Do Mixtures of Bosonic and Fermionic Atoms Adiabatically Heat Up in Optical Lattices?

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Mixtures of bosonic and fermionic atoms in optical lattices provide a promising arena to study strongly correlated systems. In experiments realizing such mixtures in the quantum-degenerate regime the temperature is a key parameter. We investigate the intrinsic heating and cooling effects due to an entropy-preserving raising of the optical lattice, identify the generic behavior valid for a wide range of parameters, and discuss it quantitatively for the recent experiments with ^{87}Rb and ^{40}K atoms. In the absence of a lattice, we treat the bosons in the Hartree-Fock-Bogoliubov-Popov approximation, including the fermions in a self-consistent mean-field interaction. In the presence of the full three-dimensional lattice, we use a strong coupling expansion. We find the temperature of the mixture in the lattice to be always higher than for the pure bosonic case, shedding light onto a key point in the analysis of recent experiments.

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Interacting bosonic and fermionic systems play a key role in several contexts in physics, quite prominently in the BCS theory of superconductivity. Systems of dilute atomic gases (in optical lattices) offer the perspective of simulating such mixtures or purely bosonic or fermionic systems under extraordinarily controlled conditions [1,2]. Bose-Fermi mixtures in optical lattices exhibit a rich physical behavior, including a wealth of novel phases, charge density waves, and supersolids [3]. Recent experiments have succeeded in preparing such mixtures in optical lattices [4], notably the realization of a stable bosonic ^{87}Rb and fermionic ^{40}K mixture in three-dimensional optical lattices [5,6].

To achieve realizations of such strongly correlated systems in the quantum-degenerate regime, very low temperatures have to be reached. This is not only a difficult prescription but also, while thermometry methods in the absence of a lattice are established, it is not entirely clear how to measure the temperature in its presence. Indeed, following recent experiments with cold bosonic atoms, an intriguing and fruitful controversy [7] has arisen concerning the general question relevant to experiments with ultracold atoms in optical lattices: How cold, after all, is the system in the optical lattice expected to be? For Bose-Fermi mixtures, this question is even harder to answer as the additional degrees of freedom leave more room for different explanations. Interactions between bosons and fermions result in an effectively reduced repulsion between bosons, independent of the sign of the Bose-Fermi interaction. Hence, one might well expect an increase in coherence as compared to the purely bosonic case. Quite surprisingly, however, the opposite effect (as measured via the visibility of the quasimomentum distribution) was observed [5,6]. The theoretical work Ref. [8], based on numerical quantum Monte Carlo and density-matrix-renormalization-group simulations of one-dimensional systems, points towards the possibility that this might actually be due to a finite temperature effect.

In this work, we discuss the thermodynamics of adiabatically loading trapped Bose-Fermi mixtures into optical lattices. During this procedure, the entropy remains constant and leads to intrinsic cooling or heating processes. We argue that one should expect a significant adiabatic heating of the mixture, not to be confused with experimental imperfections such as parametric heating. This is by no means a marginal effect. This resulting temperature affects the physics of the strongly correlated system once the optical lattice is present. We identify the generic behavior and discuss it on the basis of the values corresponding to the experiment described in Ref. [6]. More precisely, the presence of fermions leads either to a more distinct heating or a less distinct cooling of the mixture. We study in detail the behavior of these adiabatic heating and cooling effects—complementing results for purely (non)interacting bosonic [9–11] and noninteracting fermionic [12] systems—and analyze and flesh out the specific role of the fermions in this adiabatic process.

Our results rely on well-established approximations for the two regimes we set out to connect: (i) For trapped mixtures of bosonic and fermionic atoms we apply the Hartree-Fock-Bogoliubov-Popov (HFBP) approximation along with a mean-field approximation for the interparticle interaction; (ii) subjecting this mixture to a deep optical lattice allows us to invoke a strong-coupling expansion for the Bose-Fermi-Hubbard model. Assuming the raising of the lattice to be an adiabatic, entropy-preserving process, then enables us to connect regimes (i) and (ii) without the need for the approximation schemes to be valid in the intermediate regime. It is the strength of this type of argument that generically, the final state is path-independent in this adiabatic process.

