Self-Trapping of Bosons and Fermions in Optical Lattices

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We theoretically investigate the enhanced localization of bosonic atoms by fermionic atoms in three-dimensional optical lattices and find a self-trapping of the bosons for attractive boson-fermion interaction. Because of this mutual interaction, the fermion orbitals are substantially squeezed, which results in a strong deformation of the effective potential for bosons. This effect is enhanced by an increasing bosonic filling factor leading to a large shift of the transition between the superfluid and the Mott-insulator phase. We find a nonlinear dependency of the critical potential depth on the boson-fermion interaction strength. The results, in general, demonstrate the important role of higher Bloch bands for the physics of attractively interacting quantum gas mixtures in optical lattices and are of direct relevance to recent experiments with 87Rb - 40K mixtures, where a large shift of the critical point has been found.

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Ultracold multicomponent gases offer new insight into the atomic interspecies interaction. In optical lattices, the interplay between interaction and tunneling is reflected in the complex phase diagram of boson-fermion mixtures. The multitude of predicted phases has been studied theoretically using various approaches [1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11]. In particular, the phase separation between bosons and fermions, the supersolid phase [2, 3], and the pairing of bosons and fermions forming phases of composite particles [4] have been investigated. Mixtures of bosonic 87Rb and fermionic 40K atoms in optical lattices were recently realized [12, 13] and have drawn much attention due to an unexpected large shift of the bosonic phase transition between the superfluid phase and the Mott insulator [14, 15]. The effect, which is substantial even for a small ratio of fermionic to bosonic atoms, was controversially discussed [13, 16, 17, 18], and a relatively small influence of the boson-fermion interaction on the transition was suggested. In addition, the loss of coherence due to an adiabatic heating in the optical lattice was addressed [17, 18].

In preference for a single-band Hubbard-type Hamiltonian, the influence of interaction induced orbital changes were widely neglected in calculations performed for optical lattices. In this Letter, we show by means of exact diagonalization that the attractive interaction between bosons and fermions causes substantially modified single-site densities. The nonlinearity of the interaction leads to a mutual trapping of 87Rb and 40K atoms in the centers of the wells. For high bosonic filling factors the fermion orbitals, i.e., the local atomic wave function, are strongly squeezed, which leads to a considerable deformation of the effective potential for bosons. The latter causes a large shift of the bosonic Mott transition towards shallower potentials which coincides with experimental results [12, 13]. In this Letter, we show that the contribution of higher Bloch bands, usually neglected, can be very important for the physics of ultracold quantum gases in optical lattices.

The interaction between fully spin-polarized neutral atoms in the ultracold regime can be described by a contact potential gδ(r - r'). The strength of the repulsive interaction between 87Rb atoms is given by gB = 4πℏ2/(ℏ2 aB), where aB ≈ 200a0 is the bosonic scattering length and a0 the Bohr radius. The interaction between 87Rb and 40K atoms far from a Feshbach resonance is attractive with the strength gBF = 4πℏ2/(ℏ2aBF), where µ = (mB + mF)/2 is the reduced mass and aBF ≈ -205a0 [19]. The Hamiltonian of a Bose-Fermi mixture in an optical lattice is given by $H = H_B + H_F + H_{BF}$, where $H_B$ describes the system of interacting bosons, $H_F$ the system of noninteracting fermions, and $H_{BF}$ the interaction between bosons and fermions [1]. Using the bosonic and fermionic field operators $\hat{\psi}_B(r)$ and $\hat{\psi}_F(r)$, the three parts of the Hamiltonian can be written as

$$H_B = \int d^3r \hat{\psi}_B^\dagger(r) \left[ \frac{P^2}{2m_B} + V(r) + \frac{g_B}{2} \hat{\psi}_B^\dagger(r) \hat{\psi}_B(r) \right] \hat{\psi}_B(r),$$

$$H_F = \int d^3r \hat{\psi}_F^\dagger(r) \left[ \frac{P^2}{2m_F} + V(r) \right] \hat{\psi}_F(r),$$

$$H_{BF} = g_{BF} \int d^3r \hat{\psi}_B^\dagger(r) \hat{\psi}_F^\dagger(r) \hat{\psi}_F(r) \hat{\psi}_B(r),$$

with the periodic potential $V(r)$ of the optical lattice.

