Interaction-Dependent Temperature Effects in Bose-Fermi Mixtures in Optical Lattices

M. Cramer

Institut für Theoretische Physik, Albert-Einstein Allee 11, Universität Ulm, Germany
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We present a quantitative finite temperature analysis of a recent experiment with Bose-Fermi mixtures in optical lattices, in which the dependence of the coherence of bosons on the interspecies interaction was analyzed. Our theory reproduces the characteristics of this dependence and suggests that intrinsic temperature effects play an important role in these systems. Namely, under the assumption that the ramping up of the optical lattice is an isentropic process, adiabatic temperature changes of the mixture occur that depend on the interaction between bosons and fermions. Matching the entropy of two regimes—no lattice on the one hand and deep lattices on the other—allows us to compute the temperature in the lattice and the visibility of the quasimomentum distribution of the bosonic atoms, which we compare to the experiment.

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Ultracold atoms in optical lattices are, due to the available impressive control over system parameters, ideal candidates for "quantum simulators" that mimic condensed matter systems [1]. We have already seen them display the transition to a Mott insulator [2], Fermi surfaces have been observed [3], and, recently, the finite temperature phase diagram for bosonic superfluids in an optical lattice has been obtained experimentally [4]. Multicomponent mixtures, among them mixtures of bosonic and fermionic atoms, offer a variety of additional quantum phases of matter. Charge-density waves, supersolids, and exotic Mott-insulator and superfluid phases have been predicted [5] and we will certainly see experimental signatures of these in the near future. Of course, temperature plays a prime role for such quantum simulators and its influence needs to be understood or, better yet, be under control. But even just determining the temperature in an optical lattice is an extremely difficult task [4,6]. Thermometry methods for such systems without lattices are however well established. Hence, under the assumption that the lattice is ramped up adiabatically (which is usually a good approximation and was also recently confirmed for bosons in optical lattices [4]), i.e., without changing the entropy, one may make inferences about the temperature in the lattice using entropy-matching methods. Not only does this hold the opportunity for thermometry in the lattice but also offers the possibility to further cool the atoms [7].

Here, we study interaction-dependent temperature effects in Bose-Fermi mixtures under the assumption that the lattice is raised isentropically. We compare our results to the visibility of the quasimomentum distribution measured in Ref. [8] for a ^{87}Rb-^{40}K mixture. By matching the entropy of two very different regimes (with and without lattice), we are able to take all experimental parameters (such as the anisotropic trapping potential, the number of particles, and the lattice parameters) into account, leaving no free parameters in our theory. We show that these effects have a significant influence on the coherence of the bosonic atoms and depend strongly on the interaction between the two species, in agreement with the experiment. Hence, we are faced with a situation in which intrinsic adiabatic temperature effects play a dominant role and, as we argue below, have already been observed.

More specifically, we calculate the entropy as a function of the temperature in the absence of the lattice by invoking the Hartree-Fock-Bogoliubov-Popov mean-field approximation for the bosons and including the fermions in a self-consistent mean-field interaction. To describe the mixture in the lattice, we use the single-band Bose-Fermi-Hubbard Hamiltonian and calculate the entropy as a function of the temperature for a deep lattice perturbatively. For both regimes, we assume that the mixture is in thermal equilibrium such that we can assign one temperature to it. This results in temperature-entropy diagrams as in Fig. 1 and allows us to obtain the temperature in the lattice T_f as a function of the initial temperature T_i by matching the corresponding entropies (see Fig. 2). The resulting adiabatic heating or cooling of these isentropic processes was analyzed for purely fermionic [9] and bosonic [7,10] systems and a Fermi gas of atoms that can pair into molecules via a Feshbach resonance [11]. For fixed interparticle interaction, loss of bosonic coherence due to the presence of fermions was observed experimentally [12,13] and attributed to intrinsic temperature effects in Refs. [12,14,15], while in Refs. [16,17] different explanations were put forward. The adiabatic assumption was recently confirmed experimentally for bosons [4]. These studies show that T_f can depend strongly on the system parameters, prime among them the inhomogeneity introduced by the trapping potential, and hence realistic descriptions should take all of them into account. To the best of our knowledge, our analysis is the first to be directly comparable to the experiment over the full range of interspecies interactions and to fully take the experimental situation into account.

