Fermi-Bose Mixtures Near Broad Interspecies Feshbach Resonances

Jun Liang Song, Mohammad S. Mashayekhi and Fei Zhou

Department of Physics and Astronomy, The University of British Columbia, Vancouver, B. C., Canada V6T1Z1

(Dated: June 5, 2010)

In this Letter we have studied dressed bound states in Fermi-Bose mixtures near broad interspecies resonance, and implications on many-body correlations. We present the evidence for a first order phase transition between a mixture of Fermi gas and condensate, and a fully paired mixture where extended fermionic molecules occupy a single pairing channel instead of forming a molecular Fermi surface. We have further investigated the effect of Fermi surface dynamics, pair fluctuations and discussed the validity of our results.

Since the observations of molecules of Fermi atoms near Feshbach resonances, fascinating pairing correlations in cold Fermi gases have been successfully investigated both experimentally [1][2] and theoretically [3][4]. Near broad resonances where the atom-molecule coupling is very strong, pair correlations can also be closely related to the ones in the BEC-BCS crossover theory pioneered near Feshbach resonances such as molecular Fermi surfaces might reasonably what kind of many-body correlations are developed near broad resonances can distinctly differ from that near narrow resonances? and according what kind of many-body correlations are developed in a quantum Fermi-Bose mixture? And physics near broad resonances can distinctly differ from that near narrow resonances; some basic concepts introduced for narrow resonances such as molecular Fermi surfaces might not be directly applicable here. Motivated by these considerations, we carry out a study on Fermi-Bose mixtures near broad interspecies Feshbach resonances which serves as a potential reference for more sophisticated analyses. Apart from the phase diagrams in terms of interspecies scattering lengths $a_{BF}$ and Bose($m_B$)-Fermi($m_F$) mass ratio $m_B/m_F$, we focus on bound state properties of near-resonance Fermi-Bose mixtures which can be potentially probed in experiments. Our results are useful for the understanding of correlations in $^6$Li-$^{23}$Na, $^6$Li-$^{87}$Rb, and $^{40}$K-$^{87}$Rb mixtures. For simplicity, we employ a simplest one-channel Hamiltonian which captures most important aspects near broad resonances,

$$H = \sum_k \varepsilon_k f_k^\dagger f_k + \sum_k \varepsilon_k^B b_k^\dagger b_k$$

$$+ \frac{V_{BF}}{\Omega} \sum_{k,k',Q} f_{k,k'}^\dagger f_k b_{k',Q}^\dagger b_{k,{-Q}} - \frac{m_B}{m_F} f_{k,k'}^\dagger f_k b_{k',Q}^\dagger b_{k,{-Q}}$$

(1)

where $f_{k}^\dagger$($f_k$) ($b_k$) are creation (annihilation) operators for Fermi and Bose atoms respectively, and $\varepsilon_k$ are kinetic energies for fermions ($\varepsilon_k^B$) are kinetic energies for bosons and $\Omega$ is the volume. $V_{BF}$ is the strength of interaction that is related to interspecies scattering lengths $a_{BF}$ via

$$\frac{1}{V_{BF}} = \frac{m_R}{2\pi a_{BF} \hbar^2} - \frac{1}{\Omega} \sum_k \frac{1}{\varepsilon_k^B}$$

(2)

here $m_R = m_R m_F/(m_B + m_F)$, $\varepsilon_k^B = \hbar^2 k^2/2m_R$. We assume that the background boson-boson interactions are repulsive so that the mixture is stable; to illustrate the idea, here we only include interspecies scattering.

Bound states and Pauli blocking effects We first consider the binding energy of a pair of Fermi and Bose atoms with opposite momenta ($\mathbf{k}, -\mathbf{k}$), in the presence of a condensate(BEC) and a Fermi surface of Fermi atoms which blocks all states below its Fermi momentum $\hbar k_F$. Pauli blocking effects of a Fermi sea indeed lead to dressed bound states at arbitrary small negative scattering lengths but with an anomalous dispersion, or a negative effective mass (see also discussions before Eq(4)). Furthermore, the energy $W_B$ it takes to create a bound state from a non-interacting ground state
can be either positive or negative depending on scattering lengths $a_{bf}$, a unique feature of Fermi-Bose systems. This is because to form a pair of atoms with opposite momenta $(\mathbf{k}, -\mathbf{k})$ near the Fermi surface $|\mathbf{k}| = k_F$, a Bose atom has to be promoted to right above the Fermi surface which results in an energy penalty $\epsilon_b^B = \hbar^2 k_F^2 / 2 m_B$. For a bound state with an arbitrary total momentum $\mathbf{Q}$ or a kinetic energy $\epsilon_Q^B = \hbar^2 \mathbf{Q}^2 / 2 (m_F + m_B)$, the energy cost is $W_B(\mathbf{Q}) = \epsilon_Q^B + \omega_B$. The $\mathbf{Q}$-dependent binding energy $\omega_B(< 0)$ can be obtained by solving the following two-body equation,

