Abstract

For mixtures of Bose and Fermi alkali atoms, the Fermion degrees of freedom can be integrated out in their finite temperature partition function. The final result can be expanded as a power series in the Boson density. Under appropriate conditions, the pairwise interaction between the bosons can be changed from positive to negative at a low enough temperature by the Fermion-mediated term and the Boson cloud may then collapse. For attractive Fermion-Boson interactions, there is also a collapse of the Fermion cloud. This transition is first order (discontinuous) because the leading order nonlinear interaction term between the Bosons is third order in Boson density with a negative coefficient. We discuss the finite temperature phase diagram of this transition. Our result may provide for an explanation of recent experimental observations by Modungo and coworkers.

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There is much recent interest in mixtures of Bose and Fermi alkali atoms in traps experimentally. This includes different hyperfine states of the Li6-Li7 system, Na23-Li6 and K40-Rb87. The original motivation was to study possible superconductivity in the Fermions. In these systems, the Fermions are essentially non-interacting. From the Fermi exclusion principle, no two Fermions can be at the same place, the s-wave scattering between them cannot occur. As a result, evaporative cooling of the Fermions alone is ineffective. To evaporatively cooled the Fermions the Bosons were used as a refrigerant experimentally. Much of the current theoretical interest is focused on estimating the possible superconducting properties of the Fermion system. Nevertheless, mixtures of Bosons and Fermions are interesting in their own right. Modugno and coworkers recently studied mixtures of $^{40}K$ and $^{87}Rb$ with an attractive interaction between the Boson and Fermion and found that as the number of Boson is increased there is a “instability value” $N_{Bc}$ at which a discontinuous leakage of the Boson and Fermion occurs. They observed a first order collapse transition of the Boson and Fermion clouds. This paper explores the origin and the nature of this collapse transition. The nature of the transition depends on the higher order term of the Boson interaction. Because there is no direct interaction between the Fermions, it is possible to formally exactly integrate out their degree of freedom in their finite temperature partition function. The final result can be expanded as a power series in the Boson density. An effective interaction between the Bosons is obtained. We found that the pairwise effective interaction can become attractive for a large enough number of Bosons and at a sufficiently low temperature and the Boson cloud collapses. This is analogous to earlier experiments with fixed attractive Boson interaction where the Boson cloud also collapses. In the present case, the effective interaction depends on the atom densities and can change during the collapse. In addition, in contrast to the one component case, the Boson interaction involve powers of the Boson density higher than the second. The leading nonlinear interaction term is proportional to an odd (third) power of the Boson density ($n_B^3$) with a negative coefficient. As a result the transition is discontinuous and physical quantities change discontinuously. Using the experimental parameters, we estimate the instability Boson number $N_{Bc}$ for the Boson cloud to collapse. We found $N_{Bc}$ to be extremely sensitive to the precise value of the Boson Fermion scattering length $a_{BF}$. For $N_f = 2 \times 10^4$, $N_{Bc} \approx 10^5$ when $a_{BF} \approx -16.7 nm$, in good agreement with experimental results.
The Boson-Fermion system may also exhibit a superconducting transition. The Boson induced Fermi interaction is attractive and thus the superconducting transition always occurs at zero temperature. The superconducting transition temperature for the Fermions is usually very low, because it is an exponential function of the dimensionless coupling constant $a$: 

$$T_{sc} = T_F \exp(-1/a).$$

As a result the superconducting transition is difficult to observe experimentally. Thus it is important to know if the same difficulty applies to the collapse transition. The renormalized Boson interaction can change from attractive to repulsive at a sufficiently high temperature. A phase diagram of $N_{Bc}$ as a function of the temperature $T$ is worked out. We found that the collapse transition is much easier to observe than the superconducting transition. A possible interpretation of the observation of Modugno and coworkers from the above picture is as follows: As a result of the Fermion-Boson attraction, the collapse transition will happen to both the Boson and the Fermion. When the density is high enough, they disappear from the trap. If the amount of Fermion is smaller than the Bosons, they will be gone first. Once the Fermion density is small enough, the Bosons will stop collapsing. We now discuss our results in detail.

We first integrate out the Fermion degrees of freedom in the path integral for the system. Our starting point is the functional-integral representation of the grand-canonical partition function of the Bose-Fermi mixture. It has the form [7, 8, 9, 10]:

$$Z = \int D[\phi^*]D[\phi]D[\psi^*]D[\psi] \exp \left\{ -\frac{1}{\hbar} \left( S_B(\phi^*, \phi) + S_F(\psi^*, \psi) + S_{int}(\phi^*, \phi, \psi^*, \psi) \right) \right\}. \quad (1)$$

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

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

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 noninteracting form: 

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

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

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

where $g_B = 4\pi \hbar^2 a_B/m_B$ and $g_{BF} = 2\pi \hbar^2 a_{BF}/m_I$, $m_I = m_B m_F/(m_B + m_F)$.

