Pis'ma v ZhETF, vol. 80, iss. 4, pp. 305 – 310

Stability of Bose system in Bose-Fermi mixture with attraction between bosons and fermions

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Submitted 24 June 2004

Resubmitted 12 Jule 2004

An effective Hamiltonian for the Bose system in the mixture of ultracold atomic clouds of bosons and fermions is obtained by integrating out the Fermi degrees of freedom. An instability of the Bose system is found in the case of attractive interaction between components in good agreement with the experiment on the bosonic ^{87}Rb and fermionic ^{40}K mixture.

PACS: 03.75.Fi, 67.57.Fg, 67.90.+z

Since the first realization of Bose-Einstein condensation in ultracold atomic gas clouds [1 – 3], studies in this direction have yielded unprecedented insight into the quantum statistical properties of matter. Besides the studies using the bosonic atoms, growing interest is focused on the cooling of fermionic atoms to a temperature regime where quantum effects dominate the properties of the gas [4 – 6]. This interest is mainly motivated by the quest for the Bardeen-Cooper-Schrieffer (BCS) transition in ultarcold atomic Fermi gasses [7 – 9].

Strong s-wave interactions that facilitate evaporative cooling of bosons are absent among spin-polarized fermions due to the exclusion Pauli principle. So the fermions are cooled to degeneracy through the mediation of fermions in another spin state [4, 6 – 9] or via a buffer gas of bosons [5, 10, 11] (sympathetic cooling). The Bose gas, which can be cooled evaporatively, is used as a coolant, the fermionic system being in thermal equilibrium with the cold Bose gas through boson-fermion interaction in the region of overlapping of the systems.

However, the physical properties of Bose-Fermi mixtures are interesting in their own rights and are the subject of intensive investigations including the analysis of ground state properties, stability, effective Fermi-Fermi interaction mediated by the bosons, and new quantum phases in an optical lattices [12 – 16]. Several successful attempts to trap and cool mixtures of bosons and fermions were reported. Quantum degeneracy was first reached with mixtures of bosonic ^{7}Li and fermionic ^{6}Li atoms [5, 10]. Later, experiments to cool mixtures of ^{23}Na and ^{6}Li [17], as well as ^{87}Rb and ^{40}K [11, 18], to ultralow temperatures succeeded.

In this article we study the instability and collapses of the trapped boson-fermion mixture due to the boson-fermion attractive interaction, using the effective Hamiltonian for the Bose system [14]. We analyze quantitatively properties of the ^{87}Rb and ^{40}K mixture with an attractive interaction between bosons and fermions recently studied by Modugno and co-workers [11]. They found that as the number of bosons is increased there is an instability value N_{Bc} at which a discontinues leakage of the bosons and fermions occurs, and collapse of boson and fermion clouds is observed. Using the experimental parameters we estimated the instability boson number N_{Bc} for the collapse transition as a function of the fermion number and temperature and found a good agreement with experimental results.

First of all we briefly discuss the effective boson Hamiltonian [14]. Our starting point is the functional-integral representation of the grand-canonical partition function of the Bose-Fermi mixture. It has the form [15, 19, 20]:

$$Z = \int D[\phi^*]D[\phi]D[\psi^*]D[\psi]\exp\Big\{ -\frac{1}{\hbar}(S_B(\phi^*,\phi) + + S_F(\psi^*,\psi) + S_{\rm int}(\phi^*,\phi,\psi^*,\psi))\Big\} \qquad (1)$$

and consists of an integration over a complex field $\phi(\tau,\mathbf{r})$, which is periodic on the imaginary-time interval $[0,\hbar\beta]$, and over the Grassmann field $\psi(\tau,\mathbf{r})$, which is antiperiodic on this interval. Therefore, $\phi(\tau,\mathbf{r})$ describes the Bose component of the mixture, whereas $\psi(\tau,\mathbf{r})$ corresponds to the Fermi component. The term describing the Bose gas has the form:

