High-Temperature Atomic Superfluidity in Lattice Boson-Fermion Mixtures

Fabrizio Illuminati and Alexander Albus
Dipartimento di Fisica, Università di Salerno, INFM - UdR di Salerno, and INFN,
Sezione di Napoli - Gruppo collegato di Salerno, Via S. Allende, I–84081 Baronissi (SA), Italy
(Dated: June 8, 2004)

PACS numbers: 03.75.Ss, 03.75.Lm, 32.80.Pj

We consider atomic Bose-Fermi mixtures in optical lattices and study the superfluidity of fermionic atoms due to $s$-wave pairing induced by boson-fermion interactions. We prove that the induced fermion-fermion coupling is always attractive if the boson-boson on site interaction is repulsive, and predict the existence of an enhanced BEC–BCS crossover as the strength of the lattice potential is varied. We show that for direct on-site fermion-fermion repulsion, the induced attraction can give rise to superfluidity via $s$-wave pairing, at striking variance with the case of pure systems of fermionic atoms with direct repulsive interactions.

The quest for superfluidity of fermionic atoms in dilute, degenerate quantum gases is the current object of widespread theoretical and experimental efforts [6, 14, 15]. In the present work we propose a new mechanism for fermion pairing in atomic systems. We consider mixtures of bosonic and fermionic atoms in optical lattices. The fermions are assumed to belong to the same atomic species, but trapped in different potentials created by the interference patterns of intersecting laser beams. Atoms can be confined to different lattice sites, and by varying the amplitude of the periodic potential, it is possible to tune the interatomic interactions at will. Therefore, optical lattices provide an ideal tool to reach strong coupling regimes even in the dilute limit [6]. The theory of neutral bosonic atoms in optical lattices has been developed [6] by assuming that the atoms are confined to the lowest Wannier band of the periodic potential. It can then be shown [6] that the system is effectively described by a single–band Bose–Hubbard model Hamiltonian [6]. In such a model the superfluid–insulator transition is predicted to occur when the on-site boson–boson interaction energy becomes comparable to some multiple of the hopping energy between adjacent lattice sites. This situation can be experimentally achieved by increasing the strength of the lattice potential, which results in a strong suppression of the kinetic (hopping) energy term. In this way, the superfluid–Mott-insulator quantum phase transition has been realized in a series of beautiful experiments by loading an ultracold atomic Bose–Einstein condensate in an optical lattice [6]. The theory of dilute mixtures of interacting bosonic and fermionic neutral atoms subject to an optical lattice has been recently developed by deriving an effective single–band Bose–Fermi Hubbard (BFH) Hamiltonian from the underlying microscopic many-body dynamics [3]. The zero-temperature phase diagram of the BFH model has been analyzed both in the homogeneous and inhomogeneous cases [6, 10, 11, 12]. These recent studies have shown that Bose–Fermi mixtures are very fundamental systems of condensed matter exhibiting complex phase diagrams and a potentially very rich physics that is just beginning to be unravelled.

The recent spectacular acceleration in the experimental manipulation [1, 2, 3, 4] and theoretical understanding [5, 6] of systems of neutral atoms in optical lattices is leading to new and far reaching possibilities in the study of complex systems of condensed matter physics. Besides opening the way to the controlled simulation and experimental testing of models of strongly correlated systems [5, 7], such as, e.g., high-$T_c$ superconductors and Hall systems, atomic physics in optical lattices hints at the possibility of discovering and probing new quantum phases of matter. Among others, very interesting recent studies in this direction are concerned with lattice boson–fermion mixtures [8, 9, 10, 11, 12]. These recent studies have shown that Bose–Fermi systems with repulsive interactions, for which $s$-wave pairing is impossible and superfluidity might be achieved, at much lower temperatures, via higher-order mechanisms such as anisotropic $d$-wave pairing.

