Properties of a Dilute Bose Gas near a Feshbach Resonance

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Abstract

In this paper, properties of a homogeneous Bose gas with a Feshbach resonance are studied in the dilute region at zero temperature. The stationary state contains condensations of atoms and molecules. The ratio of the molecule density to the atom density is $\pi na^3$. There are two types of excitations, molecular excitations and atomic excitations. Atomic excitations are gapless, consistent with the traditional theory of a dilute Bose gas. The molecular excitation energy is finite in the long wavelength limit as observed in recent experiments on $^{85}\text{Rb}$. In addition, the decay process of the condensate is studied. The coefficient of the three-body recombination rate is about 140 times larger than that of a Bose gas without a Feshbach resonance, in reasonably good agreement with the experiment on $^{23}\text{Na}$. 

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I. INTRODUCTION

Feshbach resonance\cite{1} has been observed in $^{23}\text{Na}$\cite{2}, $^{85}\text{Rb}$\cite{3}, and a few other alkali systems. In these systems, two atoms can collide and fall into a molecular state with a different spin. The scattering length can be tuned by changing the energy difference between the atomic and molecular states through a magnetic field. In the $^{85}\text{Rb}$ system, the scattering length was tuned to the negative region to study the critical particle number of the condensate$\cite{4}$. In the positive region, an unusual processes of particle loss were observed$\cite{5}$. Recently oscillations between atomic and molecular states were discovered$\cite{6}$.

One of the motivations to study Feshbach resonance is to create a Bose system with a large and positive scattering length $a$. In the traditional theory of a dilute Bose gas$\cite{7,8,9}$, every physical quantity is expressed as a power series in the gas parameter $\sqrt{8\pi na^3}$, with higher order terms coming from high order perturbations. But the perturbation breaks down when the density $n$ is of the order of $1/a^3$. It is a challenge to find out what happens to the system beyond the dilute region. In recent experiments$\cite{6}$, $na^3$ can be tuned as high as 0.5.

However, even in the dilute region $na^3 \ll 1$, the system with a Feshbach resonance is different from the system without a Feshbach resonance because of the molecular states. The observation of oscillations between the atomic and molecular states$\cite{6}$ indicates macroscopic occupation of molecular states. In fact, in addition to photoassociation$\cite{10,11}$, Feshbach resonance is considered as another method to study the mixture of atomic and molecular condensates.

In Ref.$\cite{12}$, a two-channel model was constructed to study Feshbach resonance, with the Hamiltonian given by

$$H = \frac{\hbar^2}{2m} \nabla\psi^\dagger \cdot \nabla\psi + \frac{\hbar^2}{4m} \nabla\phi^\dagger \cdot \nabla\phi + \frac{g_0}{2} \psi^2 \psi^2 - \gamma (\phi^\dagger \psi^2 + \text{h.c.}) + \hbar \phi^\dagger \phi,$$

where $\phi$ is the molecular field operator and $\psi$ is the atomic field operator. The magnetic detuning energy is given by $\hbar$. The coupling constant of atomic fields is given by $g_0$. The coupling constant between atomic and molecular states is given by $\gamma$. The sign of $\gamma$ is chosen to be positive by gauge transformation.

Most studies$\cite{12,13,14,15}$ of this model have been focused on condensate properties. When multiple modes were included, the condensates were found to be depleted over time$\cite{16}$. In Ref.$\cite{17}$, a Hartree-Fock method was used to take into account the contribution
from atom pairs with opposite momentum, and the dynamics of the correlation between the condensates and atom pairs was studied numerically. However some properties of this model such as the complete excitation spectrum and the decay process are still unclear. In this paper, we study these problems in the dilute region where the scattering length $a$ is much bigger than the scattering length far off the resonance $a_0$ but much smaller than the interparticle distance, $a_0 \ll a \ll 1/\sqrt{n}$. A simple saddle-point method is developed to handle this case.