Trapped mixture without optical lattice.—Subsequently, we will discuss the thermodynamics of the Bose-Fermi mixture in an isotropic harmonic trap in the absence of an optical lattice. We will insist on being close to an experimental situation in our description, and take the full three-dimensional situation into account. We start from the grand-canonical Hamiltonian

$$\hat{H} = \int d\boldsymbol{r}\Big(\hat{\Phi}^{\dagger}\Big[\hat{h}_B + \frac{g}{2}\hat{\Phi}^{\dagger}\hat{\Phi} + f\hat{\Psi}^{\dagger}\hat{\Psi}\Big]\hat{\Phi} + \hat{\Psi}^{\dagger}\hat{h}_F\hat{\Psi}\Big),$$

where we denoted the bosonic (fermionic) field operators by $\hat{\Phi}$ ($\hat{\Psi}$), the interaction amplitudes g, f are related to the respective scattering lengths as $g = 4\pi\hbar^2 a_{BB}/m_B$, $f = 2\pi\hbar^2 a_{FB}(m_B + m_F)/(m_F m_B)$, the free part of the bosonic Hamiltonian is given by $\hat{h}_B = -\hbar^2\boldsymbol{\nabla}^2/(2m_B) + V_B - \mu_B$, $V_B = m_B\omega_B^2\boldsymbol{r}^2/2$, and accordingly for $\hat{h}_F$. We thus restrict ourselves to isotropic traps, taking geometrical averages of the trapping frequencies in the actual experiment.

For the bosonic sector, we invoke the standard local-density HFBP approximation, which is a self-consistent mean-field scheme that has proven applicable to a wide temperature regime [13,14]. The interspecies interaction is treated in the self-consistent mean-field approximation $\hat{\Phi}^{\dagger}\hat{\Phi}\hat{\Psi}^{\dagger}\hat{\Psi} \approx \hat{\Phi}^{\dagger}\hat{\Phi}\langle\hat{\Psi}^{\dagger}\hat{\Psi}\rangle + \langle\hat{\Phi}^{\dagger}\hat{\Phi}\rangle\hat{\Psi}^{\dagger}\hat{\Psi} - \langle\hat{\Phi}^{\dagger}\hat{\Phi}\rangle\langle\hat{\Psi}^{\dagger}\hat{\Psi}\rangle$ [15], where we define the fermionic density $\langle\hat{\Psi}^{\dagger}\hat{\Psi}\rangle := m$ and the total bosonic density $\langle\hat{\Phi}^{\dagger}\hat{\Phi}\rangle := n = n_0 + n_T$, composed of the condensate n_0 and noncondensate density n_T. This yields the following set of coupled equations: (i) The finite temperature Gross-Pitaevskii equation in the Thomas-Fermi approximation (which may be safely applied for the high number of atoms considered), governing the condensate density, $n_0 = \max\{0, (\mu_B - V_B - fm)/g - 2n_T\}$, where the chemical potential is fixed by the given total number of bosons, $N_B = N_0 + N_T = \int d\boldsymbol{r}n_0 + \int d\boldsymbol{r}n_T$. (ii) The thermal density of bosons ($k_B T = 1/\beta$) $n_T = \int d\boldsymbol{p}[(u_+^2 + u_-^2)(e^{\beta\epsilon} - 1)^{-1} + u_-^2]/(2\pi)^3$, where the Bogoliubov amplitudes are given by $2u_{\pm}^2 = (\hbar^2\boldsymbol{p}^2/(2m_B) + V_B - \mu_B + 2gn + fm)/\epsilon \pm 1$, and the quasiparticle spectrum reads $\epsilon^2 = (\hbar^2\boldsymbol{p}^2/(2m_B) + V_B - \mu_B + 2gn + fm)^2 - g^2 n_0^2$. Finally, (iii) the fermionic density in local-density approximation $m = \int(e^{\beta\delta} + 1)^{-1}d\boldsymbol{p}/(2\pi)^3$, $\delta = \hbar^2\boldsymbol{p}^2/(2m_F) + V_F - \mu_F + fn$, where the chemical potential is fixed by the given total number of fermions $N_F = \int m d\boldsymbol{r}$.

For given temperature T and particle numbers N_B, N_F, we solve (i)–(iii) self-consistently in the following way: Starting with no interaction between bosons and fermions and $n_T = 0$, we (a) compute n_0 and μ_B by solving (i) under the particle number restriction, (b) obtain n_T from (ii), (c) iterate (a) and (b) until convergence, (d) solve (iii), which yields m and μ_F, (f) iterate (a)–(d) until convergence.