The single-band BFH system in an optical lattice with nearest-neighbor hopping and on-site direct boson-boson, boson-fermion, and fermion-fermion interaction is described
by the Hamiltonian \[ \hat{H} = -J_B \sum_{\langle i,j \rangle} \left( \hat{a}^\dagger_i \hat{a}_j + \text{h.c.} \right) - J_F \sum_{\langle i,j \rangle, \sigma} \left( \hat{c}^\dagger_{i,\sigma} \hat{c}_{j,\sigma} + \text{h.c.} \right) + \frac{U_{BB}}{2} \sum_i \hat{n}^B_i (\hat{n}^B_i - 1) + U_{BF} \sum_i \hat{n}^B_i \hat{n}^F_i + U_{FF}^{\text{dis}} \sum_i \hat{n}^B_{i,\uparrow} \hat{n}^B_{i,\downarrow} \right], \tag{1}

where \( J_B \) and \( J_F \) are, respectively, the boson and fermion hopping amplitudes between adjacent lattice sites, and \( U_{BB}, U_{BF}, \) and \( U_{FF}^{\text{dis}} \) are, respectively the direct boson-boson, boson-fermion, and fermion-fermion on-site interaction strengths. The operators \( \hat{a}_i \) are the on-site bosonic annihilation operators, and \( \hat{c}_{i,\sigma} \) are the on-site fermionic annihilation operators for states with spin \( \sigma \). The bosonic on-site occupation number is \( \hat{n}^B_i = \hat{a}^\dagger_i \hat{a}_i \), while \( \hat{n}^F_{i,\sigma} = \hat{c}^\dagger_{i,\sigma} \hat{c}_{i,\sigma} \) denotes the fermionic on-site occupation number for states with spin \( \sigma \), and, finally, \( \hat{n}^B_{i,\sigma} = \hat{n}^F_{i,\uparrow} + \hat{n}^F_{i,\downarrow} \) denotes the total fermionic on-site occupation number. The bosonic and fermionic lattice potentials \( V_B \) and \( V_F \) are produced by a standing laser wave: 

\[ V_{B,F}(x, y, z) = V_{B,F}(\sin^2 \kappa x + \sin^2 \kappa y + \sin^2 \kappa z), \]

where \( k = \pi/a \) is the wave vector of the laser field, \( a \) denotes the lattice spacing, and the lattice strenghts \( V_{B,F} \) that are felt by the bosons and the fermions depend on the intensity of the laser light and the detuning of the laser frequency against the respective atomic frequencies. Scaling the tunable lattice amplitudes \( V_{B,F} \) with the bosonic and fermionic recoil energies, respectively \( E^B_F = (\pi \hbar)^2/2a^2 m_B \) and \( E^F_F = (\pi \hbar)^2/2a^2 m_F \), one can define the dimensionless bosonic and fermionic lattice amplitudes \( \eta_{B,F} = V_{B,F} / E^B_F \). Given the wavelength \( \lambda_B \) of the laser field, and the internal-state wavelengths \( \lambda_{B,F} \) for bosons and fermions, one has \( \eta_F/\eta_B = ((\lambda_F/\lambda_B)^4 \cdot (\Gamma_F \Delta \lambda_B E^B_F(an_{BB})/(\Gamma_B \Delta \lambda_F E^F_F), \)

where \( \Delta \lambda_{B,F} = \lambda_{B,F} - \lambda_L \) are the boson and fermion detunings from the laser field, and the ratio of the natural line widths \( \Gamma_F/\Gamma_B \) is usually of order one. By properly adjusting the detunings (blue or red) with the gauging of the laser field wavelength \( \lambda_L \), one can realize lattices whose depths can either be very different or nearly equal for the bosons and the fermions. The hopping and on site energy amplitudes exhibit a characteristic behavior as a function of the optical lattice: 

\[ J_{B,F} = E^B_F a_{BB,F,F} k \sqrt{8/\pi} \eta_{B,F}^{3/4}, \]

where \( a_{BB} \) and \( a_{FF} \) are the direct boson-boson and fermion-fermion s-wave scattering lengths, and \( U_{BF} = E^B_F a_{BF} k (4/\sqrt{\pi})(1+m_B/m_F)(\eta_B^{1/2} + \eta_F^{1/2} - 3/2) \), where \( a_{BF} \) is the direct boson-fermion s-wave scattering length. The ratio of the hopping amplitudes reads 

\[ J_B / J_F = \left[ (E^B_F / E^F_F) \right]^{3/4} \cdot \exp \left[ -2(\eta_B - \eta_F) \right]. \]

