The three-body recombination of a condensed Bose gas near a Feshbach resonance

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(Dated: July 6, 2005)

Abstract

In this paper, we study the three-body recombination rate of a homogeneous dilute Bose gas with a Feshbach resonance at zero temperature. The ground state and excitations of this system are obtained. The three-body recombination in the ground state is due to the break-up of an atom pair in the quantum depletion and the formation of a molecule by an atom from the broken pair and an atom from the condensate. The rate of this process is in good agreement with the experiment on $^{23}\text{Na}$ in a wide range of magnetic fields.
I. INTRODUCTION

Two-body and three-body recombinations are the main reasons for particle loss in cold Bose gases. Usually the two-body recombination is dominant in the dilute limit and the three-body recombination becomes more important when either the particle density or the interaction strength increases. In systems with Feshbach resonances, near a resonance the scattering length becomes very large. It was found in the experiment on $^{23}\text{Na}$ \cite{1} that the particle-loss rate increases enormously when close to a Feshbach resonance. The three-body recombination rate obtained from the experimental data is much higher than an earlier theoretical estimate for a simple dilute Bose gas \cite{3}.

The large particle-loss rate in $^{23}\text{Na}$ was explained by one of us in terms of the many-body effect due to the special ground-state structure of a dilute condensed Bose gas with a Feshbach resonance \cite{2}. The ground state contains both the condensate and the quantum depletion. One pair of atoms from the quantum depletion can break up. One atom from the broken pair and an atom from the condensate can form a molecule. Therefore in the final state, these three atoms become a molecule and an atom with opposite momenta. The rate of this process was found to be in good agreement with the experimental data close to the resonance \cite{2}.

There have been considerable progress in the study of the three-body recombination in few-body systems \cite{4, 5, 6, 7, 8}. (See Ref. \cite{4} for a complete review on this subject). Particularly, in Ref. \cite{8}, the large particle-loss rate in $^{23}\text{Na}$ was explained in terms of the few-body physics. One important prediction from these studies is that the three-body recombination rate displays periodic behavior due to Efimov states, which has not been observed in experiments so far.

However both theoretical results from Ref. \cite{2} and Ref. \cite{8} can only fit the experimental data of the particle-loss rate \cite{1} very close to the resonance. Theoretical explanation is still needed for the experimental data away from the resonance. In this paper, we adopt an approach which is valid not only close to the resonance, but also quite far away from the resonance, and study a dilute homogeneous system at zero temperature.
II. THE TWO-CHANNEL MODEL

The starting point of our approach is the two-channel model for systems with a Feshbach resonance,

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

where \( m \) is the atom mass, \( \phi \) is the molecular-field operator, and \( \psi \) is the atomic-field operator. The magnetic detuning energy is given by \( \hbar \). The coupling constant of atoms in absence of the resonance is given by \( g_0 = 4\pi \hbar^2 a_0/m \), where \( a_0 \) is the asymptotic scattering length far away from the resonance. The coupling constant between atoms and molecules is given by \( \gamma \), from which we can define a length scale \( a_\gamma \equiv 2\pi \hbar^4/(m^2\gamma^2) \), corresponding to the effective range in the two-atom scattering problem.

In the two-channel model, there are conversions between atoms and molecules. It is usually convenient 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.

III. THE GROUND STATE STRUCTURE

In the dilute region, at zero temperature, both the atoms and the molecules condense. The condensed atoms and molecules have phase coherence with each other, and together form the condensate. The condensate provides the dominant contribution to the grand potential, which is given by

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

where \( \psi_0 \) and \( \phi_0 \) are the expectation values of the atomic and molecular fields. The value of \( \psi_0 \) and \( \phi_0 \) are determined from the saddle-point equations

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

\[ \frac{\partial F_0}{\partial \phi_0} = (h - 2\mu) \phi_0^* - \gamma \psi_0^2 = 0. \]
In the general solution of these saddle-point equations, the molecular field is always in phase or out of phase with the square of the atomic field. For convenience, we choose the expectation value of the atomic field to be positive, $\psi_0 > 0$.

In the region with the repulsive interaction, the detuning energy is negative, $h < 0$, and the chemical potential is positive, $\mu > 0$. The non-trivial solution of the saddle-point equations are given by

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

(6)

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

(7)

where $g_{\text{eff}} = g_0 - 2\gamma^2/(h - 2\mu)$ is the effective coupling constant between atoms. The scattering length is proportional to the effective coupling constant,

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

(8)

where the width of the resonance is given by $\Delta = 2\gamma^2/g_0$. In the ground state of a dilute Bose gas, most of the particles are condensed atoms $\psi_0^2 \approx n$, where $n$ is the total particle density. The chemical potential $\mu$ is much smaller than other energy quantities which do not have density dependence.