After convergence, we are equipped with the spectra and can compute the entropy of the mixture [16], $S/k_B = \int[s_B + s_F]d\boldsymbol{p}d\boldsymbol{r}/(2\pi)^3$, with individual contributions $s_B = \beta\epsilon/(e^{\beta\epsilon} - 1) - \log(1 - e^{-\beta\epsilon})$, $s_F = \beta\delta/(e^{\beta} + 1) + \log(1 + e^{-\beta})$. In Fig. 1, we show the obtained results for the parameters of the experiments in Ref. [6] for different ratios N_F/N_B. The critical temperature for condensation is ≈ 205 nK and no thermal cloud was discernible in the

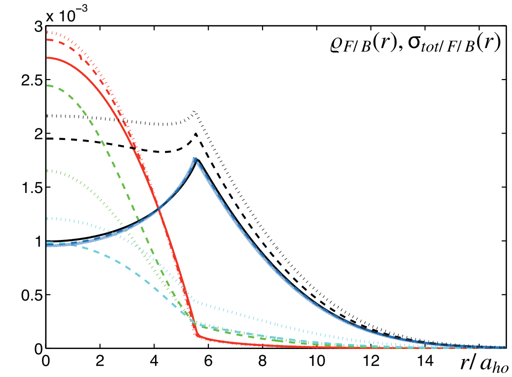

FIG. 1 (color). Densities $\varrho_B = na_{\text{ho}}^3/N_B$ (red), $\varrho_F = ma_{\text{ho}}^3/N_F$ (green) and entropy densities $\sigma_{B/F} = s_{B/F}a_{\text{ho}}^3/10^4$ (blue and cyan, scaled by 10^4 for clarity), $\sigma_{\text{tot}} = \sigma_B + \sigma_F$ (black line), in units of the bosonic harmonic oscillator length a_{ho}. The shown data sets correspond to the experiment in Ref. [6] and a temperature of 95 nK. The mixture consists of 10^5 ^{87}Rb atoms and no (solid lines), $N_F = 0.03N_B$ (dashed lines), and $N_F = 0.07N_B$ (dotted lines) 40 K atoms.

experiment, corresponding to a condensate fraction of at least 80% and a initial temperature below 95 nK. The bosonic entropy is highest at the condensate boundary, where the density of the thermal cloud has its maximum. In turn, s_F is highest in the center of the trap. We can see that the bosonic contribution to the total entropy remains basically unaltered by the presence of the fermions, their main contribution stemming from s_F itself.

Trapped mixture in deep optical lattices.—To describe the system in the presence of the lattice, we use the single-band Bose-Fermi-Hubbard Hamiltonian [3,17] $\hat{H} = \hat{J} + \sum_i \hat{h}_i$, $\hat{J} = -J_F\sum_{\langle i,j\rangle}\hat{f}_i^{\dagger}\hat{f}_j - J_B\sum_{\langle i,j\rangle}\hat{b}_i^{\dagger}\hat{b}_j$, $\hat{h}_i = U\hat{n}_i(\hat{n}_i - 1)/2 + V\hat{n}_i\hat{m}_i - \mu_i^B\hat{n}_i - \mu_i^F\hat{m}_i$. Here, the operator $\hat{b}_i$ ($\hat{f}_i$) annihilates a boson (fermion) at site i and $\hat{n}_i = \hat{b}_i^{\dagger}\hat{b}_i$, $\hat{m}_i = \hat{f}_i^{\dagger}\hat{f}_i$. $\hat{J}$ accounts for the tunneling of atoms from one site to neighboring sites, U, V are the intraspecies, respectively, interspecies on-site interactions, and $\mu_i^{B/F} = \mu_{B/F} - V_i$ are on-site chemical potentials controlling the particle number via $\mu_{B/F}$ and accounting for the harmonic confinement V_i, which is approximately the same for both species. For deep lattices the tunneling may be treated as a perturbation in $J_{B/F}$. Up to second order and within local-density approximation (assuming that the trapping potentials are the same at neighboring sites), the free energy is found to be $F = -\log(Z)/\beta = -\sum_i\log(z_i)/\beta - 3\sum_i(J_B^2 b_i + J_F^2 f_i)/z_i^2$, where $b_i = \sum_{n,n'=0}^{\infty} n(n'+1)b_i^{n,n'}$, $f_i = \sum_{n,n'=0}^{\infty}\exp[-\beta(\epsilon_i^{n,1} + \epsilon_i^{n',0})][\exp(\beta V(n' - n)) - 1]/(V(n' - n))$,

