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Finite temperature effects on the collapse of trapped Bose-Fermi mixtures

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By using the self-consistent Hartree-Fock-Bogoliubov-Popov theory, we present a detailed study of the mean-field stability of spherically trapped Bose-Fermi mixtures at finite temperature. We find that, by increasing the temperature, the critical particle number of bosons (or fermions) and the critical attractive Bose-Fermi scattering length increase, leading to a significant stabilization of the mixture.

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The recent experimental achievement in the trapping and cooling of degenerate Bose-Fermi mixtures of alkali-metal atoms have introduced interesting new instances of a quantum many-body system [1, 2, 3, 4, 5]. Similar to the purely Bose gases such mixtures provide a unique opportunity of investigating fundamental quantum phenomena. Up to date a number of theoretical analyses of trapped Bose-Fermi mixtures have been presented, addressing, for example, the static property [6], the phase diagram [7], the behavior of low-lying collective excitations [8, 9, 10, 11, 12, 13, 14], the expansion [15], as well as the relevant implications for the achievement of Bardeen-Cooper-Schrieffer (BCS) transition to a superfluid phase of the fermionic components [16, 17, 18]. The last point is particularly interesting and is highly favorable by tuning the Bose-Fermi interaction by means of Feshbach resonance [19, 20], in order to induce a large effective attraction between fermionic components by exchanging density fluctuations of the bosonic background [16, 17, 18]. It has been suggested in Ref. [20] that the optimal conditions for boson-induced Cooper pairing are reached when the Bose-Fermi mixtures are close to a critical point, beyond which the system will become unstable and collapse.

This kind of collapse is indeed observed very recently in a binary ^{40}K$-^{87}$Rb mixture [21]. The observation indicates a *large* attractive interaction between bosonic and fermionic atoms, and therefore highlights the possibility of inducing a boson-mediated effective attraction between two fermionic components once another hyperfine state of fermionic atoms is populated. On the theoretical side, the collapse or the instability of a trapped Bose-Fermi mixture at *zero* temperature has already been considered by several authors [6, 22, 23, 24, 25]. In Refs. [23, 24], the mean-field instability of a spherically trapped Bose-Fermi mixture is studied using a standard two-fluid model for the condensate and degenerate Fermi gas. Most recently, the same mean-field model has been used in Ref. [25], in which the precise geometry of the experiment is taken into account. Its prediction has been compared with the experimental stability diagram of ^{40}K-^{87}Rb mixtures to give a better estimate of the s -wave Bose-Fermi scattering length [25].

In the present paper we investigate the effects of the temperature on the stability of a spherically trapped Bose-Fermi mixture by only a mean-field approach. The motivation is twofold: At first, in the experiment there is a detection limit for determining the temperature. This limit is around $0.67T_c$, where T_c is the transition temperature of the Bose-Einstein condensation (BEC). Below this characteristic temperature, though no uncondensed fraction of the BEC is practically detectable, the possible role played by the thermal cloud of bosons in the stability of the mixture should be clarified. On the other hand, in the context of boson-induced BCS superfluidity, the critical temperature for the formation of s-wave Cooper pairing increases exponentially as the mixtures move to the collapse point. The qualitative or quantitative understanding of the collapse of Bose-Fermi mixtures at finite temperature is therefore crucial to optimize the experimental conditions to achieve the BCS transition.

Our investigation is based on the simplest self–consistent mean-field theory — the Popov version of the Hartree-Fock-Bogoliubov (HFB) theory — that has been generalized by us to the system of Bose-Fermi mixtures in previous works [14, 26]. For a weakly interacting Bose gas, it was shown that the HFB-Popov theory gives the correct thermodynamic properties with a very good accuracy [27], though it fails to predict the correct behavior of collective excitations at high temperatures [28]. In Ref. [29], this theory has been applied to study the collapse of attractive Bose-Einstein condensates.

