Thermodynamics of a trapped Bose-Fermi mixture

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By using the Hartree-Fock-Bogoliubov equations within the Popov approximation, we investigate the thermodynamic properties of a dilute binary Bose-Fermi mixture confined in an isotropic harmonic trap. For mixtures with an attractive Bose-Fermi interaction, we find a sizable enhancement of the condensate fraction and of the critical temperature of Bose-Einstein condensation with respect to the predictions for a pure interacting Bose gas. Conversely, the influence of the repulsive Bose-Fermi interaction is less pronounced. The possible relevance of our results in current experiments on trapped ^{87}Rb-^{40}K mixtures is discussed.

The recent experimental realization of ultracold trapped Bose-Fermi (BF) mixtures of alkali-metal atoms introduces an interesting new instance of a quantum many-body system [1–3], and has also stimulated a number of theoretical investigations that address, for example, the static property [4], the phase diagram and phase separation [5], stability conditions [6], and collective excitations [7–9] of trapped BF mixtures. These investigations have mainly concentrated at zero temperature using the standard Gross-Pitaevskii (GP) equation for the Bose gas, in which all the bosonic atoms are assumed to be in the Bose condensate. An extension of these theories at finite temperatures where the condensate is strongly depleted is therefore of high interest, and will also have practical applications. In the theory for a pure Bose gas, the simplest generalization of the GP equation including the effect of the noncondensed atoms in a self-consistent manner is the Popov version of the Hartree-Fock-Bogoliubov (HFB) approximation [10]. As discussed in Ref. [10], this approximation is expected to be good for both low and high temperatures.

In this paper, we generalize the HFB-Popov approximation to binary BF mixtures and address the question of how the BF interaction affects the thermodynamic properties of mixtures. We calculate *self-consistently* the temperature-dependent density profiles of mixtures, as well as the condensate fraction and the critical temperature of Bose-Einstein condensation (BEC), at various BF interaction strengths. Our present results provide the self-consistent calculation of these thermodynamic quantities within the HFB-Popov theory which goes beyond the semiclassical approximation used previously for determining the critical temperature [11,12] and density profiles of binary BF mixtures [13]. Our calculations also show a highly *nonlinear* dependence of these quantities on the BF interaction. In the presence of the BF attraction, the thermal depletion of the condensate is remarkably decreased and the critical temperature is shifted towards high temperatures. Conversely, the repulsive BF interaction affects the condensate fraction and critical temperature in the opposite direction. However, its influence is less pronounced compared to the attractive case.

The HFB-Popov mean-field theory for an inhomogeneous interacting Bose gas has been derived in detail by Griffin in Ref. [10]. The generalization of this theory to a dilute binary BF mixture is straightforward. Here we merely give a summary of basic equations and emphasize the necessary modification in the presence of the BF interaction. The trapped dilute mixture is portrayed 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. The density Hamiltonian of the system is given by (in units of $\hbar = 1$)

$$\mathcal{H} = \mathcal{H}_b + \mathcal{H}_f + \mathcal{H}_{bf},$$

$$\mathcal{H}_b = \psi^\dagger(\mathbf{r}) \left[-\frac{\nabla^2}{2m_b} + V_{trap}^b(\mathbf{r}) - \mu_b \right] \psi(\mathbf{r}) + \frac{g_{bb}}{2} \psi^\dagger \psi^\dagger \psi \psi,$$

$$\mathcal{H}_f = \phi^\dagger(\mathbf{r}) \left[-\frac{\nabla^2}{2m_f} + V_{trap}^f(\mathbf{r}) - \mu_f \right] \phi(\mathbf{r}),$$

$$\mathcal{H}_{bf} = g_{bf} \psi^\dagger(\mathbf{r}) \psi(\mathbf{r}) \phi^\dagger(\mathbf{r}) \phi(\mathbf{r}), \tag{1}$$