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Starting from the microscopic model of a mixture of bosonic atoms of mass m_B and fermionic atoms of mass m_F subject to their respective trapping potentials, and interacting via contact interactions parametrized by the s wave scattering lengths a_{BB} (Bose-Bose) and a_{BF} (Bose-Fermi), we invoke the Hartree-Fock-Bogoliubov-Popov approximation [18,19] for the bosons and include the fermions in a self-consistent mean-field approximation [20]. This yields a set of coupled equations, which we solve self-consistently with an iterative numerical scheme (see, e.g., Ref. [14] for more details).

After convergence, we are in the position to compute the entropy of the mixture in thermal equilibrium. For the parameters [21] of the experiment in Ref. [8], we show the resulting entropy as a function of the temperature in Fig. 1. We can see that it depends only weakly on the interaction a_{BF}—in stark contrast to the situation including the lattice, as we will see below. Furthermore, over the whole range of interactions, it is higher than the entropy for a purely bosonic system. Note that this is not the same as the noninteracting situation due to the fermionic contribution to the entropy of the mixture.

For sufficiently deep optical lattices, the system may be described [23] by the single-band Bose-Fermi-Hubbard Hamiltonian [24], $\hat{H} = \hat{J} + \hat{H}_0$, $\hat{J} = -J_B \sum_{\langle i,j \rangle} \hat{b}_i^\dagger \hat{b}_j - J_F \sum_{\langle i,j \rangle} \hat{f}_i^\dagger \hat{f}_j$, $\hat{H}_0 = \sum_i [U \hat{n}_i(\hat{n}_i - 1)/2 + V \hat{n}_i \hat{m}_i - \mu_i \hat{n}_i - \nu_i \hat{m}_i]$, where $\hat{n}_i = \hat{b}_i^\dagger \hat{b}_i$, $\hat{m}_i = \hat{f}_i^\dagger \hat{f}_i$, the $\hat{b}_i$ ($\hat{f}_i$) are bosonic (fermionic) annihilation operators, and the site-dependent chemical potentials account for the trapping potentials and control the number of particles. This model is obtained from the microscopic model by expanding the field operators in the Wannier basis and neglecting all bands above the lowest band [23] and contributions beyond nearest neighbors. The amplitudes $J_{B/F}$, U, μ_i, ν_i, $V \propto a_{BF}$ are then obtained from a band-structure calculation for appropriate lattice parameters [21]. While the influence of higher bands cannot be completely ruled out and can have an effect on the bosonic coherence [16,25], we are in a regime in which their occupation is expected to be small [23]. For a discussion of the validity of the single band approximation and contact interaction, we refer the reader to Refs. [16,25,26].

We obtain the entropy as a function of temperature employing the thermodynamic interaction picture, treating $\hat{J}$ as a perturbation up to first order. For a given temperature this yields the partition function and the total number of bosons and fermions as a function of the chemical potentials. Numerically solving $\langle \sum_i \hat{n}_i \rangle = N_B$, $\langle \sum_i \hat{m}_i \rangle = N_F$ then yields the entropy for a given temperature and particle numbers up to first order in $\hat{J}$. We consider the full three-dimensional anisotropic experimental situation.