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$$S_B(\phi^*,\phi)=\int_0^{\hbar\beta}d\tau\int d\mathbf{r}\Big\{\phi^*(\tau,\mathbf{r})\Big(\hbar\frac{\partial}{\partial\tau}-\frac{\hbar^2\nabla^2}{2m_B}+ +V_B(\mathbf{r})-\mu_B\Big)\phi(\tau,\mathbf{r})+\frac{g_B}{2}|\phi(\tau,\mathbf{r})|^4\Big\}. \quad (2)$$

Because the Pauli principle forbids s-wave scattering between fermionic atoms in the same hyperfine state, the Fermi-gas term can be written in the form:

$$S_F(\psi^*,\psi)=\int_0^{\hbar\beta}d\tau\int d\mathbf{r}\Big\{\psi^*(\tau,\mathbf{r})\Big(\hbar\frac{\partial}{\partial\tau}-\frac{\hbar^2\nabla^2}{2m_F}+ +V_F(\mathbf{r})-\mu_F\Big)\psi(\tau,\mathbf{r})\Big\}. \quad (3)$$

The term describing the interaction between the two components of the Fermi–Bose mixture is:

$$S_{\rm int}(\phi^*,\phi,\psi^*,\psi)=g_{BF}\int_0^{\hbar\beta}d\tau\int d\mathbf{r}|\psi(\tau,\mathbf{r})|^2|\phi(\tau,\mathbf{r})|^2, \quad (4)$$

where $g_B=4\pi\hbar^2a_B/m_B$ and $g_{BF}=2\pi\hbar^2a_{BF}/m_I$, $m_I=m_Bm_F/(m_B+m_F)$, m_B and m_F are the masses of bosonic and fermionic atoms respectively, a_B and a_{BF} are the s wave scattering lengths of boson-boson and boson-fermion interactions.

Integral over Fermi fields is Gassian, we can calculate this integral and obtain the partition function of the Fermi system as a functional of Bose field $\phi(\tau,\mathbf{r})$. Let us rewrite the integral over $\psi(\tau,\mathbf{r})$ in the form:

$$Z_F=\int D[\psi^*]D[\psi]\exp\Big(-\frac{1}{\hbar}\Big(S_F(\psi^*,\psi)+ +S_{\rm int}(\phi^*,\phi,\psi^*,\psi)\Big)\Big)= =\int D[\psi^*]D[\psi]\exp\Big\{\int_0^{\hbar\beta}d\tau\int d\mathbf{r}\int_0^{\hbar\beta}d\tau'\int d\mathbf{r}'\times \times\psi^*(\tau,\mathbf{r})\mathbf{G}^{-1}(\tau,\mathbf{r},\tau',\mathbf{r}')\psi(\tau',\mathbf{r}')\Big\}, \quad (5)$$

where

$$\mathbf{G}^{-1}=\mathbf{G}_0^{-1}-\mathbf{\Sigma} \quad (6)$$

is the Dyson equation, and $\Sigma(\tau,\mathbf{r},\tau',\mathbf{r}')$ is a selfenergy,

$$\mathbf{G}_0^{-1}(\tau,\mathbf{r},\tau',\mathbf{r}')=-\frac{1}{\hbar}\Big(\hbar\frac{\partial}{\partial\tau}-\frac{\hbar^2\nabla^2}{2m_F}+ +V_F(\mathbf{r})-\mu_F\Big)\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau'); \quad (7)$$

$$\mathbf{\Sigma}(\tau,\mathbf{r},\tau',\mathbf{r}')=\frac{g_{BF}}{\hbar}|\phi(\tau,\mathbf{r})|^2\delta(\mathbf{r}-\mathbf{r}')\delta(\tau-\tau'). \quad (8)$$

Using the formula for the gaussian integral over the Grassmann variables [19, 20]

$$\int\prod_n d\psi_n^*d\psi_n\exp\Big\{-\sum_{n,n'}\psi_n^*A_{n,n'}\psi_{n'}\Big\}=e^{\mathrm{Sp}[\ln A]} \quad (9)$$

one has:

$$Z_F=\exp\left(\mathrm{Sp}\ln\left(-\mathbf{G}^{-1}\right)\right)=\exp\Big(-\frac{1}{\hbar}S_{eff}\Big). \quad (10)$$