where $\psi(\mathbf{r})$ [$\phi(\mathbf{r})$] is the Bose (Fermi) field operator that annihilates an atom at position $\mathbf{r}$. Here we consider a spherically symmetric system, with trap potentials $V_{trap}^{b,f}(\mathbf{r}) = m_{b,f} \omega_{b,f}^2 r^2/2$, where $m_{b,f}$ are the atomic masses and $\omega_{b,f}$ are the trap frequencies. The interaction between bosons and between bosons and fermions are described by the contact potentials and are parametrized by the coupling constants $g_{bb} = 4\pi\hbar^2 a_{bb}/m_b$ and $g_{bf} = 2\pi\hbar^2 a_{bf}/m_r$ in terms of the s-wave scattering lengths a_{bb} and a_{bf}, with $m_r = m_b m_f/(m_b + m_f)$ being the reduced mass. We neglect here the fermion-fermion interactions, since we are considering a spin-polarized Fermi gas where s-wave collisions are forbidden by the Pauli principle. In the dilute regime, we may treat the density Hamiltonian describing the BF coupling in a self-consistent mean-field manner, namely

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

This kind of decomposition has been used extensively for theoretical investigations of BF mixtures at zero temperature [17].

To the Bose field operator $\psi(\mathbf{r},t)$, we shall apply the usual decomposition into a c-number part plus an operator with vanishing expectation value: $\psi(\mathbf{r},t)=\Phi(\mathbf{r})e^{-i(\varepsilon_0-\mu_b)t}+\widetilde{\psi}(\mathbf{r})$. $\Phi(\mathbf{r})$ represents the condensate wave function with eigenvalue ε_0 and the operator $\widetilde{\psi}(\mathbf{r})$ represents the excitations of the condensate. This ansatz is then inserted in the equation of motion for $\psi(\mathbf{r},t)$:

$$i\frac{\partial\psi}{\partial t}=\left[-\frac{\nabla^2}{2m_b}+V_{trap}^b-\mu_b\right]\psi+g_{bb}\psi^\dagger\psi\psi+g_{bf}\langle\phi^\dagger\phi\rangle\psi. \quad (2)$$

The statistical average over Eq. (2) and the replacement of the cubic term $\widetilde{\psi}^\dagger\widetilde{\psi}\widetilde{\psi}$ by the average in the mean-field approximation $2\langle\widetilde{\psi}^\dagger\widetilde{\psi}\rangle\widetilde{\psi}$ with neglecting the anomalous expectation value $\langle\widetilde{\psi}\widetilde{\psi}\rangle$ and its complex conjugate lead to the generalized GP equation,

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

where $\mathcal{L}_{GP}\equiv-\nabla^2/2m_b+V_{trap}^b-\varepsilon_0+g_{bb}[n_c(\mathbf{r})+2\widetilde{n}(\mathbf{r})]+g_{bf}n_f(\mathbf{r})$ with the local density of the condensate $n_c(\mathbf{r})=|\Phi(\mathbf{r})|^2$, of the depletion $\widetilde{n}(\mathbf{r})=\langle\widetilde{\psi}^\dagger(\mathbf{r},t)\widetilde{\psi}(\mathbf{r},t)\rangle$, and of the Fermi gas $n_f(\mathbf{r})=\langle\phi^\dagger(\mathbf{r},t)\phi(\mathbf{r},t)\rangle$. The condensate wave function in Eq. (3) is normalized to $N_c=1/(e^{\beta(\varepsilon_0-\mu_b)}-1)$ with $\beta=(k_BT)^{-1}$.

The subtraction of Eq. (3) from Eq. (2) gives rise to two coupled equations of motion for $\widetilde{\psi}(\mathbf{r},t)$ and its adjoint, which can be solved by the usual Bogoliubov transformation, $\widetilde{\psi}(\mathbf{r},t)=\Sigma_i[u_i(\mathbf{r})\hat{\alpha}_ie^{-i\epsilon_it}+v_i^*(\mathbf{r})\hat{\alpha}_i^\dagger e^{i\epsilon_it}]$, to the new Bose operators $\hat{\alpha}_i$ and $\hat{\alpha}_i^\dagger$. This gives the coupled Bogoliubov–de Gennes (BdG) equations,

$$[\mathcal{L}_{GP}+g_{bb}n_c(\mathbf{r})]u_i(\mathbf{r})+g_{bb}n_c(\mathbf{r})v_i(\mathbf{r})=\epsilon_iu_i(\mathbf{r}),$$

$$[\mathcal{L}_{GP}+g_{bb}n_c(\mathbf{r})]v_i(\mathbf{r})+g_{bb}n_c(\mathbf{r})u_i(\mathbf{r})=-\epsilon_iv_i(\mathbf{r}). \quad (4)$$