The integral over the Fermi fields $\psi$ is Gaussian. We can calculate this integral and obtain
the partition function of the Fermi system as a functional of the Bose field $\phi(\tau, r)$. To proceed we rewrite the partition function as $Z = \int D[\phi^*]D[\phi]Z_F \exp \left\{ -\frac{1}{\hbar} (S_B(\phi^*, \phi)) \right\}$. $Z_F$ is the integral involving $\psi(\tau, r)$: $Z_F = \int D[\psi^*]D[\psi] \exp \left\{ -\frac{1}{\hbar} (S_F(\psi^*, \psi) + S_{int}(\phi^*, \phi, \psi^*, \psi)) \right\} = \int D[\psi^*]D[\psi] \exp \left\{ \int_0^{\hbar} d\tau \int d\tau' \int d\tau'' d\tau''' \int d\tau'''' \int d\tau'''' \int d\tau''''' \int d\tau'''''' \int d\tau''''''' \phi^*(\tau, r) R^{-1}(\tau, r, r', \tau'') \psi(\tau', r') \right\},$ where $G^{-1} = G^{-1}_F - \Sigma G^{-1}_F$. To illustrate our approach we rewrite the partition function as $Z = \int D[\phi^*]D[\phi]Z_F \exp \left\{ -\frac{1}{\hbar} (S_B(\phi^*, \phi)) \right\}$. Using the formula for the gaussian integral over the Grassmann variables $\int D[\psi^*]D[\psi] \exp \left\{ -\frac{1}{\hbar} (S_F(\psi^*, \psi) + S_{int}(\phi^*, \phi, \psi^*, \psi)) \right\} = \int D[\phi^*]D[\phi] \exp \left\{ -\frac{1}{\hbar} (S_B(\phi^*, \phi) + S_F(\phi^*, \phi) - H_B) \right\}$, we have $Z_F = \exp (Tr \ln (-G^{-1})) G$ contains the additional interaction between the Bosons due to the presence of the Fermions. The properties of the Fermions can also be calculated. For example, the Fermion density can be calculated from the functional derivative $<\psi^*(r)\psi(r)> = <\delta Z_F/\delta G^{-1}(\tau, r, \tau, r)>$. To illustrate the applicability of this result, we consider its contribution to the effective interaction between the Bosons.

In the absence of the Fermions, the Boson wave function can be represented as a wave function $\phi_0$ which is given in the Thomas-Fermi approximation by $|\phi_0|^2 = (\mu_B - 0.5m_B \omega^2_B(x^2 + y^2 + \lambda^2 z^2)/g_B$. Multiboson interaction can be obtained from an expansion of $\ln(-G^{-1})$ in powers of the deviation of the boson density from $|\phi_0|^2$: $|\phi|^2 = |\phi_0|^2 + |\phi|^2$. In this spirit, we write $\Sigma = \Sigma_0 + \delta \Sigma$ where $\Sigma_0(\tau, r, \tau', r') = g_B |\phi_0|^2 |\phi|^2 (\tau - \tau')/h$. The corresponding Green’s function is defined as $G^{-1}_0 = G^{-1}_F - \Sigma_0$. We have $G^{-1} = G^{-1}_0 - \Sigma = G^{-1}_0 (I - G_0 \delta \Sigma)$, $Tr(\ln(-G^{-1})) = Tr(\ln(-G_0^{-1})) - \infty \sum_{n=1}^{\infty} Tr([G_0 \delta \Sigma]^n)/n = -\infty \sum_{n=1}^{\infty} S_n/h$. The pair interaction comes from the term $S_2 = Tr(G_0 \delta \Sigma)^2/2$. The resulting expression can be evaluated in the Thomas-Fermi approximation and assuming that the Fermions move faster than the Bose condensates. To illustrate our approach we consider the term $S_1 = Tr(G_0 \delta \Sigma)$. Let us rewrite $G_0$ in the form: $G_0(\tau, r, \tau', r') = \sum_{\omega, n} -\hbar \xi_n(r) \xi_n^*(r') e^{-i\omega(\tau - \tau')}/(-i\hbar \omega + \epsilon_n - \mu_F)/h \beta$, where $\omega = \pi (2s + 1)/\hbar \beta$; $s = 0, \pm 1, \ldots$, $(-\hbar^2 \nabla^2/2m_F + V_F(r) + g_B |\phi_0|^2) \xi_n(r) = \epsilon_n \xi_n(r)$ becomes $S_1 = TrG_0 \Sigma = \int d\tau dr G_0(\tau, r, \tau, r) g_B |\phi(\tau, r)|^2/h = g_B (h/\beta) \int_0^{\hbar} d\tau dr \delta[\phi(\tau, r)]^2 \sum_{\omega, n} \xi_n(r) \xi_n^*(r)/[i\hbar \omega - (\epsilon_n - \mu_F)] = g_B (h/\beta) \int_0^{\hbar} d\tau dr \delta[\phi(\tau, r)]^2 \sum_{\omega, n} \xi_n(r) \xi_n^*(r)/[\epsilon^2(\epsilon_n - \mu_F) + 1].$ In the semiclassical Thomas-Fermi approximation one has:

$$\sum_n \frac{\xi_n(r) \xi_n^*(r)}{e^{\beta(\epsilon_n - \mu_F)} + 1} = \frac{1}{\beta \hbar} \int dp \frac{1}{e^{\beta (H(0, p, r) - \mu_F)} + 1},$$

(2)
For $D=3$, we find using the low temperature expansion
\[ \mu = \frac{g_{BF} \hbar}{\hbar \beta} \int_0^{\hbar \beta \tau \delta} d\tau d\delta |\phi(\tau, r)|^2 \left[ \frac{1}{(2\pi \hbar)^D} \int d\mathbf{p} e^{\beta H_0(\mathbf{p}, r) - \mu} + 1 \right] \]  
(3)

Similarly we get
\[ S_2 = -\frac{\beta g_{BF}^2}{2\hbar} \int_0^{\hbar \beta \tau \delta} d\tau d\delta (|\phi(\tau, r)|^2)^2 \left[ \frac{1}{(2\pi \hbar)^D} \int d\mathbf{p} e^{\beta H_0(\mathbf{p}, r) - \mu} \right] \]
(4)

where $H_0(\mathbf{p}, r) = p^2/(2m_F) + V_F(r) - g_{BF} |\phi_0(r)|^2$.

We can write the effective Bosonic Hamiltonian in a power series in $\delta|\phi|^2$:
\[ H_{GP} = \int d\mathbf{r} \left\{ \frac{\hbar^2}{2m_B} |\nabla \phi|^2 + V_{eff}(r) \delta|\phi|^2 + \frac{g_{eff}}{2} (\delta|\phi|^2)^2 \right\}, \]
(5)

where
\[ V_{eff} = 0.5 D^\gamma_D g_{BF} \int_0^\infty e^{D/2-1} e^\mu d\epsilon \]
(6)
\[ g_{eff} = g_B - \beta \kappa_D g_{BF} \int_0^\infty e^{D/2-1} e^{\epsilon+V_F-\mu} d\epsilon \]
(7)
\[ \bar{\mu} = \mu_F - V_F(r) - g_{BF} |\phi_0(r)|^2, \]
\[ \kappa_D = (2m_F/\hbar^2)^{D/2}/(2\pi C_D), \quad C_1 = 1, \quad C_2 = 2, \quad C_3 = 2\pi; \]
\[ \gamma_D = (2m_F/\hbar^2)^{D/2}/(2\pi C'_D), \quad C'_1 = 1/2, \quad C'_2 = 2, \quad C'_3 = 3\pi; \quad c = (2m_F/\hbar^2)^{D/2}/(12\mu_F^5 \pi C_D). \]

For $D=3$, we find using the low temperature expansion
\[ V_{eff} = g_{BF} \left( \gamma_3 \bar{\mu}^{3/2} + \frac{\pi^2}{12 \bar{\mu}^{1/2} \kappa_3 (k_B T)^2} \right), \]
(8)
\[ g_{eff}(T) = g_B - g_{BF}^2 \kappa_3 \bar{\mu}^{1/2} \alpha. \]
(9)

\[ \alpha = [1 - \frac{\pi^2}{24} (k_B T/\bar{\mu})^2]. \]

In the same approximation, we get, for $D=3$, $n_F(r) = \kappa_3 \int_0^\infty \frac{e^\epsilon}{1 + e^{\epsilon+V_F-\mu}} d\epsilon$, and

at low temperatures we have:
\[ n_F(r) = 2 \kappa_3 \bar{\mu}^{3/2} / 3 + \frac{\pi^2 \kappa_3}{12 \bar{\mu}^{1/2} (k_B T)^2}. \]
(10)

We thus expect the Fermion density $n_F$ to increase as the Boson density increases. As usual, $\mu_F$ can be determined from the equation $N_F = \int d\mathbf{r} n_F(\mathbf{r})$.