The bosonic and fermionic dispersion relations in a 3-D optical lattice with nearest-neighbor hopping take the following form: 

\[ \epsilon_{B,F}(q) = 4J_{B,F} \left[ \sin^2 \frac{q a_B}{2} + \sin^2 \frac{q a_F}{2} \right] \tag{2} \]

where \( J_B \) and \( J_F \) are, respectively, the bosonic and fermionic hopping amplitudes. The bosonic energy spectrum in the Bogoliubov approximation reads 

\[ \omega_B(q) = \sqrt{\epsilon_B(q) [\epsilon_B(q) + 2n_B U_{BB}]} \tag{3} \]

In the low momentum limit for the bosons, we recover the standard quadratic single particle spectrum \( \epsilon_B(q) \approx 3J_B q^2 \), where \( q^2 = q_x^2 + q_y^2 + q_z^2 \). Correspondingly, the phononic Bogoliubov excitation spectrum in the long wavelength regime reads \( \omega_B(q) \approx \sqrt{3J_B (q a_B^2) 2n_B U_{BB}} \) where \( c_B = \sqrt{6n_B U_{BB}} \) is the velocity of sound.

Let us next consider the momentum and frequency dependent bosonic dynamic response function \( \chi_B(\omega, q) \):

\[ \chi_B(\omega, q) = \frac{2n_B U_{BB}(q)}{\omega^2 - \omega_B^2(q)}. \tag{4} \]

Regarding the effects induced on the fermions, it is possible to show that the bosonic dynamic response function can be replaced by its static limit approximation. Let us focus on the fermion-fermion interaction \( U_{FF}(\omega, q) \) induced by the bosons. If the frequency contribution is not neglected, the gap function \( \Delta(\omega, q) \) for the fermions depends on frequency averages over the off-diagonal fermionic propagator \( G_{12}(\omega, q) \).

\[ \Delta(\omega, q) = \int U_{FF}^{\text{ind}}(\omega' - \omega, q' - q) G_{12}(\omega', q') d\omega d q'. \tag{5} \]

The maximum scale of integration for the fermions is fixed by the Fermi energy: \( h \omega_{\text{max}} \approx E_F \). The condition \( \omega_{\text{max}}^2 < \omega_B^2(q) \approx \omega_B^2(q)_{q=q_F} \) can be satisfied for widely different scenarios of fermion filling factors. We will consider half-band fermion filling \( n_F \approx 1 \). This amounts to \( q_F a \approx \pi/2 \) and \( E_F \approx 6J_F \). We then have \( h^2 \omega_{\text{max}}^2 \approx 36J_F^2 \), and \( \omega_B^2(q) \approx \omega_B^2(q)_{q=q_F} \approx 36J_F^2 + 12J_B n_B U_{BB} \), so that the static limit condition reads \( \omega_B^2 < 3J_B^2 + J_B n_B U_{BB} \).