Numerically, we perform an exact diagonalization of the Hamiltonian [11] in a many-particle basis [20] that includes higher orbital states and is truncated at a sufficiently high energy (see [21] for details). In our calculation, the bosonic and the fermionic subspace are diagonalized separately using a self-consistent interaction potential, which converges within a few cycles. For a known fermionic density $\rho_F(r) = \langle \hat{\psi}_F^\dagger(\hat{\psi}_F) \rangle$ the effective Hamiltonian of the bosonic subsystem is given by

$$H_B^{\text{eff}}(\rho_B) = H_B + g_{BF} \int d^3r \rho_B(r) \hat{\psi}_B^\dagger(r) \hat{\psi}_B(r).$$

The latter term
represents the interaction with the fermionic density and leads to a bosonic effective potential $V_{B}^{\text{eff}}(\rho_B) = V(r) + g_{BF} \rho_B(r)$. Starting with the density of noninteracting fermions, we determine the boson density $\rho_B(r) = \langle \Psi_B^\dagger \Psi_B \rangle$ by diagonalization of $H_B^{\text{eff}}$. Afterwards, a new fermion density can be calculated using the fermionic effective potential $V_{F}^{\text{eff}}(\rho_F) = V(r) + g_{BF} \rho_B(r)$.

We discuss the experimental situation, where one fermion ($n_F = 1$) and several bosons ($1 \leq n_B \leq 10$) are present at each lattice site. To study the effect caused by the mutual interaction, it is instructive to restrict the particles to a single lattice site. Hence, we perform the diagonalization for atoms in a symmetric well with the shape $V_0[\sin^2(kx) + \sin^2(ky)] + \sin^2(kz)$ [22]. To illustrate the orbital changes, we fit Gaussians to the calculated densities for bosons and fermions $\rho_{BF}(r) = \rho_{BF}(\sqrt{2\pi}\sigma_{BF})^{-3} \exp(-r^2/2\sigma_{BF}^2)$ [23]. The width of the Gaussians $\sigma_{BF}$ as a function of the bosonic filling $n_B$ is shown in Fig. 1 for the lattice depths $V_0 = 8E_R$, $14E_R$, and $20E_R$, where $E_R = \hbar^2 k^2 / 2m_B$ is the recoil energy of $^{87}\text{Rb}$ atoms. Since $^{40}\text{K}$ atoms are much lighter than $^{87}\text{Rb}$ atoms, the resulting density profile for a $^{40}\text{K}$ atom on a single lattice site is much broader than for the $^{87}\text{Rb}$ atoms. For a pure bosonic system (dashed lines), we observe an increase of the bosonic width with an increasing number of $^{87}\text{Rb}$ atoms, due to the boson-boson repulsion. The interaction with the single fermion leads to a compression of the boson density (solid lines), which becomes even narrower than the single-particle boson density. In fact, the bosonic width decreases slightly with an increasing $n_B$ and reaches a minimum at $n_B = 7 - 8$. This effective attractive behavior is surprising, since the attractive interaction between bosons and fermions scales linearly with $n_B$, whereas the repulsion of the bosons is proportional to $n_B^2$. This effect is caused by the strong squeezing of the fermion density due to its effective potential $V_{F}^{\text{eff}} = V(r) + g_{BF} \rho_B(r)$, that is deepened linearly with the number of bosons $n_B$ (inset of Fig. 2). The increasing curvature of the fermionic effective potential, which equals $\partial^2 V_{F}^{\text{eff}} / \partial r^2 \approx V_0 k^2 + \sqrt{2\pi} |g_{BF}| / \sigma_{BF}^2$ using the Gaussian approach, causes the width of the fermion density to be similar to the bosonic one for $n_B = 3 - 4$ and even narrower for $n_B > 4$. In our calculation, the occupation of higher single-particle fermion orbitals, due to the squeezing of the fermion density, is roughly 10% for $n_B = 4$ and reaches 40% for $n_B = 10$.

The effective potential $V_{B}^{\text{eff}}(\rho_F)$ experienced by the $^{87}\text{Rb}$ atoms is plotted in Fig. 2 for $V_0 = 14E_R$. The curvature of the the bosonic effective potential $\partial^2 V_{B}^{\text{eff}} / \partial r^2 \approx 2V_0 k^2 + \sqrt{2\pi} |g_{BF}| / \sigma_{BF}^2$ is strongly enhanced by the nonlinear dependence on the fermion width $\sigma_F$, which leads to a deepening of the bosonic effective potential with increasing $n_B$. The resulting energy gain in $\langle H_{BF} \rangle$ overcompensates the repulsion energy of the bosons. Instead of a stronger repulsion, an increasing $n_B$ causes a self-trapping of the bosons in the deepened center of the effective potential. This effect is mediated by the squeezing of the fermion orbital due to the higher boson density. The compression of boson and fermion densities should be observable in the experiments by imaging a broadened momentum distribution or by using atomic clock shifts to measure the peak density directly [24].