In the following we briefly summarize the main points of HFB-Popov theory. The trapped binary mixture is considered as a thermodynamic equilibrium system under the grand canonical ensemble whose thermodynamic variables are N_b and N_f, respectively, the total number of trapped bosonic and fermionic atoms, T, the absolute temperature, and μ_b and μ_f, the chemical potentials. In the second quantization language, the density Hamiltonian of the mixture reads($\hbar=1$),

$$\begin{aligned}\mathcal{H} &= \mathcal{H}_b+\mathcal{H}_f+\mathcal{H}_{bf},\\ \mathcal{H}_b &= \psi^+(\mathbf{r})\left[-\frac{\bigtriangledown^2}{2m_b}+V^b_{ext}(\mathbf{r})-\mu_b\right]\psi(\mathbf{r})+\frac{g_{bb}}{2}\psi^+\psi^+\psi\psi,\\ \mathcal{H}_f &= \phi^+(\mathbf{r})\left[-\frac{\bigtriangledown^2}{2m_f}+V^f_{ext}(\mathbf{r})-\mu_f\right]\phi(\mathbf{r}),\\ \mathcal{H}_{bf} &= g_{bf}\psi^+(\mathbf{r})\psi(\mathbf{r})\phi^+(\mathbf{r})\phi(\mathbf{r}),\end{aligned}\tag{1}$$

where $\psi(\mathbf{r})$ ($\phi(\mathbf{r})$) is the Bose (Fermi) field operator that annihilates an atom at position $\mathbf{r}$. The first and second terms in the brackets contain the kinetic-energy operators and the external trapping potentials $V^b_{ext}(\mathbf{r})=m_b\omega_b^2r^2/2$ and $V^f_{ext}(\mathbf{r})=m_f\omega_f^2r^2/2$ for the bosonic and the fermionic species with masses m_b and m_f, respectively. In the dilute regime, we have considered two types of contact interactions: the interactions between bosons, and the interactions between bosons and fermions. They are parametrized by the coupling constants $g_{bb}=4\pi\hbar^2a_{bb}/m_b$ and $g_{bf}=2\pi\hbar^2a_{bf}/m_r$, respectively, in terms of the s-wave scattering length a_{bb} and a_{bf}, with $m_r=m_bm_f/(m_b+m_f)$ being the reduced mass. We have neglected here the fermion-fermion interactions since for spin-polarized fermions the s-wave contact interaction is prohibited by the Pauli principle. The next leading order, p-wave interaction is small at low energy [30] and will not be considered in the following.

We consider the many-body ground state $|\Psi\rangle$ of Hamiltonian (1) as a direct product of a symmetric N_b-body state $|\Psi_b\rangle$ for the bosonic species and an antisymmetric N_f-body state $|\Psi_f\rangle$ for the fermions. With this choice we are not considering the possible correlation effects beyond the mean-field approximation [31]. The density Hamiltonian describing the Bose-Fermi coupling can therefore be decoupled in a self-consistent mean-field manner, namely,

$$\mathcal{H}_{bf}\simeq g_{bf}\left[\psi^+\psi\langle\phi^+\phi\rangle+\langle\psi^+\psi\rangle\phi^+\phi-\langle\psi^+\psi\rangle\langle\phi^+\phi\rangle\right].\tag{2}$$

As a result, the bosonic and fermionic atoms experience, respectively, the effective potentials $V^b_{eff}(\mathbf{r})=V^b_{ext}(\mathbf{r})+g_{bf}n_f(\mathbf{r})$ and $V^f_{eff}(\mathbf{r})=V^f_{ext}(\mathbf{r})+g_{bf}n_b(\mathbf{r})$, with $n_b(\mathbf{r})$ and $n_f(\mathbf{r})$ being the bosonic and fermionic density distributions, respectively. It is then straightforward to apply the HFB-Popov theory for the bosonic species, following Ref. [32]. After invoking the Bose symmetry breaking in the equation of motion for the Bose field operator $\psi(\mathbf{r})$, we obtain, respectively, the modified Gross-Pitaevskii (GP) equation for the condensate wave function $\Phi(\mathbf{r})$,

$$\mathcal{L}_{GP}\Phi(\mathbf{r})=0,\tag{3}$$

and the modified Bogoliubov-deGennes (BdG) equations for the thermal quasiparticle amplitudes $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$,

$$\begin{aligned}\left[\mathcal{L}_{GP}+g_{bb}n_c(\mathbf{r})\right]u_i(\mathbf{r})+g_{bb}n_c(\mathbf{r})v_i(\mathbf{r}) &= \epsilon_iu_i(\mathbf{r}),\\ \left[\mathcal{L}_{GP}+g_{bb}n_c(\mathbf{r})\right]v_i(\mathbf{r})+g_{bb}n_c(\mathbf{r})u_i(\mathbf{r}) &= -\epsilon_iv_i(\mathbf{r}),\end{aligned}\tag{4}$$