S_{eff} can be expanded in powers of $|\phi(\tau,\mathbf{r})|^2$ by using the series:

$$\mathbf{G}^{-1}=\mathbf{G}_0^{-1}-\mathbf{\Sigma}=\mathbf{G}_0^{-1}(\mathbf{I}-\mathbf{G}_0\Sigma), \quad \mathrm{Sp}(\ln(-\mathbf{G}^{-1}))=\mathrm{Sp}(\ln(-\mathbf{G}_0^{-1}))- -\sum_{n=1}^{\infty}\frac{1}{n}\mathrm{Sp}\left[(\mathbf{G_0}\Sigma)^n\right]. \quad (11)$$

To proceed let us rewrite $\mathbf{G_0}$ in the form:

$$\mathbf{G}_0(\tau,\mathbf{r},\tau',\mathbf{r}')=\sum_{\omega,n}\frac{-\hbar}{-i\hbar\omega+\epsilon_n-\mu_F}\times \times\xi_n(\mathbf{r})\xi_n^*(\mathbf{r}')\frac{e^{-i\omega(\tau-\tau')}}{\hbar\beta}, \quad (12)$$

where $\omega=\pi(2s+1)/\hbar\beta;\ s=0,\pm1,\dots$ and

$$\Big(-\frac{\hbar^2\nabla^2}{2m_F}+V_F(\mathbf{r})\Big)\xi_n(\mathbf{r})=\epsilon_n\xi_n(\mathbf{r}).$$

Because of large number of fermionic atoms in the system one can use the semiclassical Thomas-Fermi approximation [21]:

$$\sum_n\xi_n(\mathbf{r})\xi_n^*(\mathbf{r})F(\epsilon_n)=\frac{1}{(2\pi\hbar)^3}\int d\mathbf{p}F(H_0(\mathbf{p},\mathbf{r})), \quad (13)$$

where $H_0(\mathbf{p},\mathbf{r})=p^2/2m_F+V_F(\mathbf{r})$ and $F(x)$ is an arbitrary function.

We suppose that all $|\phi(\tau_i,\mathbf{r}_i)|^2$ have one and the same argument $(\tau_1,\mathbf{r}_1)$ (see, for example, [19]). Using Eq. (13) $S_{\rm eff}$ may be written in the form:

$$S_{\rm eff}=\int_0^{\hbar\beta}d\tau d\mathbf{r}f_{\rm eff}(|\phi(\tau,\mathbf{r})|), \quad (14)$$

$$f_{\rm eff}=-\frac{3}{2}\kappa\beta^{-1}\int_0^{\infty}\sqrt{\epsilon}d\epsilon\ln\left(1+e^{\beta(\tilde\mu-\epsilon)}\right)= =-\kappa\int_0^{\infty}\frac{\epsilon^{3/2}d\epsilon}{1+e^{\beta(\epsilon-\tilde\mu)}}, \quad (15)$$

where $\epsilon = p^2/2m_F$, $\tilde{\mu} = \mu_F - V_F(\mathbf{r}) - g_{BF}|\phi(\tau, \mathbf{r})|^2$ and $\kappa = 2^{1/2} m_F^{3/2}/3\pi^2\hbar^3$.