II. CONDENSATE PROPERTIES

In the two-channel system, the numbers of atoms and molecules are not constants. It is easier to work in the grand canonical ensemble with the grand thermodynamical potential given by

$$F = H - \mu(\psi^\dagger \psi + 2\phi^\dagger \phi),$$

where $\mu$ is the chemical potential. At zero temperature in the dilute region, both atoms and molecules condense. The dominant contribution to the grand potential comes from the condensation, given by

$$F_0 = \frac{g_0}{2} |\psi_0|^4 - \frac{\gamma}{2} (\phi_0^* \psi_0^2 + \text{c.c.}) + h|\phi_0|^2 - \mu(|\psi_0|^2 + 2|\phi_0|^2),$$

where $\psi_0$ and $\phi_0$ are the expectation values of the atomic and molecular fields. The values of $\psi_0$ and $\phi_0$ are determined from the saddle-point equations given by

$$\frac{\partial F_0}{\psi_0} = (g_0|\psi_0|^2 - 2\gamma\phi_0 - \mu)\psi_0^* = 0,$$

$$\frac{\partial F_0}{\phi_0} = (h - 2\mu)\phi_0^* - \gamma\psi_0^2 = 0.$$

In the region with positive scattering lengths, $h < 0$ and $\mu > 0$, the nontrivial solution of the above equations is given by

$$\psi_0^2 = \frac{\mu}{g_{\text{eff}}},$$

$$\phi_0 = \frac{\gamma\psi_0^2}{h - 2\mu},$$

where $g_{\text{eff}} = g_0 - 2\gamma^2/(h - 2\mu)$. This solution is a minimum of the grand potential in the subspace of $\psi_0$ and a maximum in the subspace of $\phi_0$ because molecules have lower energy than atoms. It is dynamically stable in the condensate space\cite{12}.
Compared to the traditional theory, the relation between the chemical potential and the atomic condensate density given by Eq. (1) remains the same, with \( g_{\text{eff}} \) now as the effective coupling constant of the atoms. The scattering length is proportional to the effective coupling constant,

\[
a = mg_{\text{eff}}/(4\pi\bar{\hbar}^2) = a_0(1 - \frac{\Delta}{h - 2\mu}),
\]

where the scattering length in the absence of the resonance is given by \( a_0 = mg_0/(4\pi\bar{\hbar}^2) \), and the constant \( \Delta \) is given by \( \Delta = 2\gamma^2/g_0 \). The scattering length in the form of Eq. (8) have been observed in the experiments\(^{[2, 6]}\).

In the dilute region, the interparticle distance is much larger than any other length scale. Since the chemical potential \( \mu \) is a function of the atomic condensate density, the absolute value of the detuning energy \(|\hbar|\) is much larger than the chemical potential \( \mu \). As a consequence, the molecular condensate density is much less than the atomic condensate density,

\[
\frac{\phi_0^2}{\psi_0^2} \approx \frac{\gamma^2\psi_0^2}{\hbar^2} < \frac{\mu}{2|\hbar|} \ll 1.
\]

These condensate properties are consistent with the findings in Ref.\(^{[12]}\).

As shown in the next section, due to the coupling between atoms and molecules, the total molecule density is bigger than the molecular condensate density by a factor of \( 1/Z \) as given in Eq. (20), because the molecular eigenstates also contains atom pairs. However, in the dilute region, the total molecule density is still much smaller than the atomic condensate density. The ratio of the molecule density to the atom density \( n_m/n_a \) is approximately given by

\[
\frac{n_m}{n_a} \approx \frac{\gamma^2\psi_0^2}{Z\hbar^2} \approx \pi na^3.
\]

III. EXCITATIONS AND QUANTUM DEPLETION

In the dilute region, the system contains two types of excitations, the molecular excitation and the atomic excitation. The bare energy of a molecule is given by the detuning energy \( \hbar \). The coupling to the atomic states strongly renormalizes the molecule energy, and the molecular eigenstate becomes a superposition of the bare molecular state and pairing states of atoms. This renormalization can be easily demonstrated in the vacuum case where there are few particles.
In the vacuum, at zero temperature, the propagator of the molecular field is given by

$$G_m(q, \Omega) = \frac{1}{\Omega - \frac{\epsilon_q}{2} - h + 2\mu - \Sigma_m(q, \Omega) + i\delta},$$  

and the propagator of the atomic field is given by

$$G_a(k, \omega) = \frac{1}{\omega - \epsilon_k + \mu + i\delta},$$

where $$\Sigma_m(q, \Omega)$$ is the self energy of the molecular propagator generated by the coupling between atoms and molecules,

$$\Sigma_m(q, \Omega) = 2\gamma^2 \int \frac{d\omega}{2\pi} \int \frac{d^3k}{(2\pi)^3} G_a(k, \omega) G_a(q - k, \Omega - \omega)$$  

$$= 2\gamma^2 \int \frac{d^3k}{(2\pi)^3} \frac{1}{\Omega - \epsilon_k - \epsilon_{k-q} + 2\mu + i\delta},$$

and $$\epsilon_k = \hbar^2 k^2 / (2m)$$.