However as in the traditional theory of a dilute Bose gas, the condensate is not the complete picture of the ground state. The ground state also contains the quantum depletion which is made of pairs of atoms with opposite momenta. To describe the quantum depletion, we need to look at the gaussian fluctuation around the condensate. In the long-wavelength and low-energy limit, the gaussian fluctuation in the grand potential is given by

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

(9)

where $\epsilon_k$ is the kinetic energy of the atom, $\epsilon_k = \hbar^2 k^2/(2m)$. The molecular part of the fluctuation is not included in equation (9) because molecules have finite energy in the long-wavelength limit. However through the virtual excitation of a molecule, the atoms acquire a diagonal self-energy approximately given by $-2\gamma^2\psi_0/(h - 2\mu)$, which is included in the r.h.s. of Eq. (9).

After applying Bogoliubov transformation, we obtain

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

(10)
where the transformation is given by $c_k = u_k \psi_k + v_k \psi_{-k}^\dagger$, with $u_k^2 = [1 + (\epsilon_k + \mu)/E_k]/2$ and $v_k^2 = u_k^2 - 1$. The atoms have a gapless phonon mode with the excitation energy given by

$$E_k = \sqrt{\epsilon_k(\epsilon_k + 2\mu)}.$$  \hfill (11)

In the ground state $|G\rangle$, there are no phonon excitations, $c_k|G\rangle = 0$, which is only possible if in the ground state atoms with opposite wave-vectors $k$ and $-k$ are paired up. The paired atoms form the quantum depletion with the depletion energy $C$ given by

$$\frac{C}{V} = \frac{8}{15\pi^2} \left( \frac{m\mu}{\hbar^2} \right)^{\frac{3}{2}} \mu,$$  \hfill (12)

where $V$ is the total volume of the system. As we will discuss in the later sections, the ground state obtained here is not the state with the lowest energy, but a metastable state. Nonetheless, in the contest of the traditional theory of a dilute Bose gas, we still name this state as the ground state in this paper.

IV. VACUUM RENORMALIZATION TO THE MOLECULAR EXCITATIONS

Beside the ground state and phonon excitations, the system also contains molecular excitations. From equation (11), the bare molecular excitation energy is simply given by the detuning energy $\hbar$ in the long-wavelength limit. However, the molecule energy is strongly renormalized by the repetitive process of molecules turning into and forming from atoms. In the dilute region, the renormalization to the molecule energy due to the many-body interaction is much smaller than vacuum renormalization because the gas parameter is much smaller than one, $\sqrt{8\pi n a^3} \ll 1$. In the following, we study the vacuum renormalization in detail.

In the vacuum, the propagator of the molecular field is given by

$$G_m(q, \Omega) = \frac{1}{\Omega - \frac{\epsilon_q}{2} - \hbar + 2\mu - \Sigma_m(q, \Omega) + i\delta},$$  \hfill (13)

where $\Sigma_m(q, \Omega)$ is the self-energy due to the vacuum renormalization. The self-energy diagrams of the molecular propagator are shown in Fig. 1. As discussed in earlier references \cite{2, 11, 12}, the self-energy of molecules is given by

$$\Sigma_m(q, \Omega) = 2\gamma^2 D(q, \Omega)[1 + g_0 D(q, \Omega)],$$  \hfill (14)
FIG. 1: The self-energy diagrams of the molecular propagator. The solid lines represent the atom propagator and the dashed lines represent the molecule propagator. The vertex represents the coupling constant $g_0$.

where

$$D(q, \Omega) \equiv i \int \frac{d\omega}{2\pi} \int \frac{d^3k}{(2\pi)^3} G_a(k, \omega)G_a(q - k, \Omega - \omega),$$

and the propagator of the atomic field is given by

$$G_a(k, \omega) = \frac{1}{\omega - \epsilon_k + \mu + i\delta}. \quad (16)$$

In Ref. \[2\], the second term in the r.h.s of equation (14) was dropped. As a result, the calculations in Ref. \[2\] can only be applied when the system is close to the resonance. Here we keep both terms in the expression of the molecular self-energy in equation (14).

As discussed in Ref. \[2\], the divergence in the $D$-function in equation (15) can be removed following the standard renormalization procedure by introducing a counter term, which yields

$$D(q, \Omega) = \int \frac{d^3k}{(2\pi)^3} \left( \frac{1}{\Omega - \epsilon_k - \epsilon_{k-q} + 2\mu + i\delta} + \frac{1}{2\epsilon_k} \right) \equiv \frac{m^{3/2}}{4\pi\hbar^3} \sqrt{\frac{\epsilon_q}{2} - 2\mu - \Omega}. \quad (17)$$

The molecular self-energy is thus given by

$$\Sigma_m(q, \Omega) = \nu \sqrt{\frac{\epsilon_q}{2} - 2\mu - \Omega} + c\left(\frac{\epsilon_q}{2} - 2\mu - \Omega\right), \quad (18)$$

where the parameters $\nu$ and $c$ are given by

$$\nu \equiv \frac{m_3^{3/2}a_0^2}{2\pi\hbar^3} = \sqrt{-\frac{h(a - a_0)}{a_\gamma}}, \quad (19)$$

$$c \equiv \frac{m_3^2g_0^2}{8\pi^2\hbar^6} = \frac{a_0}{a_\gamma}. \quad (20)$$
Although the self-energy given by equation (18) looks rather complicated, the main feature of the molecular propagator is a pole which is given by

\[ \Omega_q = \frac{\varepsilon_q}{2} - 2\mu - \frac{[\sqrt{\nu^2 - 4(c+1)\hbar - \nu}]^2}{4(c+1)^2}. \]  