$$b_i^{n,n'} = \sum_{m,m'=0,1} e^{-\beta(\epsilon_i^{n,m} + \epsilon_i^{n',m'})}\frac{e^{\beta[U(n'-n-1)+V(m'-m)]} - 1}{U(n' - n - 1) + V(m' - m)},$$

and the unperturbed on-site energies and corresponding partition functions are given by $\epsilon_i^{n,m} = Un(n-1) - \mu_i^B n - \mu_i^F m + Vnm$, $z_i = \sum_{n=0}^{\infty}[\exp(-\beta\epsilon_i^{n,0}) + \exp(-\beta\epsilon_i^{n,1})]$. Starting from the above expression for the free energy, we calculate the chemical potentials for given particle numbers by numerically solving $N_{B/F} = -\partial F/\partial\mu_{B/F}$, where the right-hand side is obtained by numerically differentiating the free energy with respect to the chemical potentials. Similarly, by differentiating with respect to β, we then compute the entropy of the mixture in the lattice [16]: $S/k_B = \beta^2\partial F/\partial\beta$.

Discussion.—We are now in the position to assess the situation when raising the lattice is an adiabatic process. Figure 2 shows the entropy as a function of temperature in a system of 10^5 ^{87}Rb atoms in a three-dimensional trap. In this figure, we use the experimental parameters of Ref. [6], but the findings are valid for a wide range of parameters. Both the entropy without and in the presence of the optical lattice is depicted for the purely bosonic case and a small admixture of fermions. We see that generally, for fixed lattice depth V_0, below a certain temperature $\bar{T}$, the adiabatic ramp-up gives rise to adiabatic cooling, whereas above $\bar{T}$ we find adiabatic heating. Because of the trapping potential and its dependence on V_0 [the trapping frequencies change according to $\omega_i^2 \to \omega_i^2 + 8V_0/(m_B w_i^2)$, $i = x, y, z$; see [6]], the entropy is not a monotonic function of V_0 for fixed temperature; see Ref. [9] for a discussion of this effect in noninteracting bosonic systems. Both above and below the threshold $\bar{T}$, the presence of the fermions results in a higher final temperature as compared to the same situations with bosons only. This is most dramatic at initial temperatures for which pure bosons are adiabatically cooled and in the mixture adiabatic heating occurs: For an initial temperature of 90 nK and a final lattice depth of $15E_R$, the temperature is $\approx$40 nK higher in the presence of $0.07N_B$ fermions, corresponding to an increase of $\approx$67%; see Fig. 3. This affects the contrast of the interference pattern [8] analyzed in those experiments. This behavior is generic, valid, in particular, for both experiments of Refs. [5,6] as well as for experiments performed in an isotropic and shallower trap [18], where the initial temperature was always below the threshold: For any initial temperature, the entropy without the lattice is always much higher in the presence of fermions, even for a relatively small admixture of ^{40}K atoms. While below $\bar{T}$ adiabatic cooling occurs, this effect is lessened compared to the purely bosonic case. Above $\bar{T}$ and in the presence of the lattice, the entropy including fermions is higher, thus reducing the heating effect. However, this cannot compensate for the high initial difference of entropies; see Fig. 3.