We now address the consequences of more than a single site but only one fermionic “impurity.” We use the same diagonalization method as above that includes the deformation of orbitals for small quasi-one-dimensional chains [21] with $5 - 7$ sites, a bosonic filling factor $1 \leq n_B \leq 3$, and $15E_R \leq V_0 \leq 20E_R$. The self-trapping causes a local deepening of the bosonic effective potential for the fermion occupied site. The gain in energy, due to the boson-fermion interaction, leads to a binding of several bosons to one fermion, which is a phenomenon resembling polaron physics [25][26]. Remarkably, we find that the fermionic impurity causes, for the above parameters, the localization of six additional bosons at its site. In experimental setups an additional confining potential is used [12][13], which establishes a finite atomic cloud, so that bosons and fermions occupy only the central lattice sites.
Because of the self-trapping, the bosons are attracted to sites that are occupied by fermions. If the fermionic filling $n_F < 1$ or the fermionic cloud is smaller than the bosonic one (as in Ref. [13]), this leads to an increase of the bosonic filling factor in mixtures in comparison with pure bosonic systems. In experiments, the predicted high bosonic site occupation will be accompanied by high losses due to three-body recombinations.

In the following, we discuss commensurately filled macroscopic cubic lattices and the implications on the Mott insulator phase transition that result from the deformation of the effective potential. In optical lattices, the bosonic superfluid to Mott insulator transition is triggered by the boson-boson interaction strength relative to the hopping amplitude. In the Bose-Hubbard framework [14, 15, 27], this is described by the ratio between the on-site interaction $U$ and the hopping parameter $J$ that both depend on the depth of the lattice potential $V_0$. For boson-fermion mixtures, both $U$ and $J$ also depend explicitly on the filling factor. However, to estimate how the interaction with the fermions influences the phase transition, we use an effective Bose-Hubbard model, where the lattice potential is substituted by the bosonic effective potential $V_{\text{eff}}^B(n_B)$ for a specific static filling factor $n_B$. This approach leads to a renormalization of the parameters $U$ and $J$ in the effective bosonic system. The on-site interaction $U$ is obtained directly from $V_{\text{eff}}^B(n_B)$ and the hopping $J$ by band-structure calculations using a finite periodic continuation of $V_{\text{eff}}^B(n_B)$ [29]. Qualitatively, the bosonic effective potential, which is shown in Fig. 3, reveals two important aspects: First, even for a single boson the minimum is deepened substantially and decreases further with an increasing number of $^{87}\text{Rb}$ atoms; second, the shape of the effective potential deviates strongly from the $V_0 \sin^2(kx)$ potential, leading to a broader barrier between neighboring lattice sites. Both effects lead to a reduced hopping between neighboring sites, whereas the on-site interaction energy is mainly increased by the stronger curvature of the effective potential. The decrease in $J$, which is larger than the effect on $U$ (inset of Fig. 3), causes narrower bands.

The ratio $U/J$ of the effective potential $V_{\text{eff}}^B(n_B)$ is plotted in Fig. 3 as a function of the lattice depth $V_0$, where the dashed black line corresponds to a pure bosonic system. The interacting system is represented by solid lines which are split for different filling factors $n_B$, since the deformation of the effective potential grows with an increasing filling factor $n_B$. Even for $n_B = 1$ the self-trapping causes a large shift of $U/J(V_0)$ towards higher values, which is further enhanced with an increasing $n_B$. In the following, we use the renormalized values of $U/J$ and known results for the critical point $(U/J)_c$ to calculate the shift of the critical potential depth $V_0^c$. Following the mean field results, the critical ratio depends on the lattice factor $n_B$ and obeys the relation $(U/J)_c = n_B(n_B + 1 + 2\sqrt{n_B(n_B + 1)})$, where $z = 6$ for a cubic lattice [29]. In Fig. 3 the critical values for different filling factors $n_B$ are depicted as horizontal grey lines. The critical lattice depths $V_0^c(n_B)$ for the pure bosonic system are given by the intersections of the dashed black line with the horizontal lines (open circles). According to the relation above, the phase transition for a pure bosonic system shifts to deeper lattices for an increasing filling factor $n_B$. For boson-fermion mixtures, the intersections representing the critical potential depths are indicated by solid circles. In comparison with the pure bosonic system, the phase transition in mixtures is shifted substantially towards shallower lattices.