So we can write the effective bosonic Hamiltonian in the form:

$$H_{\text{eff}} = \int d\mathbf{r} \left\{ \frac{\hbar^2}{2m_B}|\nabla\phi|^2 + (V_B(\mathbf{r}) - \mu_B)|\phi|^2 + \right. \\ \left. + \frac{g_B}{2}|\phi|^4 + f_{\text{eff}}(|\phi|) \right\}. \quad (16)$$

The first three terms in (16) have the conventional Gross-Pitaevskii [22] form, and the last term is a result of boson-fermion interaction. In low temperature limit $\tilde{\mu}/k_B T \gg 1$ one can write $f_{\text{eff}}(|\phi|)$ in the form:

$$f_{\text{eff}}(|\phi|) = -\frac{2}{5}\kappa\tilde{\mu}^{5/2} - \frac{\pi^2}{4}\kappa(k_B T)^2\tilde{\mu}^{1/2}. \quad (17)$$

As usual, μ_F can be determined from the equation

$$N_F = \int d\mathbf{r} n_F(\mathbf{r}). \quad (18)$$

where

$$n_F(\mathbf{r}) = \frac{3}{2}\kappa \int\limits_0^\infty \frac{\sqrt{\epsilon}d\epsilon}{1 + e^{\beta(\epsilon - \tilde{\mu})}}. \quad (19)$$

At low temperatures we have:

$$n_F(\mathbf{r}) = \kappa\tilde{\mu}^{3/2} + \frac{\pi^2\kappa}{8\tilde{\mu}^{1/2}}(k_B T)^2. \quad (20)$$

In general case the Bose and Fermi systems have different temperature scales, and Eqs. (17) and (20) may be useful for studying the temperature behavior of Bose system, including the calculation of the critical temperature. For example, the characteristic temperature for the Bose system - the transition temperature for the ideal Bose gas - is [22]: $k_B T_c^0 = 0.94\hbar\omega_B(\lambda N_B)^{1/3}$. The Fermi temperature for a pure system is [21] $k_B T_F = \hbar\omega_F(6\lambda N_F)^{1/3}$. Taking into account that $\omega_F = \sqrt{m_B/m_F}\omega_B$, one can see that for $m_B > m_F$ and approximately the same numbers of bosons and fermions one can safely use Eqs. (17) and (20) to describe the behavior of the Bose system.

Let us consider now the ^{87}Rb and ^{40}K mixture with an attractive interaction between bosons and fermions [11]. The parameters of the system are the following: $a_B = 5.25\,\text{nm}$, $a_{BF} = -21.7^{+4.3}_{-4.8}\,\text{nm}$. K and Rb atoms were prepared in the doubly polarized states $|F = 9/2, m_F = 9/2>$ and $|2, 2>$, respectively. The magnetic potential had an elongated symmetry, with harmonic oscillation frequencies for Rb atoms $\omega_{B,r} = \omega_B = 2\pi \times 215\,\text{Hz}$ and $\omega_{B,z} = \lambda\omega_B = 2\pi \times 16.3\,\text{Hz}$, $\omega_F = \sqrt{m_B/m_F}\omega_B \approx 1.47\omega_B$, so that $m_B\omega_B^2/2 = m_F\omega_F^2/2 = V_0$. The collapse was found for the following critical numbers of bosons and fermions: $N_{Bc} \approx 10^5; N_K \approx 2 \cdot 10^4$.

At the zero temperature limit, expanding $f_{\text{eff}}(|\phi|)$ up to the third order in g_{BF} we obtain the effective Hamiltonian in the form:

$$H_{\text{eff}} = \int d\mathbf{r} \left\{ \frac{\hbar^2}{2m_B}|\nabla\phi|^2 + (V_{\text{eff}}(\mathbf{r}) - \mu_B)|\phi|^2 + \right. \\ \left. + \frac{g_{\text{eff}}}{2}|\phi|^4 + \frac{\kappa}{8\mu_F^{1/2}} g_{BF}^3 |\phi|^6 \right\}, \quad (21)$$

where

$$V_{\text{eff}}(\mathbf{r}) = \left(1 - \frac{3}{2}\kappa\mu_F^{1/2} g_{BF}\right)\frac{1}{2}m_B\omega_B^2\left(\rho^2 + \lambda^2 z^2\right), \quad (22)$$

$$g_{\text{eff}} = g_B - \frac{3}{2}\kappa\mu_F^{1/2} g_{BF}^2, \quad (23)$$

and $\rho^2 = x^2 + y^2$.

