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A Theoretical evaluation of energy gap of molecules with different mass ratio in Fermi-Bose mixtures near broad interspecies Fehbach resonances

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Abstract: In this paper, we have theoretically studied Fermi-Bose mixtures near broad interspecies resonances. Using Variational method, we have evaluated energy of the molecule, W_B as a function of scattering length $[K_F a_{bf}]^{-1}$ for different mass ratio, critical scattering length $[K_F a^{(1)}]^{-1}$ as a function of (m_B/m_F), pair-breaking energy Δ in the unit of (ε_F^R) and pair chemical potential $\mu(\varepsilon_F^R)$ as a function of scattering length $[K_F a_{bf}]^{-1}$ for ^{40}K-^{87}Rb.Our evaluated theoretical results are in good agreement with other theoretical workers.

Keywords: Fermi-Bose mixtures, Near broad resonances, Interspecies Feshbach resonance, Many-body correlations, Pauli blocking effect, Dilute molecular Fermi gas, Pair breaking energy, Pair chemical potential, Condensed population, Fermi gas-BEC mixture.

INTRODUCTION

Ultacold quantum gases in condensed matter physics have generated a tremendous excitement during recent years[1]. In this excitement, we have super fluid to Mott insulator transition[2], the BEC-BCS crossover in fermionic super fluids[3] and the Berezinski-Kosterlitz Thouless (BKT) transition in two dimensional Bose gas[4]. These are the new advancement in ulracold quantum gases. A large number of many-body systems may become accessible through the advent of quantum mixtures of different atomic species. In particular, Bose-Fermi mixtures with widely tunable interactions reveal boson-mediated interactions between fermions and boson-induced p-wave superfluidity[5,6]. Interactions between atoms can be strongly modified by tuning magnetic field to Feshbach resonances. Here, the molecular state has the same energy as the colliding atoms. The mechanism has been used to change the properties of ultacold bosonic gases[7-10]. However, for degenerate Fermi gases such control over the interaction strengths are crucial for super fluid phase transition. For dilute Fermi gas, the predicted phase-transition occur at temperatures that are experimentally not accessible, unless the scattering length is reasonably enhanced. Recently, interspecies Feshbach resonances in Fermi-Bose mixtures ^{6}Li- ^{23}Na, ^{40}K- ^{87}Rb and ^{6}Li- ^{87}Rb have been experimentally observed[11-15]. Recently, weakly bound ^{40}K- ^{87}Rb pairs prepared near Feshbach resonances were further converted into cold molecules at JILA[16]. This research can lead to a new opportunity of studying quantum state of matter[17]. While locations and width of resonances observed in experiments agree quite well with theories[18], many-body correlations in Fermi-Bose mixtures remain to be probed. On the other hand theoretical studies on Fermi-Bose mixtures have been mainly focused on narrow resonances[19-21]. It was seen that the phase boundaries depend on atom-molecule coupling strengths. It was also argued that molecules do not interact with each other or with Fermi atoms.

MATHEMATICAL FORMULA USED IN THE STUDY

One begins with one –channel Hamiltonian for Fermi-Bose mixtures near broad resonances

$$H=\Sigma_k \varepsilon_k{}^F f^+{}_k f_k+\Sigma_k \varepsilon_k{}^B b^+{}_k b_k+\frac{V_{bf}}{\Omega}\Sigma_{k,k',Q}\, f_{\frac{m_R}{m_B}}{}^+Q+k\ b_{\frac{m_R}{m_B}}{}^+Q-kf_{\frac{m_R}{m_B}}Q+k'b_{\frac{m_R}{m_B}}Q-k' \quad (1)$$

Where $f^+{}_k b^+{}_k(f_k b_k)$ are creation (annihilation) operators for Fermi and Bose atoms respectively and $\varepsilon^{F(B)}{}_k=\frac{\hbar^2|k|^2}{2m_{F(B)}}$ are kinetic energies for fermions (bosons) and Ω is the volume. V_{bf} is the strength of the interaction and it is related to interspecies scattering length a_{bf} by the following equation

$$\frac{1}{V_{bf}}=\frac{m_R}{2\pi a_{bf}\hbar^2}-\frac{1}{\Omega}\Sigma_k\frac{1}{\varepsilon_k{}^R} \quad (2)$$

Where $m_R={m_B m_F}/{(m_B+m_F)}$, $\varepsilon_k{}^R=\frac{\hbar^2k^2}{2m_R}$. $\frac{m_B}{m_F}$ is the Fermi-Bose mass ratio. One assumes that the boson-boson and fermion-fermion interactions are weak and practically negligible. We only consider homogeneous mixtures with an equal population of fermions and bosons.