$$-m_R \Omega = \left( \sum_{|\mathbf{Q}+\mathbf{k}| > k_F} \frac{1}{\epsilon_k^R - \epsilon_{k_F}^R - \omega_B} - \frac{1}{\epsilon_{k_F}^R} \right).$$

(3)

In the limit of small $k_F a_{bf}(< 0)$ and when $Q = 0$, Eq. (3) leads to $\omega_B = -4 \epsilon_{k_F}^R \exp(\pi \frac{m_B}{m_R} a_{bf})$, $\epsilon_{k_F}^R = \hbar^2 k_F^2 / 2 m_R$. The dispersion of bound states that can be probed using photoassociative spectroscopy is shown in Fig. 1. For small negative scattering lengths $a_{bf}$, bound states are fully gapped with positive energies $W_B(\mathbf{Q})$, and the ground state is a mixture of Fermi gas and BEC. However, $W_B(0)$, the energy gap of bound states vanishes at a critical scattering length $a^{(1)}$. In Fig. 2 we present results of $a^{(1)}$ versus $m_B / m_F$. For heavy Bose atoms, $k_F a^{(1)}$ approaches a small value of $\pi / (\ln[m_F / 4 m_B] + 2)$. To ensure the stability of $Q = 0$ molecules near the transition line $a^{(1)}$, we further examine $M_{ff}$, the effective mass near $Q = 0$. At scattering lengths $a^{(1)}$ or when $W_B(0) = 0$, we find

$$\frac{1}{M_{ff}} = \frac{1}{m_T} \left[ 1 - \frac{4 m_F}{3 m_B} g(\frac{m_R}{m_F}) \right];$$

(4)

and the dimensionless function $g(x^2) = x / [(1 - x^2)^2 (\ln[1 + x^2] + \frac{2 x^2}{x^2 + 1})]$. As far as $m_B / m_F > 0.7$ and the energy penalty $\epsilon_b^B$ is not too heavy, $M_{ff}$ is positive, although it can be are much bigger than the bare mass $m_T = m_F + m_B$ as a result of dressing in the Fermi sea. Below we focus on the limit of positive $M_{ff}$ that is most relevant to the experimental mass ratio $m_B / m_F$ (between 2.175 and 14.5). Note that the binding energy $\omega_B$ is independent of the Bose atom density when the Fermi sea is treated as a static background.

The above analysis at first sight seems to suggest that when $W_B$ becomes negative, a small fraction of Fermi and Bose atoms start forming molecules or a dilute molecular Fermi gas signifying a phase transition at $a^{(1)}$. Such a picture was in fact previously proposed for mixtures near narrow resonances. However since the extent of molecules $d_m$ is typically comparable to or much longer than the Fermi wave length $2 \pi / k_F$ near broad resonances, pairs may be accommodated, even before the two-body gap $W_B$ vanishes, in other more exotic forms without forming a molecular Fermi surface. Below we provide evidence for such a possibility. Note that a finite two-body gap $W_B$ suggests a local stability of the Fermi gas-BEC mixture against emergence of a Fermi gas of molecules, i.e. when $1/a < 1/a^{(1)}$, a molecular Fermi gas can not be a ground state. It is in this limit that we illustrate, based on an energetic analysis, that a third state or a fully paired state actually further lowers the energy.