In principle, one can study the properties of a Bose-Fermi mixture with the help of f_{eff} (17) without any expansion. However, the form of the Hamiltonian (21) gives the possibility to get a clear insight into the physics of the influence of the Fermi system on the Bose one (see discussion below). It may be easily verified that the expansion of the function $f(x) = (1 + x)^{5/2}$ (see Eq. (17)) up to the third order in x gives a reasonably good approximation for $f(x)$ even for rather large values of x, in contrast with the higher order expansions, so one can safely use Eq. (21) as a starting point for the investigation of the properties of the Bose subsystem.

In derivation of Eqs. (21)–(23) we also use the fact that due to the Pauli principle (quantum pressure) the radius of the Bose condensate is much less than the radius of the Fermi cloud $R_F \approx \sqrt{\mu_F/V_0}$, so one can use an expansions in powers of $V_F(\mathbf{r})/\mu_F$.

From Eq. (22) one can see that the interaction with Fermi gas leads to modification of the trapping potential. For the attractive fermion-boson interaction the system should behave as if it was confined in a magnetic trapping potential with larger frequencies than the actual ones, in agreement with experiment [11]. Boson-fermion interaction also induces the additional attraction between Bose atoms which does not depend on the sign of g_{BF}.

The last term in H_{eff} (21) corresponds to the three-particle *elastic* collisions induced by the boson-fermion interaction. In contrast with *inelastic* 3-body collisions which result in the recombination and removing particles from the system [23], this term for $g_{BF} < 0$ leads to increase of the gas density in the center of the trap in order to lower the total energy. The positive zero point energy and boson-boson repulsion energy (the first two terms in Eq. (21)) stabilize the system. However, if the central density grows too much, the kinetic energy and boson-boson repulsion are no longer able to prevent the collapse of the gas. Likewise the case of Bose condensate with attraction (see, for example, [22–24]), the collapse is expected to occur when the number of particles in the condensate exceeds the critical value N_{Bc}.

The critical number N_{Bc} can be calculated using the well-known ansatz for the Bosonic wave function [22]:

$$\phi(\mathbf{r}) = \left(\frac{N_B\lambda}{w^3a^3\pi^{3/2}}\right)^{1/2} \exp\left(-\frac{(\rho^2+\lambda^2z^2)}{2w^2a^2}\right), \quad (24)$$

where w is a dimensionless variational parameter which fixes the width of the condensate and $a=\sqrt{\hbar/m_B\omega_B}$.

In this case the variational energy E_B has the form:

$$\frac{E_B}{N_B\hbar\omega_B} = \frac{2+\lambda}{4}\frac{1}{w^2} + bw^2 + \frac{c_1N_B}{w^3} + \frac{c_2N_B^2}{w^6}, \quad (25)$$

$$b = \frac{3}{4}\left(1-\frac{3}{2}\kappa\mu_F^{1/2}g_{BF}\right),$$

$$c_1 = \frac{1}{2}\left(g_B - \frac{3}{2}\kappa\mu_F^{1/2}g_{BF}^2\right)\frac{\lambda}{(2\pi)^{3/2}\hbar\omega_B a^3},$$

$$c_2 = \frac{\kappa}{8\mu_F^{1/2}}g_{BF}^3\frac{\lambda^2}{3^{3/2}\pi^3\hbar\omega_B a^6}.$$

This energy is plotted in Fig.1 as a function of w for several values of N_B. It is seen that when $N_B < N_{Bc}$ there is a local minimum of E_B which correspond to a metastable state of the system. This minimum arises due the competition between the positive first three terms in Eq. (25) and negative fourth term. The local minimum disappears when the number of bosons N_B exceeds the critical value which can be calculated by requiring that the first and second derivatives of E_B vanish at the critical point. In this case the behavior of E_B is mainly determined by the second and fourth terms in Eq. (25). For $N_K = 2\cdot10^4$ and $a_{BF} = -19.44$ nm we obtain $N_{Bc}\approx 9\cdot 10^4$ in a good agreement with the experiment [11]. It is interesting to note that the critical number of Bose atoms in Bose-Fermi mixture is about two orders larger than the critical number for the condensate with a purely attractive interaction. For example, in the experiments with trapped ^{7}Li [3] it was found that the critical number of bosons is about 1000.