Modugno and coworkers recently studied mixtures of $^{40}\text{K}$ and $^{87}\text{Rb}$ with an attractive interaction between the Boson and Fermion and found a collapse of the Fermion cloud. The parameters of the system are the following: $a_B = 50 \text{Å}$, $a_{BF} = -217^{+48}_{-43} \text{Å}$, the aspect
ratio of the trapping potential, $\lambda = 0.076$. The corresponding Fermi wave vector is $k_F = 7.7 \times 10^{-4}/\AA$, and $T_F \approx 360nK$ when the number of Fermions, $N_f \approx 2 \times 10^4$.

Eq. (5) looks like a typical Landau free energy expansion of a system with order parameter $O = \delta|\phi|^2$ in a weak external field $V_{eff}$. As we learn from the study of critical phenomena, an instability occurs when coefficient of the $O^2$ term becomes zero. This instability condition of $g_{eff} = 0$ imposes a condition on $\tilde{\mu}$. Now $g_{eff}(r = 0) = g_B - g_{BF}^2 \kappa^3 (\mu_F - g_{BF} \mu_B/g_B)^{1/2}$.[12] With the Thomas-Fermi approximation $\mu_B = (m_B \omega_B^2)^{3/5}(15N_B g_B/4\pi \lambda)^{2/5}/2$. Substituting this expression of $\mu_B$ into the equation of $g_{eff}(r = 0) = 0$, we obtain an estimate of of the critical Boson number $N_{Bc}$ for the instability of the system:

$$N_{Bc} = \left(8\pi [(g_B \pi m_I/g_{BF} m_F a_{BF} k_F \alpha)^2 - 1] \mu_F d_B^3 (a_B/d_B)^{3/5}/g_{BF}\right)^{5/2} (\lambda/15). \quad (11)$$

$d_B = \sqrt{\hbar/m_B \omega_b}$ is the transverse harmonic length for the trapping potential of the Bosons. $\alpha$ is a finite temperature correction factor defined after eq. (9). The dependence of $N_{Bc}$ on $a_{BF}$ is extremely sensitive. In Fig. 1 we show $N_{Bc}$ as a function of $a_{BF}$ for $T/T_F = 0.3$ in units of nm. $N_{Bc}$ changes by a factor of two when $a_{BF}$ changes by 5 per cent. The experimental value of $N_{Bc} \approx 10^5$ suggests that $a_{BF} \approx -16.7nm$.

Even when $g_{eff} < 0$, there is still a tunnelling barrier for the collapse to occur. This tunnelling barrier disappears when $g_{eff} = -g_c$ where estimates of $g_cN_c$ has been given previously as a function of $\lambda$.[13] We have solved this equation iteratively, starting with the initial guess in eq. (28). We found that the corrections to $N_c$ from this condition is less than 1 per cent.

We next address the nature of the phase transition. In previous studies of attractive one component Bosons, the free energy is a function of only the first and the second power of the Boson density. There are no higher power terms. For the present two component system, the effective Boson interaction involve higher power terms of the Boson density. The nature of the transition is determined by these nonlinear terms. We found a term of the order of $c g_{BF}^3 (\delta n_B)^3$ in the free energy functional. From Landau type arguments, if an odd order term with a negative coefficient appears, then at the transition the free energy can be further lowered by a finite increase of $\delta n_B$; the transition is first order. This is in agreement with the experimental observation of a discontinuous leakage in the number of Bosons and Fermions. The usual second order phase transition require a leading nonlinear correction of the order of $n_B^4$ with a positive coefficient and no third order term. This is not the case in
the present system.

The experiment was carried out at finite temperatures. Upon increasing the temperature the induced interaction between the Bose particles can change from attractive to repulsive. From the condition that $g_{eff}(T) = 0$, we obtain a phase diagram of $N_{Be}$ as a function of $T/T_F$. This is shown in Fig. 2. The current system may also exhibit a superconducting transition. The Boson induced Fermi interaction is attractive at zero temperature. The superconducting transition temperature for the Fermions is usually very low, because it is an exponential function of the dimensional coupling constant $a$: $T_{sc} = T_F \exp(-1/a)$. As a result the superconducting transition is difficult to observe experimentally. The collapsing transition temperature is much higher and do not have this problem.