where the operator

$$\mathcal{L}_{GP}=-\frac{\bigtriangledown^2}{2m_b}+V^b_{ext}-\mu_b+g_{bb}(n_c(\mathbf{r})+2n_T(\mathbf{r}))+g_{bf}n_f(\mathbf{r}),\tag{5}$$

is the generalized GP Hamiltonian that includes the mean-field contributions generated by the interaction with the thermal cloud and the fermionic species. Once these wave functions have been determined, the local density of the condensate and of the noncondensate, and the total bosonic density distribution can be calculated according to

$$\begin{aligned}n_c(\mathbf{r}) &= |\Phi(\mathbf{r})|^2,\\ n_T(\mathbf{r}) &= \sum_i\left[\frac{\left(|u_i(\mathbf{r})|^2+|v_i(\mathbf{r})|^2\right)}{e^{\beta\epsilon_i}-1}+|v_i(\mathbf{r})|^2\right],\\ n_b(\mathbf{r}) &= n_c(\mathbf{r})+n_T(\mathbf{r}),\end{aligned}\tag{6}$$

with $\beta=1/k_BT$ being the inverse temperature. To solve the modified GP and BdG equations, one has to evaluate the fermionic density distribution $n_f(\mathbf{r})$. To this aim, we employ the finite-temperature Thomas-Fermi approximation (TFA) [30],

$$\begin{aligned}n_f(\mathbf{r}) &= \int\frac{d^3\mathbf{p}}{(2\pi)^3}\frac{1}{e^{\beta\left(\frac{\mathbf{p}^2}{2m_f}+V^f_{ext}+g_{bf}n_b-\mu_f\right)}+1},\\ &= \frac{m_f^{3/2}}{\sqrt{2}\pi^2}\int_{-\infty}^{+\infty}d\epsilon\frac{1}{e^{\beta(\epsilon-\mu_f)}+1}\left(\epsilon-V^f_{ext}-g_{bf}n_b\right)^{1/2}\end{aligned}\tag{7}$$

Specially, for the range of N_f considered here ($N_f\simeq10^4$), it was shown that TFA is a good approximation for a mixture with repulsive Bose-Fermi interaction at zero temperature [7]. In our case, this approximation is expected to work even better, since the quantum fluctuations are suppressed by the finite temperature and the increased density due to the Bose-Fermi attraction.

Equations (3)-(7) form a closed set of equations that we have referred to as the “HFB-Popov” equations for a dilute Bose-Fermi mixture. The simultaneous solution of this set of equations gives the temperature-dependent density profiles of the condensate, of the noncondensate, and of the degenerate Fermi gas, from which we can extract the stability conditions of the system. We have numerically solved these coupled equations by an iterative scheme, as described in Ref. [26].

With above tools we investigate the effects of the temperature upon the collapse of a trapped Bose-Fermi mixture induced by the attractive Bose-Fermi interaction. Rather than taking the realistic experimental conditions, in this paper we present a general analysis of finite temperature effects, and restrict ourselves to spherical symmetric systems. The reason is that for this geometry the temperature-dependent density profiles of the system are easily calculated. On the contrary, for anisotropic systems, though the formalism given in the present paper is

