canonical worm algorithm [23]. Within the canonical worm approach one starts by writing the Hamiltonian as $\hat{H}=\hat{V}-\hat{T}$, where $\hat{T}$ is comprised of the nondiagonal terms and is by necessity positive definite. The partition function $Z=\text{Tr} \ e^{-\beta\hat{H}}$ takes the form

$$Z=\text{Tr} \ e^{-\beta\hat{V}} \ e^{\beta\hat{T}i\rho d\tau} \ e^{\beta\hat{V}} \approx \text{Tr} \ e^{-\beta\hat{V}} \sum_n \int_0<\tau_1<\cdots<\tau_n<\beta \hat{T}(\tau_n) \cdots \hat{T}(\tau_1)d\tau_1 \cdots d\tau_n,$$

where $\hat{T}(\tau) = e^{i\beta\hat{V}} T e^{-i\beta\hat{V}}$. In order to sample expression (3) an extended partition function is considered by breaking up the propagator at imaginary time $\tau$ and introducing a “worm operator” $\hat{W}=\sum_{ijkl}\\bar{a}_{ijkl}\hat{b}_{ij}\hat{b}^\dagger_{kl}$ that leads to $Z(\tau) = \text{Tr} \ e^{-\beta\hat{W}} \hat{W} e^{-\beta\hat{W}}$. Complete sets of states are introduced between consecutive $\hat{T}$ operators to allow a mapping of the one-dimensional (1D) quantum problem onto a two-dimensional (2D) classical problem where a standard Monte Carlo technique can be applied. Measurements can be performed when configurations resulting in diagonal matrix elements of $\hat{W}$ occur. This way unphysical movements are exploited to help explore the Hilbert space, but are ignored when sampling for measurements.

As with pure bosonic systems, the evolution of the boson and fermion densities $\rho_B, \rho_F$ with the associated chemical potential $\mu_B, \mu_F$ identifies Mott-insulating behavior [19]. A jump in $\mu$ signals a Mott phase where the compressibility $\kappa_B=\partial\rho_B/\partial\mu_B$ or $\kappa_F=\partial\rho_F/\partial\mu_F$ vanishes.

Quantities of interest that we measure include the bosonic superfluid density and the fermionic stiffness,

$$\rho_B^I=\langle \hat{W}_B^\dagger \rangle /2\beta,$$

$$\rho_F^I=\langle \hat{W}_F^\dagger \rangle /2\beta.$$  \hspace{1cm} (4)

Here $\langle \hat{W}_\cdot \rangle$ are the associated winding numbers. Correlations between the bosonic and fermionic winding numbers [11] are determined by the combinations,

$$\rho_B^I=\langle (\hat{W}_B^\dagger + \hat{W}_F^\dagger)^2 \rangle /2\beta,$$

$$\rho_F^I=\langle (\hat{W}_B - \hat{W}_F)^2 \rangle /2\beta.$$  \hspace{1cm} (5)

In addition to the usual bosonic and fermionic Green function,

$$G_{ij}^B=\langle \hat{b}_i^\dagger \hat{b}_j \rangle,$$

$$G_{ij}^F=\langle \hat{f}_i^\dagger \hat{f}_j \rangle,$$

we also measure the composite anticorrelated two-body Green function

$$G_{ij}^*=\langle \hat{b}_i^\dagger \hat{b}_j \hat{f}_i^\dagger \hat{f}_j \rangle.$$  \hspace{1cm} (6)

In $G_{ij}^*$, the fermion and boson propagate in opposite directions (one from $j$ to $i$ and one from $i$ to $j$).

The Fourier transforms of $G_{ij}^B$ and $G_{ij}^F$ give the densities $n_B(k)$ and $n_F(k)$ in momentum space; $n_a(k)$ is the Fourier transform of the composite two-body Green function $G_{ij}^*$. We performed extensive checks of the code against other quantum Monte Carlo simulations in the pure boson and pure fermion cases, and against exact diagonalization and Lanczos calculations for mixed systems on small lattices.

