Mixture of bosonic and spin-polarized fermionic atoms in an optical lattice

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We investigate the properties of trapped Bose-Fermi mixtures for experimentally relevant parameters in one dimension. The effect of the attractive Bose-Fermi interaction onto the bosons is to deepen the parabolic trapping potential, and to reduce the bosonic repulsion in higher order, leading to an increase in bosonic coherence. The opposite effect was observed in $^{87}$Rb - $^{40}$K experiments, most likely due to a sharp rise in temperature. We also discuss low-temperature features, such as a bosonic Mott insulator transition driven by the fermion concentration, and the formation of composite particles such as polarons and molecules.

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I. INTRODUCTION

Systems of interacting bosons and fermions occur frequently in nature. Usually, the bosons act as carriers of force between the fermionic particles. In high energy physics, quarks exchange gluons via the strong force, while in solid state physics electrons can interact via light or lattice vibrations. Most prominent examples of such systems are conventional BCS superconductivity (caused by an effective attractive interaction between the fermions induced by the electron-phonon coupling), the Peierls instability (a charge density wave) and the formation of polarons, which in solids are electrons dressed by a cloud of phonons. There are only a few condensed matter systems in which the influence of fermions onto bosons has been investigated. One of them are mixtures of bosonic $^4$He and fermionic $^3$He, in which a shift of the transition temperature between normal and superfluid $^4$He as a function of $^3$He concentration was observed.

In the field of ultracold gases fermions and bosons are on an equal footing. The choice of different atomic species [1, 2, 3, 4] and optical lattice potentials [5, 6] give almost unrestricted access to all parameters of these systems, offering the possibility to study the influence of the species onto each other and to investigate open questions from other areas of physics in a new context. Theoretical approaches [10, 11, 12, 13, 14, 15, 16, 17, 18, 19] have proposed a whole variety of quantum phases present in homogeneous Bose-Fermi mixtures at low temperature, ranging from a charge-density wave, over a fermionic pairing phase, to polaronic properties, and even to phase separation.

In recent experiments two groups independently succeeded in the stabilization of bosonic $^{87}$Rb and fermionic $^{40}$K in a three-dimensional optical lattice [6, 8]. They focused on the loss of bosonic phase coherence and on the increase of the bosonic density by varying the fermionic concentration. The trapping potential and the finite temperature make the interpretation of the observed quantities however challenging.

Here, we study the interplay of a trap, finite temperature and strong interparticle interactions, which lead to physics quite different from the homogeneous case. In particular, while the addition of fermions induces a quantum phase transition from the Mott insulating to the superfluid phase at larger bosonic repulsion strength in a homogeneous lattice, the presence of a trapping potential makes the situation more involved because of an extra, effective strongly-inhomogeneous trapping potential. Despite the large Bose-Fermi coupling, it turns out that our results for the trapped, mixed system can be well understood in terms of first and second order corrections to the bosonic Hamiltonian. For low bosonic and fermionic densities, we illustrate that the formation of bound pairs invalidates the picture of a perturbational correction by the fermions on the bosons.

II. MODEL

A mixture of bosonic and spin-polarized fermionic atoms in an optical lattice can be described by the Bose-Fermi Hubbard Hamiltonian,

$$H = -\sum_{\langle i,j \rangle} \left( J_B \hat{b}_i^\dagger \hat{b}_j + J_F \hat{c}_i^\dagger \hat{c}_j + \text{h.c.} \right) +$$

$$\sum_i U_{BB} \hat{n}_{B,i} (\hat{n}_{B,i} - 1) + \sum_i U_{BF} \hat{n}_{B,i} \hat{n}_{F,i} +$$

$$\sum_i \epsilon_{B,i} \hat{n}_{B,i} + \sum_i \epsilon_{F,i} \hat{n}_{F,i},$$

where $\hat{c}_i^\dagger (\hat{c}_i)$ and $\hat{b}_i^\dagger (\hat{b}_i)$ are the corresponding creation and annihilation operators for the fermions (bosons), and $\hat{n}_{X,i}$ is the number operator on site $i$ for species $X=B,F$. The $J_X$-terms are the hopping, the $\epsilon_X$-terms describe the external trapping potential, and $U_{BB}$ and $U_{BF}$ denote the on-site interaction strength between bosonic atoms and between a fermionic and bosonic atom, respectively.
The effective parameters of the Bose-Fermi Hubbard model are deduced from the experimental parameters of Ref. [8, 9] using a tight-binding approximation [11, 20]. Taking the scattering lengths as $a_{BB}/a_B = 102 \pm 6$ and $a_{BF}/a_B = -205 \pm 5$, where $a_B$ is the Bohr radius, we note that $U_{BB}/U_{BB} \approx -2$, a ratio which is almost constant for all optical lattice depths. We took a wavelength $\lambda = 106\text{nm}$ for the optical lattice potential, and frequencies $\omega_B = 2\pi \cdot 30\text{Hz}$ and $\omega_F = 2\pi \cdot 37\text{Hz}$ for the harmonic confinement. To determine the state of the mixture we use two numerically exact methods: at finite temperatures the canonical two-body Bose-Fermi worm Quantum Monte Carlo (QMC) algorithm [10], and at zero temperature the density-matrix renormalization-group method (DMRG) [23].