These equations define the quasiparticle excitation energies ϵ_i *relative* to the condensate eigenvalue ε_0, and the quasiparticle amplitudes u_i and v_i. Once these quantities have been determined, the density of the depletion is obtained in terms of the thermal number of quasiparticles $\langle\hat{\alpha}_i^\dagger\hat{\alpha}_i\rangle=(ze^{\beta\epsilon_i}-1)^{-1}$ by

$$\widetilde{n}(\mathbf{r})=\sum_i\widetilde{n}_i(\mathbf{r})\Theta(E_c^b-\epsilon_i)+\int_{E_c^b}^\infty d\epsilon\,\widetilde{n}(\epsilon,\mathbf{r}), \quad (5)$$

$$\widetilde{n}_i(\mathbf{r})=\frac{|u_i(\mathbf{r})|^2+|v_i(\mathbf{r})|^2}{ze^{\beta\epsilon_i}-1}+|v_i(\mathbf{r})|^2,$$

$$\widetilde{n}(\epsilon,\mathbf{r})=\frac{m_b^{3/2}}{\sqrt{2}\pi^2}\left\{\frac{1}{ze^{\beta\epsilon}-1}+\frac{1}{2}-\frac{\epsilon}{2\epsilon_{HF}}\right\}[\epsilon_{HF}-V_{trap}^b+\varepsilon_0$$
$$-2g_{bb}n_b(\mathbf{r})-g_{bf}n_f(\mathbf{r})]^{1/2},$$

where $z=e^{\beta(\varepsilon_0-\mu_b)}=1+1/N_c$, $\epsilon_{HF}=[\epsilon^2+g_{bb}^2n_c^2(\mathbf{r})]^{1/2}$, and $n_b(\mathbf{r})=n_c(\mathbf{r})+\widetilde{n}(\mathbf{r})$ is the total density of the Bose gas. In the above equations, to eliminate the numerical errors due to the necessary truncation of the numerical basis set, we adopt the strategy of Ref. [18] and introduce an energy cutoff E_c^b, above which the semiclassical local-density approximation has been employed.

To solve the generalized GP and BdG equations, one has to find the local density of the Fermi gas $n_f(\mathbf{r})$. To this end, we insert $\phi(\mathbf{r},t)=\Sigma_i\varphi_i(\mathbf{r})\hat{c}_ie^{-i\epsilon_it}$ in Eq. (1) to diagonalize the quadratic Hamiltonian for $\phi(\mathbf{r,t})$ in terms of the new Fermi operator $\hat{c}_i$ that annihilates a fermion at state $\varphi_i(\mathbf{r})$. This leads to a stationary Schrödinger equation for $\varphi_i(\mathbf{r})$,

$$\left[-\frac{\nabla^2}{2m_f}+V_{trap}^f+g_{bf}(n_c+\widetilde{n})\right]\varphi_i=\epsilon_i\varphi_i. \quad (6)$$

The density of the Fermi gas is thus obtained by

$$n_f(\mathbf{r})=\sum_i n_{fi}(\mathbf{r})\Theta(E_c^f-\epsilon_i)+\int_{E_c^f}^\infty d\epsilon\,n_f(\epsilon,\mathbf{r}), \quad (7)$$

$$n_{fi}(\mathbf{r})=|\varphi_i(\mathbf{r})|^2\langle\hat{c}_i^\dagger\hat{c}_i\rangle,$$

$$n_f(\epsilon,\mathbf{r})=\frac{m_f^{3/2}}{\sqrt{2}\pi^2}\frac{1}{e^{\beta(\epsilon-\mu_f)}+1}(\epsilon-V_{trap}^f-g_{bf}n_b(\mathbf{r}))^{1/2},$$

where $\langle\hat{c}_i^\dagger\hat{c}_i\rangle=(e^{\beta(\epsilon_i-\mu_f)}+1)^{-1}$ is the Fermi distribution. Analogously to Eq. (5) we have applied the finite-temperature Thomas-Fermi (TF) approximation only for high-lying Fermi levels above an energy cutoff E_c^f to avoid the truncation errors.