Roth\cite{14} has studied the structure of the mixture numerically at zero temperature with a modified Gross-Pitaevskii equation for the bosons which self-consistently includes the mean-field interaction generated by the fermionic cloud. Numerical results were presented for the instability Boson number $N_{Be}$ as a function of $a_{BF}/d_B$ for isotropic traps. It is not possible to compare his results to the experiment because his results are expressed in terms of a single trap length $d_B$ whereas the experimental trap is anisotropic and there are two trap lengths that differ by a factor of more than three. When $a_{BF}/d_B$ changes by a factor of three, $N_{Be}$ changes by two orders of magnitude.

Viverit and coworkers\cite{15} have discussed an instability criterion based on a linear stability analysis at zero temperature. According to the estimate of ref. (13), the effective coupling for the experimental system is repulsive and far away from the instability point $g_{eff}/|g_{BF}| = 0.055$. Furthermore their instability criterion does not involve $N_B$.

If the temperature is higher than the Fermi temperature but below the Bose condensation temperature, it is still possible to derive an expression for the effective coupling for the Bosons. At high temperatures we have the Boltzman limit ($e^{-\tilde{\mu}/(k_B T)} \ll 1$). In this case Eqs. (6) and (7) take the form:

\begin{equation}
V_{eff} = V_B(r) + \frac{\sqrt{\pi}}{2} g_{BF} k_3 (k_B T)^{3/2} e^{-\tilde{\mu}/(k_B T)},
\end{equation}

\begin{equation}
g_{eff} = g_B - \frac{\sqrt{\pi}}{2} g_{BF} k_3 (k_B T)^{1/2} e^{-\tilde{\mu}/(k_B T)}.
\end{equation}

Now the Fermi energy is replaced by the temperature. As expected, the renormalization effect becomes very small.
Eqs. (8) and (9) are useful for studying other physical properties of the system. For example, for the trapped harmonic potential $U_b(r) = \frac{1}{2}m_b\omega_b^2(x^2 + y^2 + \lambda_b^2z^2)$, the interaction-induced fractional shift to the ideal BEC critical temperature is $\Delta T_0/T_0 \rightarrow -1.33(a_{bb}/d_b)(\lambda_bN_b)^{1/6}$ where $N_b$ is the atom number of Bose particles in the trap. Replacing the parameters with those obtained from eq. (18) and (19), our result provides for an easy way to estimate this change in the presence of Fermions.

Our result can also be used to calculate the density distribution of the particles of the mixture. Using the standard Thomas-Fermi approximation with the renormalized interaction one can obtain the density of the Bose particles. The Fermi density can then be obtained from Eq. (10) for $T = 0$.

$g_{eff}$ only depends on the square of the Fermion-Boson interaction $g_{BF}$. It can become negative for a repulsive $g_{BF} > 0$. In the case, as the Boson density is increased, the Fermion density decreases. The system phase separates. After the phase separation is complete $g_{eff}$ becomes positive again. Thus in that case, we can consider a negative $g_{eff}$ to be a signature of the instability towards phase separation. The present calculation provides a unified way of looking at these two different phenomena.

In this paper, we have used a 3D Thomas-Fermi approximation to describe the Fermions. This approximation will break down when the anisotropic quantization of the energy levels due to the anisotropic harmonic potential becomes important. The larger energy scale corresponds to the transverse harmonic frequency and is $\hbar\omega_{F,r} = 15.16 nK$. This value is less than the experimental temperature ($T_c = 360 nK$). We thus expect the anisotropic energy quantization effect not to be important in the present case. This quantization effect will be important in the investigation of possible superconductivity as the temperature involved is much lower.

In conclusion, we show that because there is no direct interaction between the Fermions, the part of the path integral involving the Fermion field can be carried out exactly. A description of the Bosons in increasing powers of its density with renormalized couplings is obtained. The Fermion-mediated term can rendered the Boson interaction attractive. When the Fermion-Boson interaction is attractive, the system collapses. We calculate the instability Boson number as a function of temperature and as a function of the Boson-Fermion scattering length. The transition temperature is comparable to the Fermi temperature. Because of the structure of the leading nonlinear term in the Boson interaction, the transition
is first order. This may provide for an explanation of recent experimental results of Modugno and coworkers.

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FIG. 1: The instability Boson number as a function of the Boson-Fermion scattering length in units of nm.

FIG. 2: The instability Boson number as a function of temperature normalized by the Fermi temperature for a Boson-Fermion scattering length of -16.7 nm for $N_f = 2 \times 10^4$ (solid line) and $N_f = 5 \times 10^4$ (dotted line).