Figure 1 summarizes the result of this procedure for the experimental parameters of Ref. [8]. The most prominent feature of $S(T)$ is its strong dependence on the Bose-Fermi interaction, while we found only a weak dependence without the lattice. For fixed temperature, starting

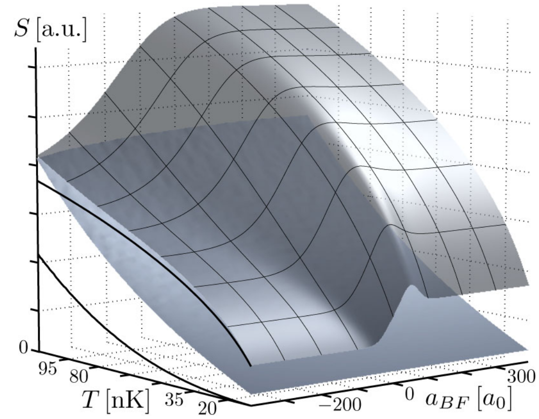

FIG. 1 (color online). Entropy as a function of temperature and Bose-Fermi scattering length a_{BF} ($\propto V$, the Bose-Fermi interaction) with (translucent surface) and without (opaque surface) a 12 recoil energies deep optical lattice. Bold lines at $a_{BF} = -400$ show the same for a purely bosonic system, for which the entropies are independent of a_{BF} (upper line, including the lattice; lower line, without lattice). The mixture consists of 4×10^5 ^{87}Rb and 3×10^5 ^{40}K atoms, and parameters [21] are as in the experiment in Ref. [8].

from a plateau for strong attraction, the entropy increases until it reaches a maximum around $a_{BF} = 0$, from which it decreases with increasing a_{BF} to a plateau for strong repulsion. It is this behavior that will crucially influence the temperature T_f in the lattice and hence also the coherence of the bosonic atoms, which displays the same strong dependence on the Bose-Fermi interaction (see below). The plateaus for large $|a_{BF}|$ are easily explained: For large repulsion, phase separation occurs, and once this phase is entered, increasing a_{BF} further does not have any effect. For large attraction on the other hand, bosons and fermions are forced to occupy the same lattice sites, and again further increasing $|a_{BF}|$ does not have any effect. Comparing the entropy of the mixture to the purely bosonic situation (note that this is not the same as the noninteracting case, as also for $a_{BF} = 0$, the fermions contribute to the total entropy), we see that the former is always higher than the latter for the considered parameter regime. As we will see below, while the adiabatic ramping up of the lattice leads to adiabatic cooling, this causes the mixture to be less cooled than bosons would be without fermions.

Having obtained the entropies with, S_f, and without, S_i, lattice, we are now in the position to obtain the temperature in the lattice, T_f, for a given initial temperature, T_i, by matching the respective entropies $S_f(T_f) = S_i(T_i)$. If the optical lattice is indeed raised adiabatically and the mixture is in thermal equilibrium, this enables us to compute T_f as a function of T_i, which can be measured, as, without lattice, thermometry methods are well established. Figure 2 shows the result obtained by matching the entropies in Fig. 1. As S_f in Fig. 1 already suggests, we find a strong dependence of the temperature in the lattice on the

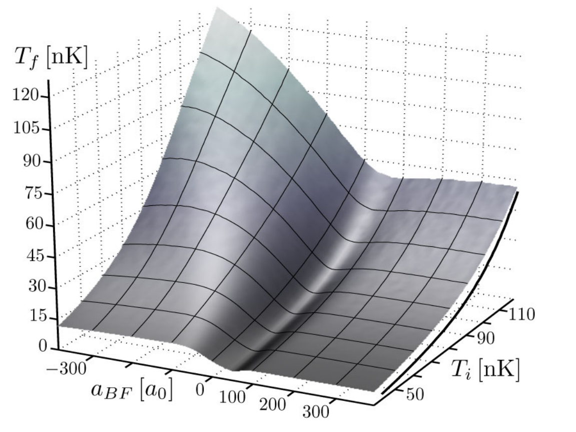

FIG. 2 (color online). Temperature of the mixture in the lattice (obtained by entropy matching from the data in Fig. 1) as a function of the Bose-Fermi scattering length a_{BF} and the initial temperature without lattice T_i. The bold line at $a_{BF} = 400$ shows the same for a purely bosonic system, for which the final temperature is independent of a_{BF}.