There is an unphysical ultra-violet divergence in the integral in Eq.(14). As shown in many examples in the effective field theory, the bare parameters are often divergent and the physical parameters are always finite. The divergence from the perturbation can be removed by introducing a divergent counter term in the Hamiltonian. (In the context of a dilute Bose gas without a Feshbach resonance, see Ref.[18].) Here we regularize the divergence by introducing a divergent part of the bare molecule energy $$-\gamma^2 \int d^3k/[2(2\pi)^3 \epsilon_k]$$. After the regularization, the self energy is given by

$$\Sigma_m(q, \Omega) = 2\gamma^2 \int \frac{d^3k}{(2\pi)^3} \left( \frac{1}{\Omega - \epsilon_k - \epsilon_{k-q} + 2\mu + i\delta} + \frac{1}{2\epsilon_k} \right)$$  

$$= \frac{\gamma^2}{2\pi} \left( \frac{m^3\gamma^4}{\hbar^6} \right)^{\frac{3}{2}} \sqrt{\frac{\epsilon_q}{2} - 2\mu - \Omega}. $$

The pole of the molecular propagator in Eq.(11) is now given by

$$\Omega_q = \frac{\epsilon_q}{2} - 2\mu - 4\left( \sqrt{\frac{m^3\gamma^4}{4\pi^2\hbar^6}} - 4\hbar - \frac{m^3\gamma^2}{2\pi\hbar^3} \right)^2.$$  

Far off the resonance, the molecule energy is simply given by $$h + \epsilon_q/2 - 2\mu$$; near the resonance $$m^3\gamma^4/(\pi^2\hbar^6) \gg 4|h|$$, the molecule energy is given by

$$\Omega_q \approx \frac{\epsilon_q}{2} - 2\mu - \frac{4\pi^2\hbar^6\epsilon_q}{m^3\gamma^4}.$$
Near the resonance and close to the pole, the propagator can be approximated as

$$G_m(q, \Omega) = \frac{Z}{\Omega - \Omega_q + i\delta}, \tag{19}$$

where the renormalization factor $Z$ is given by

$$Z = \frac{4\pi h^3}{m\gamma^2 \sqrt{|\Omega_0|/m}}. \tag{20}$$

In this region, the scattering length is approximately given by

$$a \approx \frac{\gamma^2 m}{2\pi h^2 |h|}, \tag{21}$$

and the molecular binding energy is approximately given by

$$\Omega_0 \approx -\frac{4\pi^2 h^6 h^2}{m^3 \gamma^4} - 2\mu. \tag{22}$$

The relation between the binding energy of molecules and the scattering length is similar to that in the single-channel problem,

$$\Omega_0 \approx -\frac{h^2 m a^2}{ma^2} - 2\mu, \tag{23}$$

except that there is a mean-field shift by $2\mu$.

So far the results presented in this section Eq.(18-23) are derived for the vacuum case, valid near the resonance when the scattering length $a$ is much larger than the scattering length off the resonance $a_0$. For a system with many particles, these results are still valid as long as the system is in the dilute region $a_0 \ll a \ll 1/\sqrt{n}$, because in this region the many-body contribution to the molecular energy from the condensate is proportional to the particle density $n$, much smaller than $|\Omega_0|$. However, beyond the dilute region when $na^3 \geq 1$, the many-body effect may be dominant and the results for the dilute case may no longer be accurate. In a recent experiment $[19]$, a shift to the molecular energy larger than $2\mu$ was observed, which may be due to the many-body effect.