III. PHASE DIAGRAM IN THE $\mu_B-U_{BF}$ PLANE

We begin our determination of the phase diagram by calculating the dependence of the density $\rho_B$ on chemical potential $\mu_B$, mapping out the extent that the Mott plateaus described in the Introduction survive the addition of quantum fluctuations $t_B, t_F$. We examine a system with a fixed $U_{BB}=10$ and $\rho_F=1/4$ and focus on the regions through $\rho_B \leq 3/2$ and $U_{BF} \leq 5U_{RB}/2$ in the phase diagram. The $t_B=t_F=0$ analysis suggests for $U_{BF}<2U_{RB}$ there will be plateaus with compressibility $\kappa=0$ at $\rho_B=1$ (i.e., $\rho_B=3/4$) caused by $U_{BF}$ and at $\rho_B=1$ caused by $U_{BB}$. Figure 1 exhibits these plateaus for $U_{BF}=16$ and $t_B=t_F=1$. The complete phase diagram in the $\mu_B-U_{BF}$ plane at fixed $U_{BB}=10$ is obtained by replicating Fig. 1 for different $U_{BB}$, and is given in Fig. 2(a). For weak $U_{BF}$ the phase diagram is dominated by the $\rho_B=1$ plateau where the chemical potential jumps by $2U_{BB}-U_{BF}=2U_{BB}=20$. As $U_{BF}$ increases, this plateau shrinks and finally terminates at $U_{BF}=2U_{BB}=20$. At the same time, the
The fermion density is \( \rho_F = 1/4 \) and the interaction strengths are fixed at \( U_{BF} = 10 \) and \( U_{BB} = 16 \). There are Mott plateaus at \( \rho_B = 1 - \rho_F = 3/4 \) and \( \rho_B = 1 \) as predicted by the \( t_F = t_2 = 0 \) analysis. The positions of the Mott lobes coincide for different lattice sizes \( L = 36, 44 \), and temperatures \( \beta = 32, 48 \), to within our error bars, which are smaller than the symbol size. The dependence of \( \rho_B \) on \( \mu_B \) in the absence of fermions is given for comparison.

Plateau at \( \rho_B = 1 - \rho_F \) grows to \( U_{BB} = 20 \). The explanation of the labeling of the different phases (I–VI) will be given after we discuss the superfluid response of the system. Figure 2 shows the phase diagram in the \( \mu_B \) and \( U_{BB} \) plane.

IV. SUPERFLUID RESPONSE AT \( \rho_B + \rho_F = 1 \)

After determining the positions of the Mott plateaus, we examine the stiffness and Green functions. We take a “horizontal” cut through Fig. 2(a) by fixing \( \rho_B + \rho_F = 1 \) (\( \rho_B = 3/4 \)) and increasing \( U_{BB} \). In Fig. 3 we see that for \( U_{BB} \leq 2U_{BF} = 20 \) the interaction strength \( U_{BF} \) is small enough that fermions and bosons can briefly inhabit the same site. Now, when a boson visits the site of a neighboring fermion (or vice versa) it is equally likely that the fermion will exchange as for the boson to return to its original site. Through these exchanges the bosons and fermions can achieve anticoordinated winding around the lattice. Thus, the bosonic superfluid density and the fermionic stiffness are both nonzero and identical [25]. However, as \( U_{BB} \) increases past \( U_{BB} \leq 2U_{BF} = 20 \) the cost of double occupancy becomes prohibitive. With its benefits outweighed by energy penalties exacted by \( U_{BF} \), all anticoordinated “superfluidity” ceases. Pollet et al. [11] have argued that this region exhibits phase separation. Indeed we do detect a signal of phase separation through density structure factor. But the signal is weak, about 20 times weaker than what we get at phase VI (next section), and compressibility is close to zero, so we label this region as an insulator.

From the results depicted in Fig. 3 one should notice that while for quantities like the energy and Mott gap \( \beta = 32 \) is sufficiently low for \( L = 32 \) to capture the ground state behavior, for stiffnesses one requires much lower temperatures.