Equations (3)–(7) form a closed system of equations that we have referred to as the "HFB-Popov" equations for a dilute BF mixture. We have numerically solved these equations by an iterative procedure as follows: The generalized GP and BdG equations are first solved self-consistently for $\Phi(\mathbf{r})$, $u_i(\mathbf{r})$, and $v_i(\mathbf{r})$ as described in Ref. [10] to evaluate $n_c(\mathbf{r})$ and $\widetilde{n}(\mathbf{r})$, with $n_f(\mathbf{r})$ set to the result for an ideal Fermi gas. Once $n_c(\mathbf{r})$ and $\widetilde{n}(\mathbf{r})$ are known, the eigenfunctions in Eq. (6) are obtained numerically and are used to update $n_f(\mathbf{r})$ in Eq. (7). This newly generated $n_f(\mathbf{r})$ is then inserted in the GP and BdG equations and the process is iterated to convergence. At each step, the chemical potentials for the Bose gas and the Fermi gas are fixed by the normalization conditions $\int d\mathbf{r}n_b(\mathbf{r})=N_b$ and $\int d\mathbf{r}n_f(\mathbf{r})=N_f$, respectively.

As an illustration of this procedure, we consider a mixture of 2000 ^{87}Rb (boson) and 2000 ^{40}K (fermion) atoms in an isotropic harmonic trap, for which the order parameter $\Phi(\mathbf{r})$, the quasiparticle amplitudes $u_i(\mathbf{r})$ and $v_i(\mathbf{r})$, and the orbits $\varphi_i(\mathbf{r})$ can be labeled by (n,l,m), according to the number of nodes in the radial solution n, the orbital angular momentum l, and its projection m. In addition, we use the following parameters [3]: $m_b=1.45\times10^{-25}$ kg, $\omega_b=2\pi\times216$ Hz, $m_f/m_b=0.463$, $\omega_f/\omega_b=1.47$, $a_{bb}=99a_0$, and $a_{bf}=-410a_0$, where $a_0=0.529$ Å is the Bohr radius. Because our calculations are especially delicate near the critical tem-
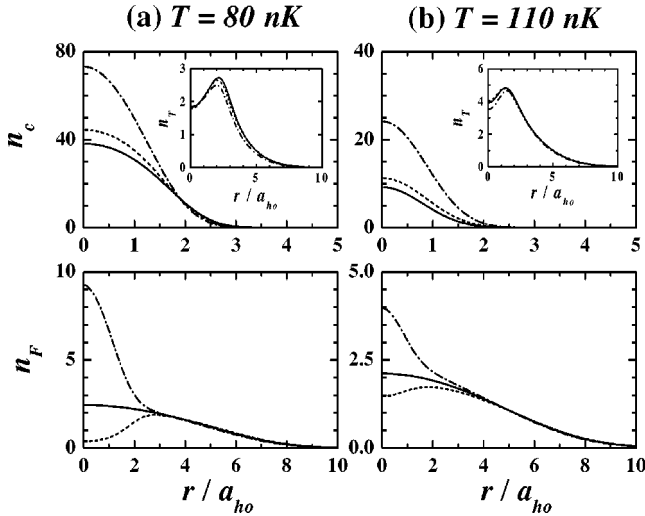
FIG. 1. The density profiles of the condensate $n_c(r)$ and of the Fermi gas $n_F(r)$ for a mixture of 2000 ^{87}Rb and 2000 ^{40}K atoms in an isotropic harmonic trap at various BF interaction: $a_{bf}=0$ (full line), $a_{bf}=+410a_0$ (dashed line), and $a_{bf}=-410a_0$ (dash-dotted line), where $a_0=0.529$ Å is the Bohr radius. Insets show the density profiles of the noncondensate $\tilde{n}(r)$. We have taken $a_{bb}=99a_0$ and $\omega_b=2\pi\times216$ Hz. The coordinate r and densities are measured in units of the harmonic-oscillator lengths a_{ho}^b and $(a_{ho}^b)^3$, respectively.

perature, we have taken $n_{max}=32$, $l_{max}=64$ and high energy cutoffs of $E_c^b=60\hbar\omega_b$ and $E_c^f=90\hbar\omega_b$ to ensure the accuracy. Throughout the paper, we also express the lengths and energies in terms of the characteristic oscillator length $a_{ho}^b=(\hbar/m_b\omega_b)^{1/2}$ and characteristic trap energy $\hbar\omega_b$, respectively.