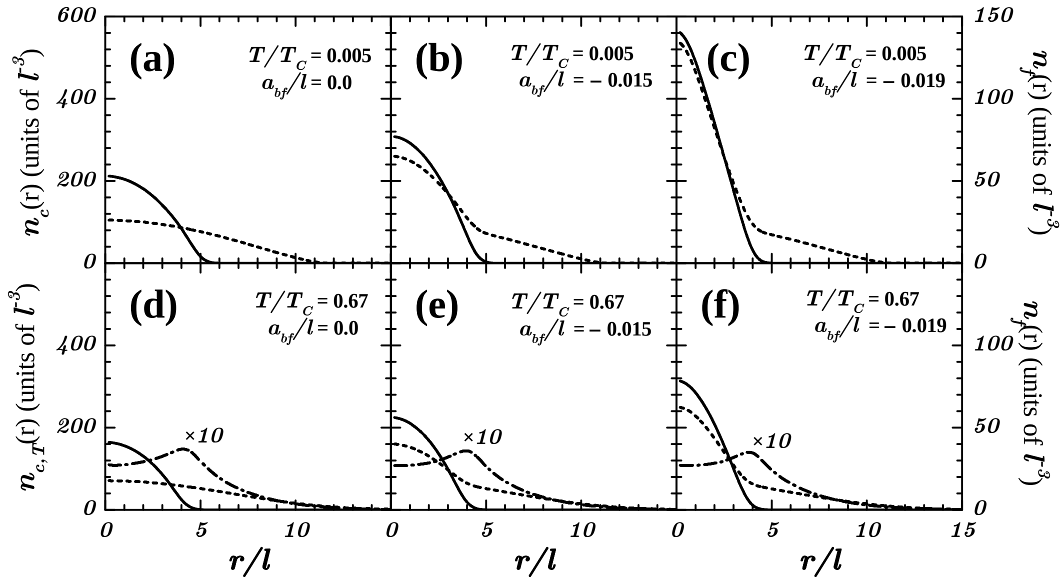

FIG. 1: Radial density profiles of a Bose-Fermi mixture with $N_b = N_f = 5 \times 10^4$ for different temperatures and Bose-Fermi interaction strengths. The condensate and noncondensate densities $n_c(r)$ and $n_T(r)$ are given, respectively, by the solid and dash-dotted lines (left scale), and the fermion density $n_f(r)$ by dashed line (right scale). To visualize $n_T(r)$ is enlarged by a factor of ten. The upper and lower rows show, respectively, examples with decreasing Bose-Fermi attraction at $T/T_C = 0.005$ and 0.67, where $T_C = 0.94\hbar\omega N_b^{1/3}/k_B$ is the transition temperature of a non-interacting Bose-Einstein condensate in the thermodynamic limit. We fix the boson-boson scattering length $a_{bb}/l = 0.005$.

suited as well, the numerical calculation is computationally much more involved. In particular, for the highly anisotropic traps used in the experiments at the European Laboratory for Non-linear Spectroscopy (LENS) [4, 21] it is unlikely to obtain useful information without the use of further approximation. In the following, we consider equal masses for the two species $m = m_b = m_f$ and identical trapping frequencies $\omega = \omega_b = \omega_f$. The oscillator length $l = (\hbar/m\omega)^{1/2}$ and trap energy $\hbar\omega$, respectively, serve as fundamental length unit and energy unit. We also take the transition temperature of a non-interacting Bose gas with $N_b = 5 \times 10^4$ atoms, $T_c = 0.94\hbar\omega N_b^{1/3}/k_B = 34.63\hbar\omega/k_B$, as a characteristic temperature. In most calculations, we have set $T = 0.67T_c$ that corresponds to a typical detection limit for the measurement of the temperature.

First we consider the effects of the temperature upon the density profiles of the mixture. The upper and lower rows in Fig. 1 show the density profiles of configurations with $N_b = N_f = 5 \times 10^4$ particles for three different values of the s-wave Bose-Fermi scattering length a_{bf}/l at two temperatures: $T = 0.005T_c$ and $T = 0.67T_c$. The value of $a_{bb}/l = 0.005$ has been fixed, which corresponds to $a_{bb} \approx 100a_{\rm Bohr}$ for a typical trap with $l = 1\mu m$. Our results at the lower temperature $T = 0.005T_c$ are in good agreement with the findings by Roth and coworkers [23, 24], that is, the mutual attraction between bosons and fermions results in an enhancement of both densities in the overlap region. In particular, as shown in Fig. (1c), both the bosonic and fermionic densities grow substantially when the mixture is close to the instability point (note that at $T = 0.005T_c$ the critical value of a_{bf}/l is -0.0193). This enhancement, however, is much reduced at a finite temperature, whose effect is a broadening of the density distributions of the condensate and of the Fermi gas and therefore reduces their center densities. As can be seen in Fig. (1f), at $T = 0.67T_c$ both densities is decreased by a factor of 2 compared to the lower temperature case. As a consequence, the mixture in this case is expected to be much stabilized against collapse.