V. SUPERFLUID RESPONSE AT \( \rho_B = 1 \)

Although it shares the property that \( \kappa_F = 0 \) with the \( \rho_B + \rho_F = 1 \) lobe, a horizontal cut (Fig. 4) through the \( \rho_B = 1 \) Mott lobe exhibits rather different superfluid response. This trajectory initially lies within the Mott lobe and then emerges into a region of nonzero compressibilities. As expected, the plateau in \( \rho_B \) (Mott gap) indicates the bosons are locked into place by the strong \( U_{BB} \), and as a consequence \( \rho_F = 0 \) (Fig. 4). Throughout this boson Mott lobe the fermions are, however, free to slide over the bosons and so \( \rho_F \) is nonzero. In this region, as expected, the fermion compressibility \( \kappa_F \) is nonzero.

The Bose-Fermi repulsion \( U_{BF} \) competes with \( U_{BB} \), and, in a window around \( U_{BF} \approx 2U_{BB} \), it is energetically equivalent for a boson to share a site with another boson as with a fermion. The Mott lobe is terminated and a superfluid win-
flow for both species stops, but the compressibilities energetically unfavorable for a boson to share a site with a spling similar. However, quickly after turning on diagram of Fig. 2. As in Figs. 1 and 2, in which gate in opposite directions “Horizontal” sweep, which is fixed den-

FIG. 3. (Color online) “Horizontal” sweep, which is fixed densities \( \rho_b = 3/4 \) and \( \rho_f = 1/4 \) and varying \( U_{BF} \), through the phase diagram of Fig. 2. As in Figs. 1 and 2, \( U_{BF} = 10 \). Top panel: Both the bosonic and fermionic species exhibit a finite stiffness at weak coupling (region II of the phase diagram), which decays as \( U_{BF} \) increases until insulating behavior occurs (region V of the phase diagram). Bottom panel: Near \( U_{BF} = 0 \) both \( \rho'_b \neq 0 \) and \( \rho'_f \neq 0 \) are very similar. However, quickly after turning on \( U_{BF} \), the correlated and anticorrelated stiffness show that the bosons and fermions propagate in opposite directions \( \rho'_b \neq 0 \), while \( \rho'_f = 0 \).

VI. SUPERFLUID RESPONSE AT GENERAL FILLING

Further insight into the physics of this phase diagram can be obtained by measuring the superfluid response along the same “vertical” cuts through the phase diagram as done in Figs. 1 and 2, in which \( \rho_b \) is varied at fixed \( U_{BF} \). In Figs. 5 and 6, we show the result. Distinctive densities in the latter figures are \( \rho_b = 3/4 \) (so that \( \rho_b + \rho_f = 1 \)) and \( \rho_b = 1 \). We discuss first (Fig. 5) the case of \( U_{BF} = 16 \), where increasing \( \rho_b \) cuts through both Mott lobes. The bosonic superfluid density vanishes at \( \rho_b = 1 \), dips at \( \rho_b + \rho_f = 1 \), and is nonzero above, below, and between the lobes. The fermion superfluid density is never driven to zero in this cut, and only dips at the special value \( \rho_b = 3/4 \) where the commensurate total density works against superfluidity. In the case of \( U_{BF} = 24 \), Fig. 6, as \( \rho_b \) increases we cut through only the \( \rho_b = 3/4 \) lobe. Here the superfluid density is pushed to zero for the entire region between \( \rho_b = 3/4 \) and \( \rho_b = 1 \), and is nonzero without.

We now fill in the labeling of the phase diagram of Fig. 2. A gapless superfluid phase (I) with \( \rho'_b \neq 0 \) and \( \rho'_f \neq 0 \) exists at low filling of the lattice \( \rho_b + \rho_f < 1 \). When the combined filling of the two species becomes commensurate, an anticorrelated (II) phase appears in which \( \rho'_b \neq 0 \) and \( \rho'_f \neq 0 \), but \( \rho'_b = \rho'_f \). This phase is characterized by superflow of the two species in opposite directions and is gapped to the addition of bosons or fermions. The usual bosonic Mott insulator, phase IV, occurs at commensurate boson densities. However, it can be melted by increasing \( U_{BF} \) since the jump in bosonic