Note that the influence of fermions is most distinguished in the absence of the lattice. This is plausible when considering the form of the unperturbed free energy in the presence of the lattice: $\epsilon_i^{n,0} = Un(n-1) - \mu_i^B n$ and $\epsilon_i^{n,1} = Un(n-1) - \mu_i^B n + Vn$ are different only by an alteration of a definition of the bosonic chemicals potentials (the total number of bosons is the same with and without fermions), leading for low temperatures to approximately the same expression for the entropy. Taking a closer look at the situation including the lattice, we see that, at low temperatures, more fermions lead to a lower entropy—the interspecies attraction reducing the mobility of the atoms and thus the number of possible microstates. In turn, at higher temperatures interactions become less important and the entropy increases with the number of fermions. While this cannot compensate the initial difference in entropies, it however reduces the heating effect for higher initial temperature; see Fig. 3. This effect could be observed in the currently available experiments: At a fixed lattice depth the difference between the situation with and

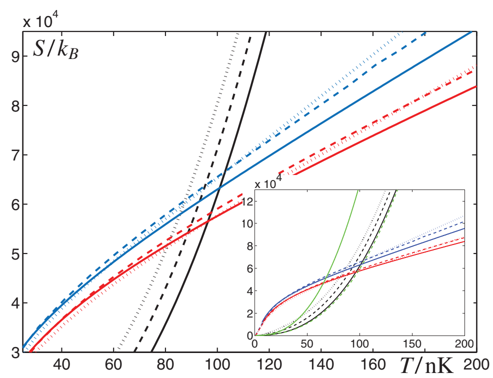

FIG. 2 (color). Entropy as a function of temperature for the parameters of Ref. [6]. The mixture consists of 10^5 ^{87}Rb atoms and $N_F = 0$ (solid lines), $0.03N_B$ (dashed lines), $N_F = 0.07N_B$ (dotted lines) ^{40}K atoms in a lattice of various depths (blue, $15E_R$; red, $30E_R$; black, no lattice; resulting in different V_i; see main text). The inset shows the same at a larger scale, including the entropy for the purely bosonic case obtained from analytical expressions (green) valid below the critical temperature (dashed line) and at ultralow T (solid line); see[20].

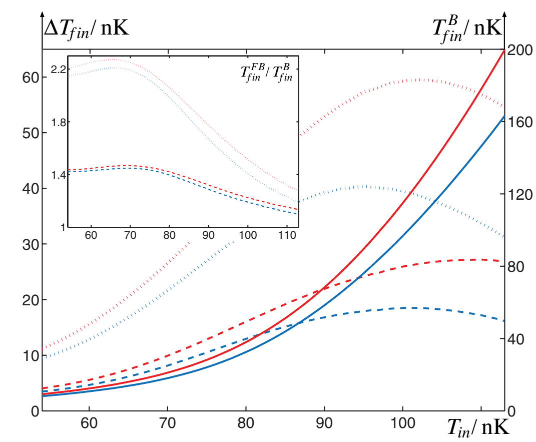

FIG. 3 (color). Difference $\Delta T_{\rm fin} = T_{\rm fin}^{FB} - T_{\rm fin}^{B}$ between the final temperature in the lattice with and without fermions as a function of the initial temperature without lattice. Parameters are as in Fig. 2. For any initial temperature, the presence of the fermions leads to higher final temperatures as compared to the purely bosonic case. Solid lines depict the final temperature $T_{\rm fin}^{B}$ without fermions (right scale).

without fermions should first increase, reach a maximum, and finally decrease with increasing initial temperature.

Summary and outlook.—We have quantitatively explored the adiabatic cooling and heating effects that are to be expected in experiments with Bose-Fermi mixtures in optical lattices, crucial when reaching a strongly correlated system. On intuitive grounds, one could have suspected that the features observed in experiments were due to a shift of the bosonic Mott lobes in the presence of fermions, their presence effectively altering the local chemical potential. This is indeed the case, but predicts an increase of coherence [8], the opposite of which was observed in experiments. We have seen that for parameters of present experiments, the resulting temperature is much larger than expected from thermometry without the lattice. Methods to assess the temperature of samples in optical lattices would clearly be a breakthrough, promising ideas being, e.g., the characterization of the shell structure of local densities [19]. A link to the expected visibility from our analysis is provided by Ref. [8]. This analysis applies to a one-dimensional situation, yet for the visibility it is expected to give a clear guideline: It is seen how the bosonic visibility decreases with increasing temperature. A clear-cut quantitative analytical analysis of the quasimomentum distribution at finite temperature is still lacking and poses—even for purely bosonic systems—an exciting challenge and constitutes a test bed for theories developed in the condensed matter context. It is the hope that the present work can significantly contribute to the clarification of the intriguing discussion on the interpretation of observed data and on the available theoretical models for mixtures of bosonic and fermionic atoms in optical lattices.

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