In a simplified model [6], the collapse or the instability of the mixture is governed by the balance between the kinetic energy of fermions and the mutually attractive mean-field generated by the Bose-Fermi interaction (see, for example, the discussion above the Eq. (11) in Ref. [6]), If the Bose-Fermi attraction becomes too strong, *i.e.*, the numbers of bosons (or fermions) or the scattering length a_{bf} becomes too large, the attractive mean field cannot be stabilized by the kinetic energy anymore, so both density distributions grow indefinitely within the overlap region and collapse. According to the study reported in Refs. [6, 23, 24, 25], the onset of this mean-field instability is monitored by the failure of the convergence during the iterative procedure. In this manner, we can determine the critical s-wave Bose-Fermi scattering length a_{bf} or critical particle numbers N_b^{crit} and N_f^{crit} beyond which the collapse occurs.

In Fig. 2, we show the critical particle number as a function of the s-wave Bose-Fermi scattering length a_{bf}/l with fixed $a_{bb}/l = 0.005$ for two temperatures. In

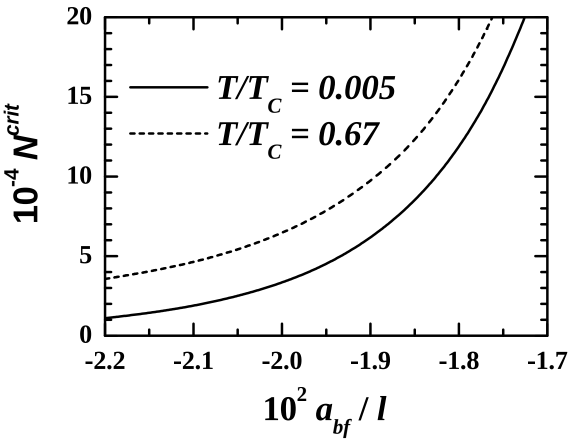

FIG. 2: Behavior of the critical particle number as a function of the s-wave Bose-Fermi scattering length a_{bf}/l for $N_b = N_f$ at two temperatures: $T/T_C = 0.005$ (solid line) and $T/T_C = 0.67$ (dashed line). $T_C = 0.94\hbar\omega N_b^{1/3}/k_B$ is the ideal transition temperature evaluated at $N_b = 5 \times 10^4$. The boson-boson scattering length $a_{bb}/l = 0.005$ is fixed.

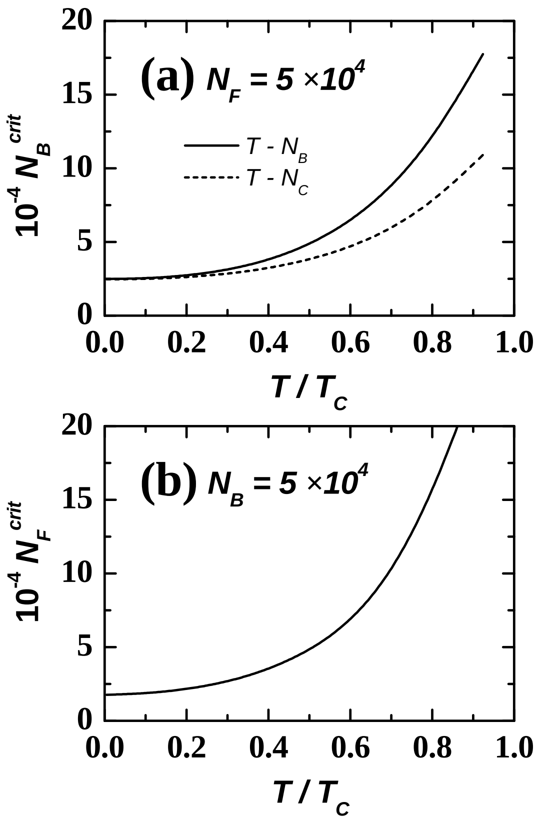

FIG. 3: (a) The critical number of bosons N_b^{crit} as a function of the rescaled temperature T/T_C with fixed number of fermions $N_f = 5\times10^4$. The dashed line shows the corresponding number of condensed bosons. (b) The critical number of fermions N_f^{crit} as a function of the re-scaled temperature T/T_C with fixed number of bosons $N_b = 5\times10^4$. In both cases $T_C = 0.94\hbar\omega N_b^{1/3}/k_B$ is the ideal transition temperature for $N_b = 5 \times 10^4$. The other parameters are: $a_{bb}/l = 0.005$ and $a_{bf}/l = -0.020$.