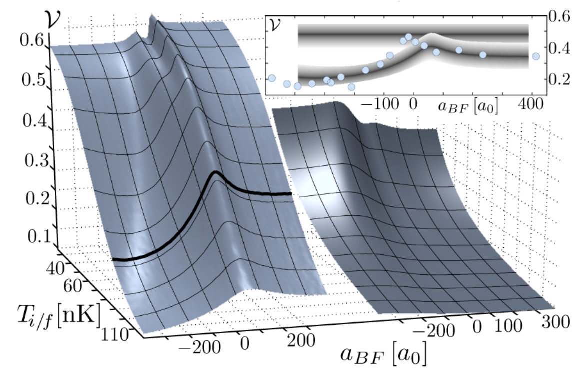

FIG. 3 (color online). Visibility, $\mathcal{V}$, of the time-of-flight distribution at a lattice depth of 12 recoil energies as a function of the Bose-Fermi scattering length a_{BF} and initial temperature without the lattice T_i (left surface, T_f obtained as in Fig. 2) and temperature in the lattice T_f (right surface). The inset shows the same at fixed T_i (the bold line on the left surface, chosen such that the purely bosonic situation matches the experiment [8]) for the purely bosonic situation (including an uncertainty of 10% in T_i) and the mixture (including an uncertainty of 15% in T_i). Circles are measurements from [8]. The mixture consists of 4×10^5 ^{87}Rb and 3×10^5 ^{40}K atoms; all parameters are as in [8]. There are no free parameters in the theory.

Bose-Fermi interaction, most pronounced for high initial temperatures. The qualitative behavior of T_f is similar to that of S_f: For fixed T_i starting from a plateau at large attraction, the temperature decreases with increasing a_{BF} and reaches a minimum around $a_{BF} = 0$, from which it increases with increasing a_{BF} to a plateau at high repulsion. We also depict T_f for a purely bosonic system, which shows that while over most of the parameter regime the mixture is cooled, the cooling is less than it would be without fermions. Being equipped with T_f, we now study the dependence of the bosonic coherence on the Bose-Fermi interaction.

Letting the atom cloud evolve freely for a time t, the density of bosons $n(\boldsymbol{p})$ is well approximated by [27,28]

$$\sum_{\boldsymbol{i},\boldsymbol{j}} \langle \hat{b}_{\boldsymbol{i}}^\dagger \hat{b}_{\boldsymbol{j}} \rangle e^{i\boldsymbol{p}a(\boldsymbol{i}-\boldsymbol{j})} e^{i(1/4\tau)(|\boldsymbol{j}|^2-|\boldsymbol{i}|^2)} w\left(\boldsymbol{p} - \frac{\boldsymbol{i}}{2a\tau}\right) w\left(\boldsymbol{p} - \frac{\boldsymbol{j}}{2a\tau}\right),$$