The Q –dependence binding energy W_B (<0) can be obtained as a solution to a two-body equation

$$-\frac{m_R\Omega}{2\pi a_{bf}\hbar^2}=[\sum_{\left|\frac{m_R}{m_B}Q+k\right|>k_F}\frac{1}{\varepsilon_k{}^R-\varepsilon_F{}^R-w_B}-\frac{1}{\varepsilon_k{}^R}] \quad (3)$$

Q is total arbitrary momentum. We have binding energy of a pair of Fermi and Bose atoms with opposite momentum (k, -k) in the presence of condensate (BEC) and Fermi surfaces of Fermi atoms which blocks all states below its Fermi momentum ℏk. We have

$$\varepsilon_F{}^B=\frac{\hbar^2k^2{}_F}{2m_B},\quad \varepsilon_Q{}^c=\hbar^2Q^2\Big/2(m_F+m_B),\quad W_B(Q)=\varepsilon_F{}^B+\varepsilon_Q{}^c+W_B$$

In the light of small k_Fa_{bf} (<0) and when Q=0.0, equation (3) reduces to

$$W_B=-4\varepsilon_F{}^R\exp(\frac{\pi}{k_Fa_{bf}})$$

$$\varepsilon_F{}^R=\frac{\hbar^2k^2{}_F}{2m_R} \quad (4)$$

From these relations, one gets the dispersion of two-body bound states. Near resonances, one considers a simplest pairing wave function ansatz

$$\left|g.s>=\exp(c_0b^+{}_0)\prod_{k\neq 0}(u_k+v_kf_k{}^+b_{-k}{}^++\eta_kf^+{}_k\right|vac> \quad (5)$$

Where u_k,v_k and η_k are three families of variational parameters. The expectation value of energy can be obtained as

$$E=F+\mu^FN_F+\mu^BN_B \quad (6)$$

$$F=\Sigma_k(\left|u_k\right|^2+\left|\eta_k\right|^2)\zeta^F{}_k\quad+\Sigma_k\left|v_k\right|^2\zeta_k{}^B+\frac{v_{bl}}{\Omega}\Sigma_{k,l}v^*{}_ku_kv_lu_l{}^* \quad (7)$$

Here, one has introduced new variables $\zeta^{F(B)}{}_k=\varepsilon^{F(B)}{}_k-\mu_k{}^{F(B)}$ where $\mu^{F(B)}$ are chemical potentials of bosons and fermions respectively. One then minimizes equation (7) with respect to u_k, v_k and η_k with respect to the normalization condition $\left|u_k\right|^2+\left|v_k\right|^2+\left|\eta_k\right|^2=1$. Equilibrium condition can then be obtained and then there are two solutions for any given value of k

- An unpaired states with η_k =1 and u_k =0 and v_k=0
- A paired state with η_k =0 and

$$v^2{}_k=\frac{1}{2}(1-\frac{\zeta_k{}^R}{E_k})$$

$$u_k{}^2=\frac{1}{2}(1+\frac{\zeta_k{}^R}{E_k})$$

$$\Delta = (-\frac{V_{bl}}{\Omega})\Sigma(1-\eta_k{}^2)u_k v_k \tag{8}$$

Where

$$E_k = \sqrt{(\zeta^R{}_k)^2 + 4\Delta^2]}$$

$$\zeta_k{}^R = \zeta_k{}^F + \zeta_k{}^B \tag{9}$$

For a given **k**, η_k can be either 0 or 1 for ground states and the pair breaking energy Δ is also a measure of pair correlation. Chemical potential μ^B,μ^F only enter the equation through an effective pair chemical potential μ, where $\mu= \mu^B+\mu^F$. The pairing gap Δ, μ as well as condensed population $|c_0|^2$ are determined self-consistently by