FIG. 4. (Color online) Same “horizontal cut” as Fig. 3 except at commensurate density for the boson species alone \( \rho_b = 1 \) and \( \rho_f = 1/4 \). Top panel: The bosons are insulating at weak \( U_{BF} \) within this Mott lobe of commensurate bosonic filling (region IV of the phase diagram). However, the fermions are free to flow on the uniform boson background and have nonzero stiffness. Upon emerging from the lobe, at \( U_{BF} = 2U_{BB} \), \( \rho_b \) becomes nonzero in a window where the two repulsions work against each other. After the peak, the system becomes phase separated and \( \rho_b \) and \( \rho_f \) go to zero. Bottom panel: The correlated and anticorrelated stiffnesses are essentially equal throughout the weak coupling because the flow is dominated by fermions. However, in the window the anticorrelated stiffness increases beyond the correlated stiffness in a weak simulacrum of phase II (as discussed in the text).
once a fermion riding atop bosons runs into a fermion alone on a site. The fermion without a boson cannot move out of the other fermion's way either. However, the boson sharing a site with the mobile fermion can then hop to the immobile fermion at low energy cost. Thus, the boson is passed from one fermion to the other, granting it mobility. Signatures of this phase are the lower value of the temperature at which the superfluid density builds up, that \( \rho_B \) exceeds \( \rho_F \), and more correlated winding than anticorrelated. However, there is nothing preventing lone fermions from acting as in the anticorrelated phase. Unfortunately this means that potential signals are masked. While we do see some of these signatures superfluid phase IV, the temperature scale at \( U_{BF} = 24 \) is increased from \( U_{BB} = 32 \) to \( U_{BF} = 108 \) in Fig. 5, both superfluid densities vanish in the insulating region of the Mott lobe at commensurate total filling.

VII. MOMENTUM DISTRIBUTION FUNCTIONS

To further explore the nature of the phases we turn to the momentum distributions for the bosons, fermions, and anticoordinated pairing—Figs. 7–12. Each plot is made at \( \beta = 108 \) and corresponds to the parameter choices: I, \( U_{BB} = 16 \) and \( N_B = 20 \); II, \( U_{BF} = 16 \) and \( N_B = 27 \); III, \( U_{BF} = 16 \) and \( N_B = 32 \); IV, \( U_{BF} = 16 \) and \( N_B = 36 \); V, \( U_{BF} = 30 \) and \( N_B = 27 \); VI, \( U_{BF} = 28 \) and \( N_B = 36 \). In the superfluid phase I, there is a peak in the boson distribution and a plateau in the fermion distribution, implying quasicondensation in the bosonic sec-
In the insulating phase real space Green function counterparts are decaying exponentially and their corresponding momentum distributions are smooth functions of $k$. In the case of phase separation (VI) the bosonic momentum distribution is similar to the superfluid, while fermionic distribution is similar to that of an insulator.

**VIII. CONNECTION TO PREVIOUS THEORETICAL WORK**

As reviewed in the Introduction, there is extensive theoretical literature on Bose-Fermi mixtures. We now make more detailed contact with previous work, first by comparing our results to the strong coupling phase diagram of Lewenstein et al. (LSBF) [8]. Figure 13 combines our results and those of LSBF. Besides the quantitative agreement, we note the following correspondences: LSBF’s region $0 \leq \mu \leq 1$ is analogous to our $0 \leq \mu \leq 20$, and $0 \leq \alpha \leq 1$ to our $0 \leq U_{BF} \leq 20$. Furthermore, our phase II (anticorrelated phase) corre-
superfluid and mott-insulator phases of one-...
We acknowledge support from the National Science Foundation Grant No. ITR-0313390, Department of Energy Grant No. DOE-BES DE-FG02-06ER46319, and useful conversations with G. G. Batrouni and T. Byrds. This work is part of the research program of the Stichting voor Fundamenteel Onderzoek der Materie (FOM), which is financially supported by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek (NWO).

[24] Unlike $n_g(k)=(\phi_{0}|b^\dagger(k)b(k)|\phi_{0})$, which is the length of a vector and hence must be positive, there is no such constraint on $n_n(k)$, which is the Fourier transform of $G_n(k)$. We have verified that the same small negative values of $n_n(k)$ in the figures are also obtained in exact diagonalization on small clusters.
[25] This phase has been termed “super-Mott” as a consequence of its combining a nonzero gap with nonzero superflow [18].