**Energy landscape of pairing states** Suggested by above discussions, we consider energetics of pairing states of Fermi-Bose atoms and from now on focus on homogeneous mixtures with equal populations of fermions and bosons, i.e. $N_F = N_B$. Although in principle pairing with a finite total momentum $hQ$ can occur in ground
states, detailed calculations show that for a range of mass ratios \( m_B/m_F > 0.2 \) that is relevant to Fermi-Bose mixtures so far studied in experiments, pairing in \( hQ = 0 \) channel is always dominating and favored, qualitatively consistent with our analyses on the two-body bound states. Below we only show results of \( Q = 0 \) pairing and adopt the simplest pairing wavefunction

\[
|g.s.> = \exp(c_0b_0) \prod_{k \neq 0} (u_k + v_k b_k^\dagger b_{-k} + \eta_k f_k^\dagger)|\text{vac}>
\]

where \( u_k, v_k \) and \( \eta_k \) are three families of variational parameters. We obtain the energy of the variational states and then minimize it with respect to \( u_k, v_k \) and \( \eta_k \) that are subject to the normalization condition \( |u_k|^2 + |v_k|^2 + |\eta_k|^2 = 1 \). Equilibrium conditions can then be obtained and there are two solutions for any given \( k \): i) a unpaired state with \( \eta_k = 1 \) and \( u_k = v_k = 0 \); ii) a paired state with \( \eta_k = 0 \) and \( v_k = \frac{1}{2} \left( 1 - \frac{\xi_k^R}{\xi_k} \right), u_k = \frac{1}{2} \left( 1 + \frac{\xi_k^R}{\xi_k} \right) \),

\[
\Delta = -\frac{\xi_k^R}{\xi_k} \sum_k (1 - \eta_k^2) u_k v_k, \quad E_k = \sqrt{\left( \frac{\xi_k^R}{\xi_k} \right)^2 + 4\Delta^2},
\]

\[
\xi_k^R = \xi_k^B - \mu \quad \text{and} \quad \mu \quad \text{is the pair chemical potential. Pairing gap} \ \Delta, \ \mu \ \text{as well as the condensed population} \ |c_0|^2 \ \text{are determined self-consistently.} \ \sum_{F} = \sum_k \left( v_k^2 (1 - \eta_k^2) + \eta_k^2 \right), \ \sum_B = |c_0|^2 + \sum_k v_k^2 (1 - \eta_k^2) \ \text{and}
\]

\[
\frac{-m_B \Omega}{2\pi a_{bf} \hbar^2} = \sum_k \frac{1 - \eta_k^2}{\sqrt{\xi_k^2 - 4\Delta^2}} - \sum_k \frac{1}{\xi_k^R}.
\]

To minimize the energy, we further choose \( \eta_k \) to be a step function, \( \eta_k = 1 \) if \( |k| \leq Xk_F \), and zero otherwise; the dimensionless variational parameter \( X \in [0, 1] \) specifies the size of residue Fermi surface of unpaired Fermi atoms. When \( N_F = N_B \), one can also verify that \( X^3 \) is equal to \( |c_0|^2/N_B \), i.e. the condensation fraction.

In Fig. 3 we present the main results of variational calculations. In Fig. 3(a) the energy per pair of atoms is shown as a function of \( X \), the size of Fermi surface of unpaired fermions. At small and negative scattering lengths, a Fermi gas-BEC mixture is a ground state and \( X_0 = 1, \mu = \epsilon_F^B + W_B (\epsilon_F^B = \hbar^2k_F^2/2m_B) \) and \( \Delta = 0 \). A fully paired state with \( X_0 = 0 \) becomes degenerate with the Fermi gas-BEC mixture (\( X_0 = 1 \)) at a critical scattering length \( a_{cr} \), beyond which the paired state becomes a ground state. However, a Fermi gas-BEC mixture remains to be locally stable until scattering lengths reach the value of \( a^{(1)} \) which is fully consistent with the above study of bound states. Our variational calculations suggest a first order phase transition between a Fermi gas-BEC mixture and a fully paired mixture. This later state of extended molecules is conceptually different from a Fermi gas of molecules; instead, all molecules, though fermionic in nature, occupy the same pairing channel with zero total momentum. A direct comparison of energies indicates that a fully paired mixture has lower energies than a Fermi gas of molecules provided \( 1/a_{bf} < 1/a^{(2)} \). For \( ^{40}\text{K}-^{87}\text{Rb} \) mixtures, \( 1/k_F a^{(2)} \) is about \( 0.25 - 0.3 \) and \( 1/a^{(2)} > 1/a^{(1)} \); further towards the molecular side, a paired mixture is expected to evolve into a Fermi gas of molecules.