If the molecule density is initially slightly away from the stationary value due to a perturbation of the molecule energy in the action $\alpha\phi^\dagger \phi$, the molecule density will oscillate. The oscillation can be calculated in the linear response theory. In the long-time $t \to \infty$ limit, it is given by

$$\langle \phi^\dagger(t) \phi(t) \rangle > \phi_0^2 \approx -i\alpha\phi_0^2 \left[ \phi_0(t) \phi_0^\dagger(0) - \phi_0^2 \right] \tag{24}$$

$$\approx -\alpha\phi_0^2 \int \frac{d\omega}{2\pi} G_m(0, \omega) e^{-i\omega t/\hbar} \tag{25}$$

$$\approx 2i \frac{\alpha \Omega_0}{|h|} \phi_0^2 e^{-\Omega_0 t/\hbar}. \tag{26}$$
The oscillation frequency is simply given by the molecular binding energy $\Omega_0$ because of the molecular condensation. It is similar to the single-channel problem where the phonon frequency coincides with the energy of the single particle excitation. In the experiment [6], the oscillation frequency fits perfectly with the molecule energy calculated from a microscopic potential [20]. This result was also obtained in the context of photoassociation [21], in the Hartree-Fock approach [17], and in Ref. [22].

In the dilute region, most of the particles are in the atomic condensate. The long-wavelength and low-energy excitations are atomic excitations, described by the gaussian fluctuation

$$\delta F_2 = \sum_k [(\epsilon_k - \mu + 2g_0\psi_0^2 - \frac{2\gamma^2\psi_0^2}{h - 2\mu})\psi_k^\dagger\psi_k + (\frac{g_0\psi_0^2}{h} - \gamma\phi_0)(\psi_k^\dagger\psi_{-k} + h.c.)].$$

(27)

The molecular part of the fluctuation is not included because molecular excitations have a gap $\Omega_0$ as shown above. However molecular excitations contribute a diagonal self-energy to the atomic propagator through the coupling between atoms and molecules

$$\Sigma_a(k, \omega) = 2\gamma^2\psi_0^2 G_m(k, \omega) \approx -\frac{2\gamma^2\psi_0}{h - 2\mu},$$

(28)

which is already included in the r.h.s. of Eq. (27).

After diagonalizing Eq. (27), we obtain a linear dispersed mode

$$\delta F_2 = C + \sum_k E_k c_k^\dagger c_k,$$

(29)

where $c_k = u_k\psi_k + v_k\psi_{-k}^\dagger$, $u_k^2 = \frac{1}{2}(\frac{\epsilon_k + \mu}{2E_k} + 1)$ and $v_k^2 = u_k^2 - 1$. The excitation energy is given by

$$E_k = \sqrt{\epsilon_k(\epsilon_k + 2\mu)},$$

(30)

and the energy of quantum depletion $C$ is given by

$$\frac{C}{V} = \frac{8}{15\pi^2} \left( \frac{m\mu}{\hbar^2} \right)^{\frac{3}{2}} \mu.$$  

(31)

The density of the quantum depletion can be easily calculated.

$$\delta n = \int \frac{d^3k}{(2\pi)^3} v_k^2 = \frac{1}{3\pi^2} \left( \frac{m\mu}{\hbar^2} \right)^{\frac{3}{2}}$$

(32)

These results are consistent with the first order results in the traditional theory. To this order, $\mu = 4\pi\hbar^2 a/m$, any physical quantity can be expressed in terms of the density of the atomic condensate $\psi_0^2$ and the scattering length $a$. 

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IV. THE THREE-BODY RECOMBINATION

In the dilute region, the condensate state is only metastable because occupation of molecular states can lower the system energy. Most of the decay is due to the three-body recombination. In the two-channel system, the picture of this process is rather simple. One pair of atoms with opposite momentum in the quantum depletion break up, and one of the them interacts with an atom in the condensate to form a molecule leaving the other atom of the original pair as an excited atom. The energy and momentum can be conserved in this process because molecules have negative energies. Mathematically the decay comes from the perturbation of the atom-molecule coupling term $-2\gamma \psi_0^{\dagger} \phi_k \psi_k$ in the Hamiltonian.

The probability density of this three-body recombination process can be calculated by Fermi’s golden rule

$$\Gamma = \frac{2\pi}{\hbar} \int \frac{d^3k}{(2\pi)^3} |\langle \mathbf{k} | 2\gamma \psi_0^{\dagger} \phi_k \psi_k | G > |^2 \delta(E_k + \Omega_k)$$