III. EFFECTS OF FERMIONS ON BOSONS

A. Induced potentials and interactions

In a mixture, the lowest order effect of the fermions is a mean-field shift $U_{BF}/\langle n_{F,i} \rangle$ of the potential experienced by the bosons [11, 24]. In a homogeneous system with a fixed particle number the shift in the potential has no consequences besides adding a constant to the energy. The next order effect is an induced attractive interaction between the bosons [11, 24]. A similar effect is well known from conventional superconductivity, where the phonons (bosons) induce an effective electron-electron interaction. The induced interaction shows up most clearly in a shift of the critical $U_{BB}/J_B$ of the bosonic superfluid-Mott transition while varying the interspecies interaction as shown in Fig. 1(a). As expected for an induced attractive interaction, we find a shift to larger values of $U_{BB}/J_B$. At small $U_{BF}$ the shift is proportional to $U_{BF}^0$ in agreement with perturbative calculations [24]. Therefore the presence of fermions can induce a phase transition from a Mott-insulating to a superfluid phase.

In the following we discuss how a parabolic trap and finite temperature change this picture. To separate the effect of the effective trapping from the induced interaction, we generate an effective site-dependent potential for the bosons by replacing the Bose-Fermi interaction operator by the effective potential $\epsilon_i n_{B,i} = U_{BF} \langle n_{F,i} \rangle \hat{n}_{B,i}$. This deviates from the disordered chemical potential approach of Ref. [9] and from a mean-field approximation: The exact fermionic density distribution of the mixture serves as input for a second, purely bosonic simulation. In Fig. 1(b), we compare the resulting bosonic density and compressibility profiles. We observe that the density profiles are quite well reproduced, confirming that the dominant effect of the fermions is to modify the effective potential for the bosons. However, looking at higher order quantities such as the density fluctuations $\langle n_{B,i}^2 \rangle - \langle n_{B,i} \rangle^2$ we find significant discrepancies. In particular, we see Mott plateaus in the approximation (signaled by dips in the variance of the density in Fig. 1(b)) that are absent in the full QMC simulation. Around these dips the difference between the two curves is around
eighty percent. This is a clear signature for a fermion-induced attractive Bose-Bose interaction, reducing the bare repulsion \( U_{BB} \) (cf. Fig. 1a). We note that the visibilities, discussed below, are rather well reproduced in the approximation, indicating that the effective potential is the dominant effect as far as this experimental quantity is concerned (which is surprising seen the large values of \( U_{BF} \)).

Having gained an understanding of the relevant mechanisms, we proceed in section III C with the results of two simulations where we vary experimental control parameters, namely the Bose-Fermi coupling and the fermionic concentration, and then compare our results to experiment in section III C.

B. Results at low and constant temperature

Fig. 2 shows density profiles for different values of the attractive interaction strength \( U_{BF} \). In the absence of a boson-fermion interaction, all particles are smeared out over the lattice. Turning the interspecies interaction on, we see in Fig. 2 that both species accumulate in the trap center. The fermions are pinned down in the trap center (cf. Fig. 2), despite their light bare mass. They lower the effective potential in the center of the trap as \( U_{BF}(n_F,i) \), causing the accumulation of bosons.

The effect of an inhomogeneous effective potential can be seen even more clearly by varying the fermionic concentration instead of the interaction strength \( U_{BF} \). In Fig. 3 we show the dependence of the bosonic visibility on the number of fermions with a fixed number of bosons, a setup similar to recent experiments [8, 9]. The bosonic visibility is defined by \( \nu = (\rho_B(0) - \rho_B(\pi))/(\rho_B(0) + \rho_B(\pi)) \) where \( \rho_B(k) \) is the value of the bosonic momentum distribution at momentum \( k \). The visibility is often taken as a measure of the coherence of the bosons.