where $\tau = \hbar t/(2m_B a^2)$ and w is the Fourier transform of the Wannier function centered at zero. This density is measured by taking an absorption image of the cloud, resulting in the column density $n(p_x, p_y) = \int dp_z n(\boldsymbol{p})$. For shallow lattices and low temperatures, i.e., in the superfluid regime, this density displays a pronounced interference pattern, which vanishes deep in the Mott regime (ultradeep lattices) and for high temperatures. Hence, the visibility of this interference pattern, $\mathcal{V} = \frac{n_{\max} - n_{\min}}{n_{\max} + n_{\min}}$ [29], is an indicator for the coherence of the ^{87}Rb atoms. We calculate $\mathcal{V}$ for a given temperature and number of particles by computing the two-point correlations $\langle \hat{b}_{\boldsymbol{i}}^\dagger \hat{b}_{\boldsymbol{j}} \rangle$ in thermal perturbation theory up to first order in $\hat{J}$. The result of this computation is shown in Fig. 3 for parameters as in Refs. [8,21] and for two different temperatures: We depict $\mathcal{V}$ as a function of the temperature in the lattice T_f (right surface) and as a function of the initial temperature T_i (left surface). This corresponds to two different scenarios: (a) where the adiabatic cooling mechanism is omitted and hence T_f does not depend on the Bose-Fermi interaction and (b) the more realistic scenario in which the final temperature does depend on a_{BF} through the entropy matching described above. As Fig. 3 shows, the two scenarios result in opposed behaviors of $\mathcal{V}$ as a function of the interaction strength a_{BF}. For all temperatures and large $|a_{BF}|$, the visibility $\mathcal{V}$ is higher on the attractive side than on the repulsive side of the interaction for scenario (a), while we see the exact opposite for (b).

The inset of Fig. 3 compares our results directly to the experiment in Ref. [8]. We assume that the initial temperature for all measurements was approximately the same as in the purely bosonic situation. We can see that the results display the same qualitative behavior: Starting at strong attraction, the visibility decreases to a minimum, from which it increases with increasing a_{BF} up to a maximum at around $a_{BF} = 0$, and finally decreases to a plateau for strong repulsion. This is in stark contrast to what one finds without taking intrinsic temperature effects into account (see right surface in Fig. 3): At the relevant temperatures, the visibility simply decreases monotonically with increasing interaction strength.

Figure 3 also shows a shift of the theoretical results relative to the experimental data. All our results are parametrized by the Bose-Fermi scattering length, which is tuned in the experiment by addressing the magnetic Feshbach resonance at around $B_0 \approx 546.9$ G [30]. Close to resonance, magnetic field B and scattering length are related by $a_{BF} = a_{\mathrm{bg}}(1 - \frac{\Delta B}{B - B_0})$, where the resonance is at B_0, a_{bg} is the background scattering length, and ΔB the width of the resonance. A faithful experimental determination of all the parameters in this relation is an extremely difficult endeavour. They depend on external parameters such as the trapping potential—and, even more so, the tight "trapping" within a lattice site [26]. In particular, the latter complicates a direct comparison to the experiment: Neither *ab initio* calculations for realistic interatomic potentials nor experimental measurements of the dependence of a_{BF} on the magnetic field are available for the situation at hand. In fact, the experimental visibility shown in Fig. 3 is really a function of the magnetic field, $a_{BF} = a_{\rm bg}(1 - \frac{\Delta B}{B - B_0})$ with $B_0 = 546.9$ G, $\Delta B = -2.9$ G, and $a_{\rm bg} = -185 a_0$ [22]. This scattering length is *a priori* not the same as the one used to model the interatomic contact potential. It will be an exciting challenge to explore whether this may explain the discrepancy between theory and experiment in Fig. 3 and might result in a better understanding of the dependence of a_{BF} on external potentials. We hope that, due to the pronounced features of the visibility—in particular the location of the maximum—the present study can contribute to the work along this direction.

In conclusion, we have studied intrinsic temperature effects in Bose-Fermi mixtures taking the full three-dimensional anisotropic experimental situation into account. Under the adiabatic assumption, we have determined the temperature in the lattice as a function of the temperature before the lattice is ramped up and found a strong dependence on the interspecies interaction. This dependence affects the coherence of the bosons and is displayed in the visibility of the time-of-flight interference pattern, which we have compared to the experiment in Ref. [8], finding qualitative agreement. Not including these temperature effects results in a very different dependence on the interaction and leads us to conclude that they need to be incorporated into any realistic description of Bose-Fermi mixtures in optical lattices.

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Note added.—After completion of this work, related results were reported in [31]. By means of generalized dynamical mean-field theory, the authors come to similar conclusions, including the discrepancy concerning the peak in the visibility.

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