$$N_F = \Sigma_k[v^2{}_k(1-\eta_k{}^2)+\eta_k{}^2] \tag{10(a)}$$

$$N_B = |c_0|^2 + \Sigma_k v^2{}_k(1-\eta_k{}^2) \tag{10(b)}$$

$$\frac{-m_R\Omega}{2\pi a_{bl}\hbar^2} = \Sigma_k \frac{1-\eta_k{}^2}{[(\varepsilon_k{}^R-\mu)^2+4\Delta^2]^{\frac{1}{2}}} - \Sigma_k \frac{1}{\varepsilon_k{}^R} \tag{10(c)}$$

Here equation 10 (c) is the gap equation for mixtures. One assumes η_k to be step function

η_k ={1 if $k<xk_F$ (11)

0 Otherwise

Here x is a dimensionless variational parameter. It specifies the size of the residue Fermi surface of unoccupied Fermi atoms. Only fermions outside the surface $k=xk_F$ are involved in pairing those bosons.

DISCUSSION OF RESULTS

In this paper, we have studied Fermi-Bose mixtures near broad interspecies resonances. We have used the theoretical formalism of S. Mahammod etal[22] in this study. In this formalism, they have used variational method where the fraction of unpaired Fermi atoms acts as a variational parameter. In Table T1, we have shown the evaluated results of energy gap of molecule W_B in the unit of $\varepsilon_F{}^R$ as a function of $[K_Fa_{bf}]^{-1}$ ($1/a_{bf} < 1/a^{(1)}$) with different mass ratios or mixtures. From our evaluated results, it appears that W_B decreases as $[K_Fa_{bf}]^{-1}$ and becomes zero for some value of $K_Fa_{bf}]^{-1}$. The value of W_B is large for K-Rb mixture and small for Li-Rb mixture. In Table T2, we have shown the evaluated results of critical scattering length $[K_Fa^{(1)}]^{-1}$ as a function of mass ratio ($m_{B/}m_F$). This evaluation gives an idea that when W_B becomes negative, a small fraction of Fermi and Bose atoms start forming a molecule or a dilute molecular Fermi gas signifying a phase transition a [1].Once all atoms form molecules, condensates becomes completely dappled implying a second critical scattering length. Such type of picture was earlier proposed for mixtures near narrow resonances[23, 24].

However, a finite two-body gap W_B only ensures a local stability of the Fermi gas BEC mixture against emergence of a Fermi gas of molecules. And since the extent of molecule d_m is typically comparable to the Fermi wave length($2\pi/K_F$) near broad resonance, anti-commutators of composite molecule fields differ from the ones of fundamental fermions with substantial deviations of order $(k_F d_m)^3$.Consequently, pairs may appear even before the two-body gap W_B vanishes. Below, one carries out calculations to differentiate the two sceneries and illustrates a pairing state without molecular Fermi surfaces[25]. In Table T3, we have shown the evaluated results of $[K_F a_{cr}]^{-1}$ scattering length at which the first order phase transition between a Fermi gas-BEC mixture and a fully paired mixture. The state of extended molecules is completely different from Fermi gas of molecules. These pairs, though fermionic in nature, occupy a state in a two particle channel with zero total momentum and therefore form a Fermi condensate of extended molecules. In Table T4, we have shown the evaluated results of pair breaking energy Δ in the unit of ε_F^R as a function of scattering length $[K_F a_{bf}]^{-1}$ near (a_{cr}) for mass ratio (m_B/m_F) =2.175. A pair of atoms with momentum (k,-k) can be broken when rf (radio frequency) pulses are applied to transfer a Fermi atom to a third hyperfine spin state[26, 27] that weakly interacts with the Fermi-Bose mixtures. Our theoretically evaluated results are in good agreement with other theoretical workers[28, 29].

We have used the formulae for the frequency shift in the rf spectroscopy

$$\hbar\Delta\omega(k) = \frac{1}{2}\{\zeta_k{}^R + \{\left|\zeta_k{}^R\right|^2 + 4\Delta^2\}^{\frac{1}{2}} \tag{12}$$

We have also repeated the calculations for pair chemical potential μ (ε_F^R) as a function of scattering length $K_F a_{bf}]^{-1}$ for mass ratio (m_B/m_F) =2.175. The evaluated results are shown in Table T5. Results were compared with other theoretical workers[28,29]. Some recent results[30-35] also reveals the same behavior.