In Fig. 1, we present our results for the density profiles of the condensate, of the noncondensate, and of the Fermi gas at two temperatures. The cases with the BF interaction and without the BF interaction are shown by the dash-dotted lines and full lines, respectively. We have also considered a fictitious case of a positive BF interaction: $a_{bf}=+410a_0$ (dashed lines). The choice of the first temperature $T=80$ nK corresponds to the situation in which the condensate and noncondensate have an approximately equal number of atoms, while the other temperature $T=110$ nK is chosen to be close to the critical temperature for a pure interacting Bose gas with the same number of bosons, $T_c\approx112$ nK. As clearly emerges from the figure, the density profiles of the condensate and of the Fermi gas are strongly affected by the BF interaction at both temperatures. In particular, the densities around the center are significantly enhanced in the case of the BF attraction. The density profile of the noncondensate (shown in the insets), on the other hand, is less influenced by the BF interaction due to its broad distribution and the strong repulsion from the condensate.

In Fig. 2, we show our predictions for the temperature dependence of the condensate fraction $N_c(T)/N_b$. The essential feature of the figure is the importance of the *attractive* BF interaction that results in a sizable quenching of the thermal depletion compared to the prediction for a pure interacting Bose gas. Contrarily, the effects of the repulsive BF in-
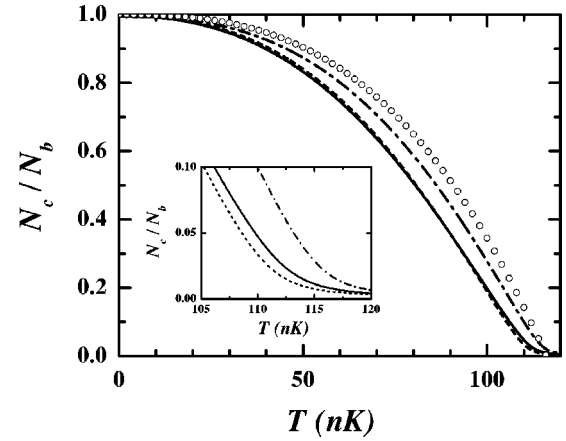

FIG. 2. Temperature dependence of the condensate fraction. The dashed and dash-dotted lines correspond to $a_{bf}=+410a_0$ and $-410a_0$, respectively. The solid lines show the result for a pure interacting Bose gas. The empty circles show ideal Bose gas result with the finite-size correction, $N_c^0/N_b=1-(T/T_c^0)^3-2.1825(T/T_c^0)^2N_b^{-1/3}$, where $k_BT_c^0=0.94\hbar\omega_bN_b^{1/3}$. The inset highlights the condensate fraction near the critical temperature. The other parameters are the same as in Fig. 1.

teraction are more subtle and are always very small. The sizable enhancement of the condensate fraction predicted by our calculation follows from the fact that in the presence of the BF attraction the condensate effectively experiences a more tightly confining potential. As a consequence, if we neglect the corrections due to the interaction between bosons and the finite-size effect, the critical temperature $T_c^0=0.94\hbar\omega_{eff}N_b^{1/3}/k_B$ is effectively increased and the condensate fraction is, therefore, enhanced according to the ideal gas result $N_c/N_b=1-(T/T_c^0)^3$.

Closely related to the condensate fraction, another important parameter characterizing the effect of the BF interaction is the shift of the critical temperature from the pure interacting Bose gas case. In Fig. 3, we report the HFB-Popov results for the relative shift of the critical temperature $\delta T_c/T_c$ as a function of a_{bf} in solid circles. Here T_c is determined as the maximum of the function d^2N_c/dT^2 [19]. The semiclassical predictions for $\delta T_c/T_c$, calculated as in Ref. [11] in the first order of a_{bf}, are also shown by the dashed line. The agreement of these two approaches is reasonably good for a weak BF interaction ($|a_{bf}|\lesssim100a_0$). However, as $|a_{bf}|$ increases, our HFB-Popov results diverge from the semiclassical predictions. In particular, for the realistic BF s-wave scattering length for ^{87}Rb-^{40}K mixtures, $a_{bf}=-410a_0$, the deviation becomes remarkable.