This condition can be satisfied in several ways, depending on the type of boson-fermion mixture that one actually considers, and on the lattice strengths and hopping amplitude ratios that can be realized in experiments. For boson-fermion mixtures with almost equal atomic masses, like \(^6\text{Li}-^7\text{Li} \), and large red detuning of the laser field from the typical \( D \) lines of the Lithium isotopes, one has \( J_B \approx J_F \), which implies a static limit condition of the form \( \Delta(FJ - J_B) < n_B U_{BB} \). This condition is well satisfied at the onset of bosonic superfluidity \( U_{BB} \approx 10J_B \) and bosonic filling factors \( n_B \geq 1 \). Alternatively, the static limit condition can be satisfied by realizing small detunings such that \( \eta_F > 2\eta_B \); this yields in general \( J_B \gg J_F \), which again allows inequality (5) to hold. In this second instance, the bosonic lattice is usually some times weaker than the fermion lattice, and the bosons are in the deep superfluid regime. This setting is suited to treat mixtures irrespective of the atomic mass differences, and is thus the one we will consider in the following when studying the degenerate mixture of \(^{40}\text{K} \) and \(^{87}\text{Rb} \). We will study quantitatively the case of half-band fermion.
filling $n_F \approx 1$, because this is a situation that can be easily realized experimentally, it provides the optimal scenario for the highest attainable critical temperatures, and finally allows a direct comparison with the work of Hofstetter et al. on the high-temperature superfluidity of pure fermionic systems in optical lattices [7]. Taking the static bosonic response function $\chi_B(0, q) = -2n_{BB}(q)/\omega_B(q)$, the resulting induced fermion-fermion interaction (due to the bosonic density-density fluctuations caused by the boson-fermion coupling $U_{BF}$) reads $U_{FF}^{ind}(0, q) = \chi_B(0, q) \omega_B(q)$. To discuss s-wave fermion pairing and evaluate the critical temperature, one must compute the average induced interaction $U_{FF}^{tot}$ over the Fermi surface [7]. Provided that the bosonic lattice is not extremely weak (i.e. $\eta_B$ not $\ll 1$), contributions from nearest-neighbor induced interactions are negligible in first approximation, and one finds $U_{FF}^{ind} = -U_{BB}^{2} / U_{BB}$. We see that, irrespective of the sign of the boson-fermion s-wave scattering length $a_{BF}$, and thus of the boson-fermion on-site coupling $U_{BF}$, the induced fermion-fermion interaction is always attractive as long as the bosons are endowed with a positive s-wave scattering length $a_{BB} > 0$ and thus with a repulsive on-site interaction $U_{BB} > 0$. This is the case we will always consider in the following. For distinguishable fermions, such as ensembles of spin unpolarized neutral atoms, the total on-site fermion-fermion coupling $U_{FF}^{tot}$ is then

$$U_{FF}^{tot} \equiv U_{FF}^{dir} + U_{FF}^{ind} = U_{BB}^{2} / U_{BB} . \tag{7}$$

Thus, regarding interatomic pairing, fermions in a lattice Bose-Fermi mixture behave as interacting particles in a pure lattice fermionic system, but for the crucial difference of acquiring a dressed atom that modifies the direct fermion-fermion interaction through the boson-fermion coupling. This has relevant consequences on the possible pairing mechanisms in the system, in view of the relative sign between the direct and the induced part of the coupling strength. Because the sign of $U_{FF}^{dir}$ is determined solely by the sign of the fermion-fermion s-wave scattering length $a_{BF}$, we need to treat separately the two possible instances $a_{BF} < 0$ of direct on-site attraction, and $a_{BF} > 0$ of direct on-site repulsion.