In Eq. (25) we use $\mu_F^0 = \hbar\omega_F[6\lambda N_F]^{1/3}$ as the chemical potential of the Fermi system μ_F. The corrections to μ_F due to interaction with the Bose system have the form: $\mu_F = \hbar\omega_F[6N_F]^{1/3}[1+m_1+m_2]$, where $m_1 = \frac{1/2\kappa g_{BF}(\mu_F^0)^{1/2}N_B}{N_F}$ and $m_2 = -\frac{3/4\kappa g_{BF}(\mu_F^0)^{-1/2}m_F\omega_F^2w^2a^2N_B}{N_F}$. It may be shown that

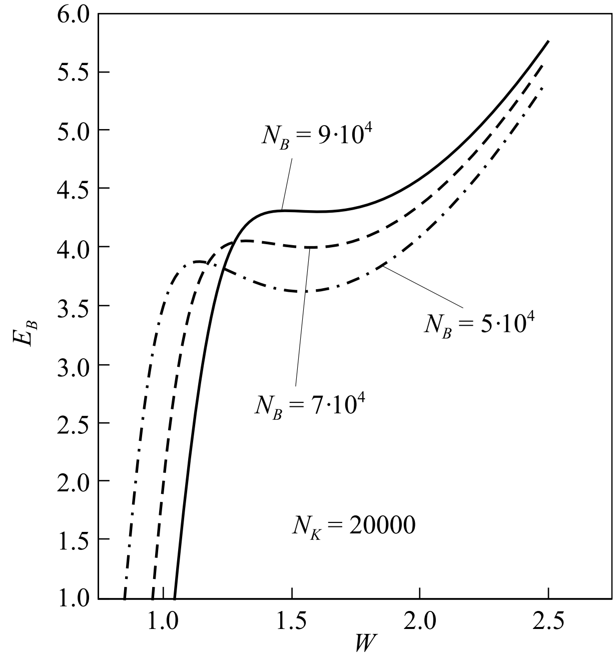

Fig.1. Variational energy $E_B/N_B\hbar\omega_B$ as a function of w for various numbers of bosons

$m_1+m_2\approx 0.09$ for the values of the parameters used in these calculations.

Upon increasing the number of fermions, the repulsion between bosons decreases leading to the collapse for the smaller numbers of the bosonic atoms. In Fig.2 the critical number of bosons N_{Bc} is represented as a function of the number of fermions.

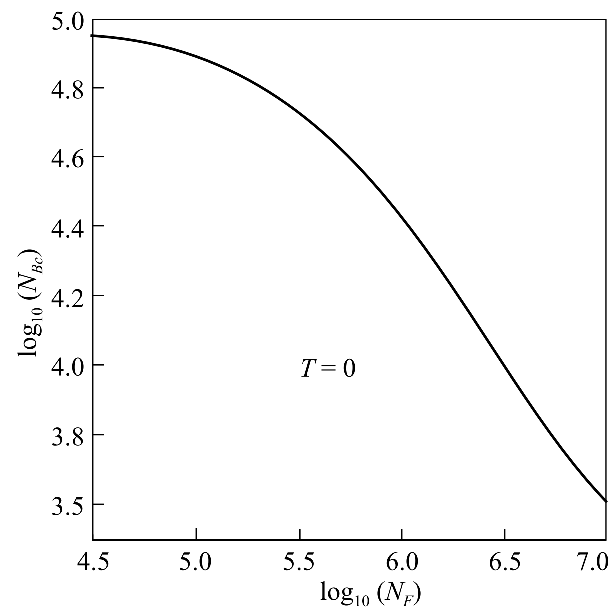

Fig.2. Critical number of bosons N_{Bc} as a function of the number of fermions N_F at $T=0$

The critical number of bosons N_{Bc} is extremely sensitive to the precise value of the boson-fermion s wave scattering length. This is illustrated in Fig.3.