In Fig. 3 we further present the results on the pair breaking energy \( \Delta \) and pair chemical potential \( \mu \). The pair breaking energy can be probed when applying rf pulses to transfer Fermi atoms to a different hyperfine spin state \( 2 \text{D}, 25 \) that weakly interacts with the Fermi-Bose mixture. The frequency shift in the rf spectroscopy should be \( \hbar \Delta (k) = \frac{1}{2} (\xi_k^R + \sqrt{\xi_k^R^2 + 4\Delta^2}) \). In the fully paired phase, Bose atoms are completely depleted and the Bose atom distribution \( n_B(k) \) follows closely the Fermi atom distribution \( n_F(k) \).

**Fermi surface dynamics and pair fluctuations**

At small negative scattering lengths when quantum fluctuations are weak, our mean-field analyses on two-body bound states as well as the fully paired states are asymptotically adequate. And \( a^{(1)}, a_{cr} \) estimated in the limit of large mass ratio \( k_F a^{(1)} \sim \pi/(|m_B|/4m_B) + 2 \) in Fig. 3(a) are quantitatively valid. However when \( k_F a \) is of order of one, the fluctuations become substantial and the bound states can be further dressed in fluctuating particle-hole pairs; the energetic analyses are subject to
corrections. To clarify this, we estimate the dominating effects of Fermi surface dynamics, i.e. the Gorkov corrections (GMB) in the two-body scattering vertex due to fluctuating particle-hole pairs\cite{22,26,27}, and the self-energy (SE) effect which mainly represents the effect of atomic Fermi surface smearing and the mass renormalization due to scattering by the condensate or Fermi sea. We then examine the pole structure of the propagator for a pair of Fermi-Bose atoms taking into account the vertex corrections and self-energy effects and obtain the binding energy $\omega_B$. The relative shift caused by the GMB effect (the leading order term $R_1$) and the SE effect (the higher order term $R_2$) is given as

$$\frac{\delta \ln |\omega_B|}{\ln |\omega_B|} = R_1(k_Fa_B) + R_2(k_Fa_B)^2 \ln |k_Fa_B|... (7)$$

where $R_{1,2}$ both are dimensionless quantities depending on the mass ratio $m_B/m_F$ and can be obtained numerically\cite{28}. For large mass ratios ($m_B/m_F$), one finds that

$$R_1 \approx -\ln(m_B/m_F)/\pi$$

and

$$R_2 \approx -2/(3\pi^2);$$

and $\omega_B$ is reduced by a factor of $m_F/m_B$ solely due to the GMB effect. The net reduction in the binding energy $\omega_B$ leads to a upward shift of $1/a^{(1)}$ (line 1) in Fig.3. In addition, we have estimated that, for the paired state, the amplitude of pair fluctuations $A_1 \approx (\Delta/\epsilon_F^p)^4 \sqrt{\kappa/m_Rk_F}$ (the compressibility of the paired mixture), and the corresponding zero point energy (in units of $\epsilon_F^p$) per particle $A_2 \approx (\Delta/\epsilon_F^p)^4 \sqrt{m_Rk_F}/\kappa$. We incorporate these quantum fluctuations (analogous to NSR effects\cite{11}) which further favor pairing, and the GMB correction into our analysis of energetics of the paired state. For $^{40}K,^{87}Rb$ mixtures, we find that

$$A_1 \approx 0.01, A_2 \approx 0.003$$

and

$$R_1 \approx -0.4 \text{ and } R_2 \approx -0.1;$$

the GMB and SE effects appear to be more dominating. The modified critical lines obtained by extrapolating the above analyses to near resonance are shown in Fig.3 and are qualitatively consistent with the mean field ones. Data suggest that quantum fluctuations tend to enlarge the window between $1/a_{cr}$ and $1/a^{(1)}$ and further stabilize the first order phase transition. Quantum Monte Carlo simulations similar to those in Ref.\cite{29} remain to be carried out.