1) Fermions with direct on-site attraction – In this case the fermions can undergo a transition to s-wave superfluidity at a higher critical temperature $T_c$ than the analogous pure Fermi case, as the direct and induced interactions are both attractive and add together (See Eq. [7]). All the considerations valid for pure fermionic systems [7, 17] hold as well in the case of a Bose-Fermi mixture, with the crucial difference that the thermodynamic properties will now depend on the total fermion-fermion interaction $U_{FF}^{tot}$ rather than the direct one $U_{BB}^{2} / U_{BB}$. Starting with a lattice of low or intermediate depth, the BCS picture for s-wave pairing holds, predicting a critical temperature for the transition with a scaling behavior $k_BT_c \approx 6J_F \exp \left(-\frac{2s}{|U_{FF}^{dir}|} \right)$. As the depth of the lattice is increased, the on-site interaction becomes at first comparable and then finally dominates over the tunneling amplitude; then the fermionic atoms form localized on-site bosonic molecules that can undergo a Bose-Einstein condensation (BEC) into the superfluid state at a transition temperature $k_BT_c \approx 6J_F \left|U_{FF}^{tot} / U_{BB}^{2} \right|$. In this situation the reduced ability of the pairs to move around in the lattice leads to a net decrease of the critical temperature. The maximum of the critical temperature $T_{max}^{c}$ is then achieved at the region of crossover between the BCS and BEC regimes, $|U_{FF}^{tot}| \approx 10J_F$ [17, 18]. In Fig. 1 we show the behavior of the critical temperature for the superfluid (SF) transition of $^6$Li atoms as a function of the strength of the optical lattice, at $n_F \approx 1$. When trapped in the state $| \uparrow, \uparrow \rangle$, the fermionic Lithium atoms are endowed with a very large and negative scattering length $a_{BF} \approx -2500a_0$. This is the most favorable case of direct fermion-fermion attraction known so far, and considered by Hofstetter et al. [7]. Their result is compared in Fig. 1 with the case of a $^6$Li-$^7$Li mixture, for which $a_{BF} \approx 38a_0$ [19]. We see that the presence of the bosons further enhances the maximum critical temperature attainable for the SF transition of the fermionic atoms. For a lattice spacing $a = 10^{-4}a_0$ the maximum critical temperature $T_{max}^{c}$ is $0.11\mu K$ for pure $^6$Li; for the mixture $^6$Li-$^7$Li we have $T_{max}^{c} = 0.14\mu K$.

II) Fermions with direct on-site repulsion – In the case of direct on-site repulsive fermion-fermion interactions, $U_{FF}^{dir} > 0$, the picture departs more radically from the analogous pure Fermi system. The direct repulsion and the induced attraction that determine the total interaction strength are now in competition, and the net total sign depends on their relative importance. In fact, because $U_{FF}^{dir}$ and $U_{BB}$ are both positive, we can evaluate the total fermion-fermion interaction as $U_{FF}^{tot} = (U_{BB}U_{FF}^{dir} - U_{BB}^{2}) / U_{BB}$. In several important instances of mixtures of alkali atoms of current experimental interest, with direct fermion-fermion repulsion, the measured value of the boson-fermion s-wave scattering length $a_{BF}$ turns out to be much larger than both the boson-boson and fermion-fermion s-wave scattering lengths $a_{BB}$ and $a_{FF}$, with the largest difference attained in degenerate mixtures of fermionic $^{40}$K and bosonic $^{87}$Rb. Namely, in this case one has that $a_{BF} = 104.8 \pm 0.4a_0$ (being the Bohr radius) in the singlet state, and $a_{BF} = 174 \pm 7a_0$ in the triplet state [20], while $a_{BB} = 100.2 \pm 1.8a_0$, and $a_{BB} = -410 \pm 80a_0$ [21]. A similar situation occurs for a mixture of fermionic
6Li with direct repulsion and bosonic 7Li, where one has $a_{FB} \simeq a_{FF} \simeq 5a_0$, and $a_{BF} \simeq 38a_0$. In these important instances the direct fermion-fermion repulsion is thus dominated by the induced fermion-fermion attraction, and high-temperature superfluidity of the fermionic atoms occurs by $s$-wave pairing. This is at striking variance with the case of systems of pure fermionic atoms with direct on-site repulsion: for such systems $s$-wave pairing is obviously always forbidden, and superfluidity can be achieved via different mechanisms of higher order, at lower critical temperatures, such as anisotropic $d$-wave pairing. Therefore, mechanism II) realizes the first atomic analogue of electron paring in crystal lattices. A further dramatic increase in the transition temperature $T_c$ can be obtained by combining the boson-induced interaction with the experimental manipulation of the $s$-wave boson-fermion scattering length via Feshbach resonances. In fact, the existence has been recently predicted of a Feshbach resonance at an applied magnetic field $B \simeq 725$ G in the degenerate mixture of $^{40}$K and $^{87}$Rb, leading to an enhancement of the boson-fermion $s$-wave scattering length to the very high value $a_{BF} \simeq -687a_0$. In Fig. 2 we show the behavior of the critical temperature for the superfluid transition of $^{40}$K atoms induced by the presence of the $^{87}$Rb atoms. Assuming the isotopes trapped at the $D$-line values of current experiments (795nm for rubidium, 767nm for potassium), and a blue-detuned laser at 764nm, we have $\eta_F \simeq 4\eta_B$, so that in the range of values of $\eta_F \simeq 7$ around the maximum critical temperature, we have $\eta_B \simeq 2$ (fully superfluid bosons) and $J_B^F \simeq 20J_F^s$ (static regime holds). We compare results for the case with (continuous curve) and without the presence of a Feshbach resonance (dotted curve). For a lattice spacing $a = 10^4a_0$ the first case yields $T_c^{\text{max}} = 0.05\mu K$, while without resonance we have $T_c^{\text{max}} = 0.04\mu K$. In conclusion, we have shown that for mixtures of bosonic and fermionic neutral atoms in optical lattices, the fermionic atoms acquire an induced on-site attraction mediated by the boson-fermion interaction, irrespective of the sign of the latter. This fact allows the fermions to undergo a high-temperature superfluid transition via total $s$-wave pairing in both instances of direct attractive and repulsive on-site fermion-fermion interactions. Recent progresses in the manipulation of mixtures of bosonic and fermionic atoms in optical lattices indicate that these predictions may be subject to experimental verification in the near future. We warmly thank Dr. K. Bongs for providing us with up-to-date values on forthcoming experiments with degenerate mixtures of $^{40}$K and $^{87}$Rb. This work has been supported by the ESF under project BEC2000+, the INFN, the INFN, and the Italian Ministry for Scientific Research, under project PRIN-COFIN 2002. We dedicate this work to Noam Chomsky on his 75th birthday, for his tireless struggle in favor of free research, human dignity and justice throughout the world.