(33)

where $| G >$ is the ground state of $\delta F_2$, $| \mathbf{k} >$ is the ground state plus a molecule with wavevector $\mathbf{k}$ and an excited atom with wavevector $-\mathbf{k}$. As defined earlier, $v_k$ is the coherence factor, and $Z$ is the probability of finding a molecule in a molecular eigenstate given in Eq.(20). In the dilute region near resonance, the decay rate is approximately given by

$$\Gamma \approx \frac{2\pi}{\hbar} \int \frac{d^3k}{(2\pi)^3} 16\psi_0^2 \mu_k^2 \sqrt{\left| \Omega_0 \right|} \left( \frac{m}{\hbar^2} \right)^\frac{3}{2} \delta(3\varepsilon_k - \frac{h^2}{ma^2})$$

(35)

$$= 32\sqrt{3}\pi^2 \frac{\hbar}{m} \psi_0^6 a^4.$$  

(36)

In Fig.(11), the particle-loss rate for the $^{23}$Na system is plotted and compared with the experimental data[2]. In the region $2a_0 \leq a \leq 10a_0$ (906G to 906.9G for the magnetic field), the theoretical result is fairly close to the experimental data, although the theoretical derivation so far is for the homogeneous case and the experimental system is inhomogeneous. In the single-channel case[23], the rate of the three-body recombination is also proportional to $n^3a^4$, but the coefficient is about 3.9, about 140 times smaller than $32\sqrt{3}\pi^2$, and cannot be fitted to the experimental result on $^{23}$Na. The increase of the coefficient reflects the fact that in the two-channel system there is a virtual process allowing two atoms to collide and fall into a molecular state, so the three-body recombination process is greater. However, in
rubidium system, the experimental results are rather intricate. A decay rate with a weak density dependence was observed, which seems to suggest that the decay is dominated by a process independent of the particle density.

In addition, the collision between atoms and molecules can also provide a three-body decay but its decay rate is much smaller. The decay of the condensate is consistent the numerical result in Ref. that when multiple modes are included the condensate is depleted over time. The energy scale of the decay rate is comparable to the chemical potential \( \mu \) when \( \psi_0^2 a^3 \) is of the order of 0.01,

\[
\frac{h \Gamma}{\psi_0^2 u} \approx 8 \sqrt{3\pi} \psi_0^2 a^3.
\]

(37)

It indicates that the condensate may not be stable enough beyond the dilute region.

V. CONCLUSION

In conclusion, we have obtained properties of a dilute Bose gas with a Feshbach resonance at zero temperature. The system contains both atomic and molecular condensates but the atom density is much higher. The molecular excitation has a energy gap and the atomic excitations are gapless. The low-energy properties are consistent with the results of the traditional theory. However, the condensed state is only metastable. The coupling between atomic and molecular states gives rise to a three-body recombination process. The decay rate is proportional to \( \psi_0^6 a^4 \) as in the single-channel case, but the coefficient is much bigger as observed in the Na experiment.

It is tempting to go beyond the dilute region in the current approach. However, there are two expansion parameters in higher orders terms neglected in this approach, \( \psi_0 a_0 \sqrt{a} \) from the atomic interaction and \( \psi_0 m^2 \gamma^2 \sqrt{a}/(\hbar^4 |\hbar|) \) from the atom-molecule coupling. The latter is of the order of \( \psi_0 \sqrt{a^2} \) which is much larger than unity near the resonance, and causes the expansion to break down beyond the dilute region. In the most recent experiment, a shift in the molecular energy was observed, which cannot be explained by any theories so far. It seems to suggest that there is a non-trivial many-body effect beyond the dilute region and more theoretical effort are needed.

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[23] P. O. Fedichev, M. W. Reynolds, and G. V. Shlyapnikov, Phys. Rev. Lett. **77**, 2921 (1996).
[24] The decay rate due to the atom-molecule collision is is proportional to $\psi_0^2 a_c^2 / \gamma^4$, where $a_c$ is the scattering length of the atom-molecule collision. Near the resonance, $a \gg a_c$ and $a \gg \frac{m^2 \gamma^2}{\hbar}$, this decay rate is much smaller than $\Gamma$. 

FIG. 1: The coefficients of the particle-loss rate for Na system $\dot{N}/N < n^2 >$ is plotted versus the magnetic field as in Fig.2 in Ref. [2]. The straight line is the theoretical result computed from Eq. (36); the squares and triangles are the experimental data taken at ramp speeds 0.13G/ms and 0.31G/ms of the magnetic field [2]. The scattering length as a function of the magnetic field is computed from Eq. (8) with the parameters given in Ref. [2].