In conclusion, we have examined dressed bound states and provided evidence of a new quantum state of extended molecules near broad interspecies resonances. As far as three- and higher-body correlations are insignificant, our results can be applied to understand Fermi-Bose mixtures near broad resonances. We thank Gordon Baym, Immanuel Bloch, Kirk Madison, Subir Sachdev, Joseph Thywissen, Jun Ye and Zhenhua Yu for stimulating discussions. This work is supported by NSERC (Canada) and Canadian Institute for Advanced Research. Note added: Upon the submission of this work, we learned that finite-temperature mixtures near broad resonance were also studied in Ref.\cite{30}.

\begin{thebibliography}{99}
\bibitem{1} C. A. Regal et al., Nature \textbf{424}, 47-50 (2003); C. A. Regal et al., Phys. Rev. Lett. \textbf{92}, 040403 (2004).
\bibitem{2} K. Strecker et al., Phys. Rev. Lett. \textbf{91}, 080406 (2003).
\bibitem{3} S. Jochim et al., Phys. Rev. Lett. \textbf{91}, 240402 (2003).
\bibitem{4} M. Zwierlein et al., Phys. Rev. Lett. \textbf{91}, 250401 (2003).
\bibitem{5} C. Chin et al., Science \textbf{305}, 1128-1130 (2004).
\bibitem{6} M. Holland et al., Phys. Rev. Lett. \textbf{87}, 120406 (2001); E. Timmermans et al., Phys. Lett. \textbf{A285}, 228 (2001); Y. Ohashi and A. Griffin, Phys. Rev. Lett. \textbf{89}, 130402 (2002).
\bibitem{7} T. L. Ho, Phys. Rev. Lett. \textbf{92}, 090402 (2004).
\bibitem{8} A. V. Andreev et al., Phys. Rev. Lett. \textbf{93}, 130402 (2004).
\bibitem{9} D. M. Eagles, Phys. Rev. \textbf{186}, 456 (1969).
\bibitem{10} J. Leggett, J. Phys. (Paris) Colloq. \textbf{41}, 7 (1980); for discussions on resonance widths, see A. J. Leggett, Quantum Liquids (Oxford University Press, 2006).
\bibitem{11} P. Nozieres and S. Schmitt-Rink, J. of Low Temp. Phys. \textbf{59}, 195 (1985).
\bibitem{12} C. A. Stan et al., Phys. Rev. Lett. \textbf{93}, 143001 (2004).
\bibitem{13} S. Inouye et al., Phys. Rev. Lett. \textbf{93}, 183201 (2004).
\bibitem{14} F. Ferlaino et al., Phys. Rev. A \textbf{73}, 040702 (2006).
\bibitem{15} S. Ospelkaus et al., Phys. Rev. Lett. \textbf{97}, 120403 (2006).
\bibitem{16} B. Deh et al., Phys. Rev. A \textbf{77}, 010701(R) (2008).
\bibitem{17} K. K. Ni et al., Science \textbf{322}, 231 (2008).
\bibitem{18} H. P. Büchler et al., Phys. Rev. Lett. \textbf{98}, 060404 (2007).
\bibitem{19} S. Powell et al., Phys. Rev. B \textbf{72}, 024534 (2005).
\bibitem{20} H. Yabu et al., Physica B \textbf{329-333}, 25 (2003).
\bibitem{21} D. C. E. Bortolotti et al., J. Phys. B \textbf{39}, 189 (2006).
\bibitem{22} C. J. Pethick and H. Smith, Bose-Einstein condensation in dilute gases (Cambridge University Press, 2008).
\bibitem{23} A. Simon et al., Phys. Rev. Lett. \textbf{90}, 163202 (2003); M. Gacesa et al., Phys. Rev. A \textbf{78}, 010701(R) (2008); Z. Li et al., Phys. Rev. A \textbf{78}, 022710 (2008); C. Marzok et al., Phys. Rev. A \textbf{79}, 012717 (2009).
\bibitem{24} Far away from resonances or for much smaller Bose-Fermi mass ratios, the dispersion can be anomalous with a minimum at $Q \neq 0$.
\bibitem{25} G. Baym et al., Phys. Rev. Lett. \textbf{99}, 190407 (2007).
\bibitem{26} L. P. Gorkov and T. M. Melik-Barkhudarov, Sov. Phys. JETP \textbf{13}, 1018 (1961).
\bibitem{27} H. Heiselberg et al., Phys. Rev. Lett. \textbf{85}, 2418 (2000).
\end{thebibliography}
The log-divergency in Eq. 7 can be removed if the compressibility of BEC is taken into account.

S. Pilati and S. Giorgini, Phys. Rev. Lett. 100, 030401 (2008).

E. Fratini and P. Pieri, Phys. Rev. A 81, 051605 (2010).