We now turn to consider the experimental relevance of our results. In current experiments, the realistic number of ^{87}Rb and ^{40}K atoms in mixtures is about ten times larger than what we assumed here [3]. For such large number of atoms, our calculation is very time consuming and we then resort to the semiclassical version of the HFB-Popov theory by setting E_c^b to an energy of a few $\hbar\omega_b$ and applying the TF approximation for the whole Fermi spectra. The accuracy of this semiclassical treatment has been checked by the comparison with the full quantum-mechanical calculations for a
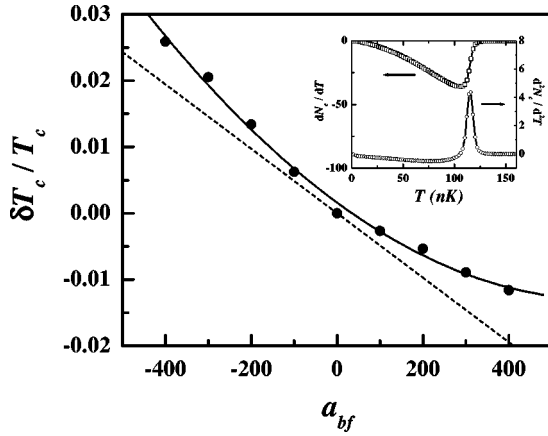
FIG. 3. The relative shift of the critical temperature as a function of the BF s-wave scattering length a_{bf} (in units of a_0). The solid circles show the result calculated using the HFB-Popov equations and the full line is a parabolic fit to guide eye. The dashed line is the result calculated by Eq. (18) in Ref. [11]. The inset shows the functions dN_c/dT and d^2N_c/dT^2 for the case of $a_{bf}=-410a_0$. T_c is extracted from the maximum of d^2N_c/dT^2. The other parameters are the same as in Fig. 1.

FIG. 4. Temperature dependence of the condensate fraction for a mixture of 2×10^4 ^{87}Rb and 5×10^4 ^{40}K atoms confined in an isotropic trap with $\omega_b=2\pi\times91.7$ Hz, calculated in the semiclassical version of the HFB-Popov theory as mentioned in the text.

small mixture. The condensate fraction obtained by these two methods coincides within 1% errors.

In Fig. 4, we present the results for $N_c(T)/N_b$ of a mixture of 2×10^4 ^{87}Rb and 5×10^4 ^{40}K atoms confined in an isotropic trap with $\omega_b=2\pi\times91.7$ Hz. This choice corresponds to the typical experimental situations at LENS [20]. Although the trap becomes more shallow, the enhancement of the condensate fraction shown in Fig. 4 is quantitatively similar to the one of Fig. 2, due to the much larger values of N_b and N_f contained in the trap. Finally, in this case we also roughly estimate the relative shift of the critical temperature due to the BF attraction, $(\delta T_c/T_c)_{bf}\simeq+4\%$, which is comparable to the shift due to the boson-boson interaction, $(\delta T_c/T_c)_{bb}\simeq-1.33(a_{bb}/a_{ho}^b)N_b^{1/6}=-3.2\%$, and the finite-size correction, $(\delta T_c/T_c)_{fs}\simeq-0.73N_b^{-1/3}=-2.7\%$ [21].
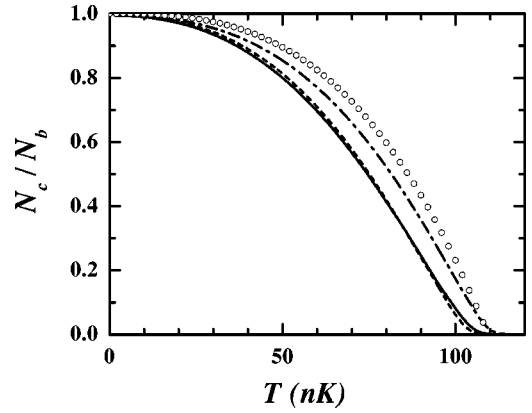
In conclusion, we have generalized the HFB-Popov theory to binary BF mixtures and have presented a detailed study of the thermodynamic properties of mixtures at finite temperature, including the density profiles, the condensate fraction, as well as the critical temperature of BEC. These quantities are found to depend on the BF interaction in a nonlinear way. Moreover, under conditions appropriate to the ^{87}Rb-^{40}K mixture in the LENS experiments, the condensate fraction and the critical temperature of BEC are significantly enhanced with respect to the prediction for a pure interacting Bose gas. This enhancement might be observable in current experiments.

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