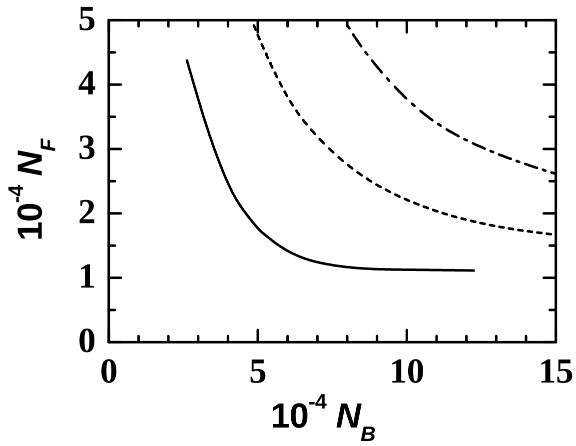

FIG. 4: Region of stability of the Bose-Fermi mixture, as a function of the number of atoms, for the case of $a_{bb}/l = 0.005$ and $a_{bf}/l = -0.020$. Lines show the boundary between the stable (left) and collapse (right) regions, for three values of the temperature: $T/T_C = 0.005$ (solid line), $T/T_C = 0.50$ (dashed line) and $T/T_C = 0.67$ (dash-dotted line), where $T_C = 0.94\hbar\omega N_b^{1/3}/k_B$ is the transition temperature for a non-interacting Bose gas with $N_b = 5 \times 10^4$.

this calculation we have kept equal numbers of bosons and fermions ($N_b = N_f$). At the lower temperature $T = 0.005T_c$, we observed that even a small decrease of Bose-Fermi attraction can reduce the critical particle number significantly, *i.e.*, N^{crit} changes by a factor of 2 when a_{bf}/l changes by 5 percent. This strong dependence of the criticality on a_{bf}/l is in accordance with the scaling law for the critical particle number: $N^{crit} \sim |a_{bf}|^{-\alpha}$ with $\alpha = 12$, as discussed in Refs. [6, 22, 25]. The presence of a moderate temperature $T = 0.67T_c$ results in a substantial increase of the critical particle number. For example, at $a_{bf}/l = -0.022$, N^{crit} grows from 1.1×10^4 to 3.6×10^4 with the inclusion of the temperature. Apart from this growth, the critical particle number is still strongly dependent on a_{bf}/l. However, the presence of the finite temperature leads to a re-normalization of the scaling exponent, *i.e.*, $\alpha \sim 8$.

In Figs. (3a) and (3b), we study the critical particle numbers of bosons and fermions as a function of the temperature. We report, respectively, the prediction on the critical particle numbers of bosons (with fixed $N_f = 5\times10^4$) and fermions (with fixed $N_b = 5\times10^4$). For comparison, in Fig. (3a), we also show the critical number of the condensed atoms against temperature(dashed line). As expected, the critical particle number for each species increase with increasing the temperature. The dependence is highly nonlinear. Below $0.5T_c$, the critical particle number varies slowly with the temperature, whereas above $0.5T_c$ it rises up steeply. In addition, the critical particle number of fermions grows more rapidly than that of bosons against the temperature.

Finally, we have built a region of stability of the Bose-Fermi mixture in Fig. 4, as a function of the number of atoms, for the cases of $a_{bb}/l = 0.005$ and $a_{bf}/l = -0.020$, for three values of the temperature: $T/T_C = 0.005$, $T/T_C = 0.50$ and $T/T_C = 0.67$. Each of the curves marks the limit of stability. For numbers of bosons or fermions below the stability limit the mixture is stable, otherwise the mixture is unstable against mean-field collapse. Figure 4 indicates that the region of the stability broadens with increasing temperature. This behavior emphasize again that the inclusion of a temperature gives rise to a significant stabilization of the mixtures.

In conclusion, we have investigated the mean-field stability of a spherically trapped binary Bose-Fermi mixture at finite temperature. We solved the coupled HFB-Popov equations numerically and obtained the critical particle number as a function of the temperature and the s-wave Bose-Fermi scattering length. We have shown that the critical particle number and the critical Bose-Fermi scattering length increase with the inclusion of a moderate temperature that corresponds to the typical experimental detection limit. This leads to a significant stabilization of the Bose-Fermi mixtures.

Acknowledgments

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