The parameters in our calculations have been chosen such that a comparison with the experiment in Ref. [13] is possible. The critical potential depth can be estimated from Fig. 3 as $12.3E_R$ for $n_B = 1$, increases to $13.8E_R$ for $n_B = 4$, and decreases slightly for higher fillings. Comparing the boson-fermion mixture and the pure bosonic system with the same bosonic filling, the shift $\Delta V_0^c$ of the phase transition is given by the difference of the respective critical lattice depths (see arrow for $n_B = 2$). The expected shift increases substantially with the filling factor, e.g., $\Delta V_0^c = -2.2E_R$ for $n_B = 1$ and $\Delta V_0^c = -5.2E_R$ for $n_B = 4$. In Refs. [12, 13], pure bosonic systems are compared to Bose-Fermi mixtures with the same number of bosonic atoms, not accounting for the increase of the local bosonic filling factor due to the self-trapping, as discussed above. In addition, the confinement in experiments causes the formation of shells with different filling factors $n_B$. Therefore, the reported shift in Ref. [13] of approximately $-5E_R$ is an average value of a system, where at the center of the filling factor $n_B > 5$ and $n_F = 1$. Accounting for the inhomogeneous filling, we average our results for $n_B \leq 5$ to $n_B \leq 7$ leading to a shift between $-4.2E_R$ and $-5.1E_R$, which is in good agreement with the experiment. Using atomic clock shifts [24], the local filling factors could be determined, which
FIG. 4: The shift of the superfluid to Mott insulator phase transition $\Delta V_0^c$ in dependence on the scattering length ratio $a_{BF}/a_B$ for the filling factors $n_B = 1$ to $n_B = 5$. The dashed lines are obtained by keeping the fermion orbital fixed.

would allow a more accurate comparison of experiment and theory. 

Uniquely, experiments with ultracold atoms allow the precise tuning of the interaction strength by Feshbach resonances. Hence, the shift of the critical potential depth $\Delta V_0^c$ can also be studied in dependence on the scattering length $a_{BF}$ between bosons and fermions, while the bosonic scattering length $a_B = 100a_0$ is kept constant. Such an experiment would allow a closer investigation of the mutual interaction and the effects due to orbital changes. In Fig. 4 we present the calculated shifts $\Delta V_0^c$ for bosonic filling factors $n_B = 1$ to $n_B = 5$, where the solid lines are calculated allowing for orbital deformations and the dashed lines by using a rigid fermion orbital obtained by $V_{\text{eff}}(r) = V(r)$. The latter corresponds to a single-band approach for fermions, leaving the orbital degrees of freedom only to the bosonic subsystem. Because of a much weaker deformation of the bosonic effective potential, both $U$ and $J$ are less affected than in the previous discussion [30]. The scattering length $a_{BF}$, which enters linearly in the Hamiltonian (1), leads to an almost linear shift $\Delta V_0^c$. In great contrast, the dependence on $a_{BF}$ for the self-consistent calculation (solid lines), which fully includes the orbital degrees of freedom, is superlinear due to the self-trapping. Thus, the mutual deformation of the effective potential is enhanced by a larger scattering length as well as by a higher bosonic filling factor as discussed above. Therefore, the assumption of a fixed fermion orbital is only suited for weak interaction and low bosonic filling.

For repulsive interaction between bosons and fermions ($a_{BF} > 0$) the shift $\Delta V_0^c$ becomes positive but remains rather small with a sublinear dependence on $a_{BF}$. In this region, however, the separation of bosons and fermions plays a role, which is not accounted for in our calculations.

In conclusion, we have shown that orbital changes in attractive Bose-Fermi mixtures ($^{87}$Rb - $^{40}$K) are nonnegligible as they lead to a substantial deformation of the effective potential and a squeezing of the effective orbitals. The results are therefore of fundamental importance for quantum gas mixtures in optical lattices. We found a self-trapping behavior of the bosons in their effective potential mediated by the interaction with the fermions. Using a model with effective Bose-Hubbard parameters $U$ and $J$, the expected shift of the critical potential depth separating the superfluid phase from the Mott insulator was estimated. Our results reveal a strong dependence of the shift on the boson-fermion interaction strength and the bosonic filling factor, which could explain a large shift and the bosonic filling factor, which could explain a large shift as reported in Refs. [12, 13], and are applicable to future experiments using Feshbach resonances to tune the interspecies interaction. Theoretically, the full inclusion of orbital changes is a challenge for the efficient calculation of lattice systems.

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