Table T1: An evaluated results of W_B the energy of the molecule in the unit of ε_F^R as a function of $[K_F a_{bf}]^{-1}$ ($1/a_{bf} < 1/a^{(1)}$) with different mass ratios or mixtures

($1/K_F a_{bf}$)	← W_B(energy of molecule) ε_F^R →		
	K-Rb	Li-Na	Li-Rb
-1.6	0.452	0.237	0.158
-1.5	0.437	0.215	0.134
-1.4	0.422	0.208	0.116
-1.2	0.408	0.186	0.102
-1.0	0.386	0.132	0.086
-0.8	0.356	0.116	0.058
-0.6	0.322	0.095	0.042
-0.4	0.286	0.047	0.035
-0.2	0.187	0.033	0.007
-0.1	0.108	0.006	0.0007
0.0	0.050	0.002	0.0002

Table T2: An evaluated results of critical scattering length $[K_F\, a^{(1)}]^{-1}$ as a function of (m_B/m_F)

(m_B/m_F)	$[K_F a^{(1)}]^{-1}$	
	Our result	Other's results
1	0.386	0.295
2	0.165	0.132
3	0.054	0.037
4	-0.128	-0.098
5	-0.189	-0.164
6	-0.226	-0.278
7	-0.354	-0.365
8	-0.428	-0.455
9	-0.509	-0.536
10	-0.556	-0.574
11	-0.622	-0.655
12	-0.658	-0.687
13	-0.702	0.722
14	-0.746	-0.767
15	-0.785	-0.798

Table T3: An evaluated results of $[K_F a_{cr}]^{-1}$(scattering length at which the first order phase transition occurs) as a function of (m_B/m_F) Results were compared with other theoretical workers.

(m_B/m_F)	$[K_F a_{cr}]^{-1}$	
	0ur results	Other results
1	0.056	0.066
2	0.008	0.012
3	-0.067	-0.042
4	-0.128	-0.147
5	-0.235	-0.258
6	-0.308	-0.337
7	-0.375	-0.398
8	-0.422	-0.446
9	-0.478	-0.508
10	-0.526	-0.545
11	-0.595	-0.607
12	-0.677	-0.646
13	-0.732	-0.705
14	-0.756	-0.766
15	-0.778	-0.785

Table T4: An evaluated results for pair breaking energy in the unit of ε_F^R as a function of scattering length $[K_F a_{bf}]^{-1}$ for mass (m_B/m_F) =2.175 (^{40}K- ^{87}Rb)

$(1/K_F a_{bf})$	$\Delta(\varepsilon^R_F)$	
	Our results	Other results
-0.30	0.056	0.025
-0.25	0.062	0.035
-0.20	0.089	0.047
-0.15	0.095	0.068
-0.10	0.456	0.395
-0.05	0.463	0.412
0.00	0.489	0.446
0.05	0.502	0.488
0.10	0.525	0.522
0.20	0.543	0.539

Table T5: An evaluated results of pair chemical potential $\mu(\varepsilon_F{}^R)$ as a function of scattering length $[K_F a_{bf}]^{-1}$ for mass (m_B/m_F) =2.175 (^{40}K- ^{87}Rb)

$(1/K_F a_{bf})$	$\mu(\varepsilon_F{}^R)$	
	Our results	Other's results
-0.30	0.897	0.922
-0.25	0.822	0.876
-0.20	0.806	0.843
-0.15	0.785	0.827
-0.10	0.625	0.607
-0.05	0.567	0.586
0.00	0.548	0.562
0.05	0.522	0.543
0.10	0.506	0522
0.20	0.467	0.506

CONCLUSION

From the above theoretical investigation and analysis, we have come across the following conclusions

(1) Variational approach works quite well in the study of molecule formation and momentum distribution in Fermi-Bose mixture

(2) Gapless molecular states and pair breaking energies can be probed using photoemission and radio frequency spectroscopy respectively.

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