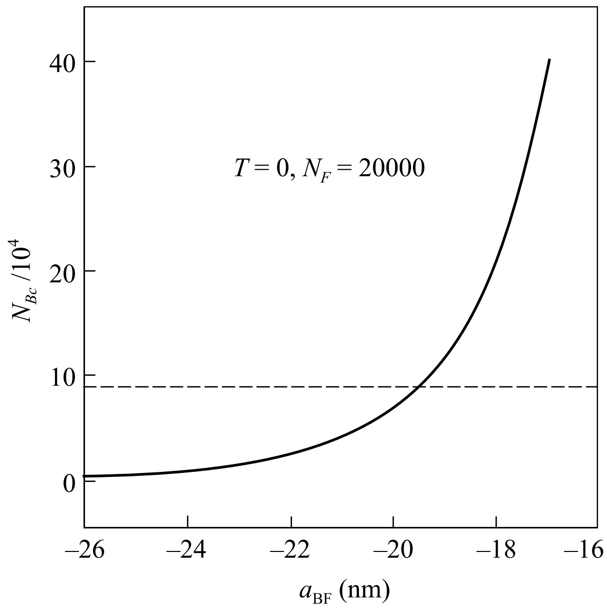

Fig.3. Critical number of bosons N_{Bc} as a function of the boson-fermion scattering length a_{BF}

Fig.4 shows the dependence of the critical number of bosons N_{Bc} on the temperature calculated with the help

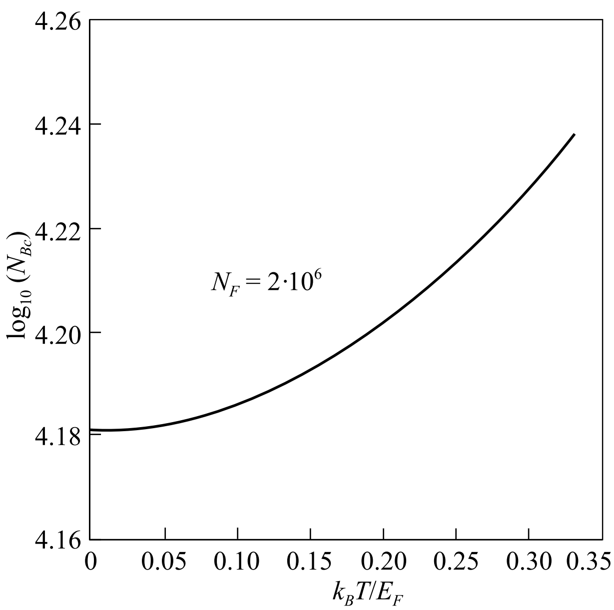

Fig.4. Critical number of bosons N_{Bc} as a function of reduced temperature k_BT/E_F for $N_F = 2 \cdot 10^6$

of the equation (17). This dependence has a simple explanation: an increase of the temperature results in the decrease of the local density of fermions and reduces the interaction energy between Bose and Fermi systems.

Finally, we make a short remark on the nature of the collapse transition. In this article we found the instability point of the Bose-Fermi mixture with attractive interaction between components. A strong rise of density of bosons and fermions (see Eq. (20)) in the collapsing condensate enhances intrinsic inelastic processes, in particular, the recombination in 3-body interatomic collisions, as is the case for the well-known ^{7}Li condensates [23]. However, recently M. Yu. Kagan and coworkers suggested the new microscopic mechanism of removing atoms from the system which is specific for the Bose-Fermi mixtures with attraction between components and is based on the formation of the boson-fermion bound states [25]. It seems that the description of the evolution of the collapsing condensate should include both these mechanisms.

VNR acknowledges valuable discussions with M. Yu. Kagan. The work was supported in part by the Russian Foundation for Basic Research (Grants # 02-02-16622 and # 02-02-16621). STC is partly supported by a grant from NASA.

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