[1] M. Greiner et al., Phys. Rev. Lett. 87, 160405 (2001).
[2] C. Orzel et al., Science 291, 2386 (2001).
[3] M. Greiner et al., Nature 415, 39 (2002); M. Greiner et al., Nature 419, 51 (2002).
[4] G. Modugno et al., Phys. Rev. A 68, 011601(R) (2003).
[5] D. Jaksh et al., Phys. Rev. Lett. 81, 3108 (1998).
[6] W. Zwerger, J. Opt. B: Quantum Semiclass. Opt. 5, S9 (2003).
[7] W. Hofstetter et al., Phys. Rev. Lett. 89, 220407 (2002).
[8] A. Albus, F. Illuminati, and J. Eisert, Phys. Rev. A 68, 023606 (2003).
[9] H. P. Büchler and G. Blatter, Phys. Rev. Lett. 91, 130404 (2003).
[10] M. Lewenstein et al., Phys. Rev. Lett. 92, 050401 (2004); H. Fechner et al., Opt. Express 12, 55 (2004).
[11] R. Roth and K. Burnett, Phys. Rev. A 69, 021601(R) (2004).
[12] M. Cramer, J. Eisert, and F. Illuminati, cond-mat/0310705.
[13] M. P. A. Fisher et al., Phys. Rev. B 40, 546 (1989).
[14] L. P. Pitaevskii and S. Stringari, Science 298, 2144 (2002).
[15] K. M. O’Hara et al., Science 298, 2179 (2002).
[16] L. Viverit, C. J. Pethick, and H. Smith, Phys. Rev. A 61, 053605 (2000); L. Viverit, ibidem 66, 023605 (2002).
[17] R. Micnas, J. Ranninger, and S. Robaszkiewicz, Rev. Mod. Phys. 62, 113 (1990).
[18] R. T. D. Scalalett et al., Phys. Rev. B 39, 4711 (1989).
[19] F. Schreck et al., Phys. Rev. Lett. 87, 080403 (2001).
[20] T. Loftus et al., Phys. Rev. Lett. 88, 173201 (2002).
[21] G. Roati et al., Phys. Rev. Lett. 89, 150403 (2002).
[22] A. Simon et al., Phys. Rev. Lett. 90, 163202 (2003).