For shallow lattice potentials, a slight increase in the visibility for an intermediate number of fermions is seen, due to an increase in the bosonic density in the center of the trap caused by the fermions. For moderate lattice potentials one observes a complex, non-monotonic behavior with large variations. If a few fermions are admixed to a bosonic system, the fermions – spreading over several sites in the center of the trap – cause a strongly inhomogeneous effective potential for the bosons. The effective potential exhibits a deep minimum in the center of the trap and causes the bosons to accumulate in this region. If the purely bosonic system was superfluid (cf. Fig. 4 \( N_F = 0, V_0 = 3E_R \)) the effective potential causes a superfluid state with higher filling in the center of the trap, slightly increasing the bosonic visibility. If the bosonic system exhibited a broad \( n_B \approx 1 \) Mott plateau (cf. inset Fig. 4 \( N_F = 0, V_0 \geq 6E_R \)), this plateaux is partially destroyed resulting in a large rise of the visibility. The mechanism holds until there are enough fermions present to form a band insulating region (cf. Fig. 4 \( N_F \approx 14 \)). For such and higher fermion numbers, the effective potential induced by the fermions follows the curvature of the external trap over the region occupied by the fermions with a sudden increase at its boundaries. The number of fermions sets the length of an effective system for the bosons, and controls the bosonic filling. In this approximately parabolically trapped effective systems insulating regions can form for \( N_B/N_F = 40/20 \) (as shown), but also for \( N_B/N_F \approx 60/30 \) or \( 20/10 \), yielding strong dips in the visibility [26, 27].
now be formed for moderately deep optical lattices. First signs of this pairing can be seen in the two-body Bose-Fermi momentum distribution shown in Fig. 5(a). The momentum distribution of these fermionic molecules shows a sharper Fermi edge compared to the bare fermion. It also tends to zero at larger momenta, showing that these molecules are a better description of the system than the bare fermions and bosons. The formation of molecules is also well supported by coinciding charge modulations in the bosonic and fermionic densities (Fig. 5(b)). For the parameters chosen in Fig. 5(b) the density modulations are Friedel oscillations due to trap, but for larger lattice depths a density wave can be formed \[10, 15\].

V. CONCLUSION

In conclusion, we have simulated the trapped one-dimensional Bose-Fermi Hubbard model. The interplay between temperature, trap, optical potential and particle number is very rich and non-universal. The dominant effect is the creation of a strongly inhomogeneous trapping potential by the fermions. In higher order the fermions induce an attractive interaction between the bosons, which should lead to an increase in the bosonic visibility. However assuming a rise in temperature when ramping up the lattice, a decrease in the visibility is found analogous to the experimental observation in the $^{87}\text{Rb}\ -^{40}\text{K}$ samples. If temperature remains low, one could observe a Mott transition driven by the fermionic concentration, and observe the formation of molecules. The same effects are expected for higher dimensions, since the underlying mechanisms do not depend on dimensionality. Our study explicitly shows that the effects of temperature, particle number, adiabatic processes and trapping potential have to be taken into account carefully when analyzing cold-atom experiments.

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C. Comparison with experiment

In apparent contradiction to our low-temperature predictions of an increase in the bosonic visibility for most numbers of admixed fermions (in Fig. 3), the experiments show a strong decrease for moderate values of the lattice potential. Assuming that entropy is conserved when ramping up the lattice, the effective temperature of a $^{87}\text{Rb}\ -^{40}\text{K}$ mixture rises dramatically because of the different temperature dependence of fermionic ($S_F \propto \frac{1}{T}$) for an ideal gas and bosonic ($S_B \propto (T/T_c)\frac{3}{2}$) for an ideal gas) contribution to the entropy. In Fig. 2 we increase the temperature (decrease $\beta = 1/k_BT$) at fixed optical potential and atom number and find a drastic drop in the visibility as the temperature is increased around $\beta \approx 2/J_B$. A rise in the temperature of the bosonic atoms in the presence of fermions can cause a large decrease of the bosonic visibility and is thus the most likely explanation for the experimental results.

IV. AT LOW DENSITIES

We finally discuss the physics at low densities. Bound pairs ("molecules") of one boson and one fermion can now be formed for moderately deep optical lattices. First signs of this pairing can be seen in the two-body Bose-Fermi momentum distribution shown in Fig. 5(a). The momentum distribution of these fermionic molecules shows a sharper Fermi edge compared to the bare fermion. It also tends to zero at larger momenta, showing that these molecules are a better description of the system than the bare fermions and bosons. The formation of molecules is also well supported by coinciding charge modulations in the bosonic and fermionic densities (Fig. 5(b)). For the parameters chosen in Fig. 5(b) the density modulations are Friedel oscillations due to trap, but for larger lattice depths a density wave can be formed 10, 15.

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