(21)

Close to the pole, the propagator can be approximated as

\[ G_m(q, \Omega) \approx \frac{Z}{\Omega - \Omega_q + i\delta}, \]  

(22)

where the renormalization factor \( Z \) is given by

\[ Z = \left[ 1 + c + \frac{\nu}{2\sqrt{\nu^2 - 2\mu - \Omega_q}} \right]^{-1} \]

\[ = \left[ 1 + c + \frac{\nu(c+1)}{\sqrt{\nu^2 - 4(c+1)\hbar - \nu}} \right]^{-1}. \]  

(23)

In the limit \( a \gg a_0 \), the molecule energy is approximately given by the shallow bound-state energy, \( \Omega_0 \approx -\hbar^2/(a^2m) \), as given in Ref. [2]. In the limit that \( a \) is very close to \( a_0 \), the molecule energy is approximately given by the detuning energy, \( \Omega_0 \approx \hbar \).

V. THE THREE-BODY RECOMBINATION

In the repulsive-interaction region, the molecules have lower energy than the atoms. Thus the system can always reduce its energy by forming more molecules. The ground state obtained so far is not the state with the lowest energy, but a metastable state. The three-body recombination is one of the main processes for the system to move away from the metastable state.

In the metastable condensed state, the three-body recombination takes place in the following manner. One pair of atoms with opposite momenta in the quantum depletion break up. One atom from the broken pair can interact with an atom in the condensate to form a molecule, leaving the other atom in the broken pair as an excited atom. Thus the final state of this process is the ground state plus a molecule and an excited atom. The probability density of the three-body recombination process can be obtained by using Fermi’s golden rule

\[ \Gamma = \frac{2\pi}{\hbar} \int \frac{d^3k}{(2\pi)^3} |\langle k | 2\gamma \psi_0 \bar{\phi}_k \psi_k | G \rangle|^2 \delta(E_k + \Omega_k) \]
\begin{align*}
&= \frac{2\pi}{\hbar} \int \frac{d^3k}{(2\pi)^3} 4\gamma^2 |\psi_0|^2 \epsilon_k Z \delta(E_k + \Omega_k) \\
&\approx \frac{2\pi}{\hbar} \int \frac{d^3k}{(2\pi)^3} 4\gamma^2 n \frac{\mu^2}{4\epsilon_k^2} Z \delta\left(\frac{3\epsilon_k}{2} + \Omega_0\right) \\
&= 16\sqrt{3\pi\gamma^2 Z a^2 n^3} \frac{a}{\sqrt{m|\Omega_0|^3}},
\end{align*}

(24)

where \(|k\rangle\) is the final state which is the ground state plus a molecule with wave vector \(k\) and an excited atom with wave vector \(-k\).

In the limit that \(a \gg a_0\), the three-body recombination rate \(\Gamma\) is proportional to \(a^4\), with a coefficient about 140 times larger than that in the single channel case. Away from this limit, although there is no simple scaling form for the rate \(\Gamma\), we can compute its numerical value from equation (24). Here the theoretical value of the particle-loss rate in the \(^{23}\text{Na}\) system is plotted and compared with the experimental data in Fig. 2. The experimental data is the loss rate divided by the product of total particle number \(N\) and the average of the density squared. The theoretical value is the loss rate divided by the product of \(N\) and the homogeneous density squared. All the parameters used in the calculation are taken from the experiment, \(a_0 = 3.3\text{nm}\) and \(\Delta = 2\mu_B G\). The theoretical result is fairly close to the experimental data in a wide range of magnetic fields in the repulsive-interaction region, although the theoretical derivation so far is for the homogeneous system and the experimental system is inhomogeneous.

**VI. CONCLUSIONS**

We have studied a homogeneous dilute Bose gas with a Feshbach resonance is studied at zero temperature. In the ground state, there are both the condensate and the quantum depletion. There are two types of excitations, phonon excitations and molecular excitations. The three-body recombination in the ground state is due to the formation of a molecule from an atom in the condensate and an atom from the quantum depletion. The excellent agreement between our calculation and the experimental results in a wide range of magnetic fields leads us to conclude that the many-body effect due to the ground-state structure plays a major role in the three-body recombination process.

An interesting question is whether or not such theoretical description is still valid when
FIG. 2: The coefficients of the particle-loss rate for the Na system, $\dot{N}/N\langle n^2 \rangle$ is plotted vs the magnetic field as in Fig. (2) of Ref. [1]. The straight line is the theoretical result computed from Eq. (24); the squares and triangles are the experimental data taken at ramp speeds 0.13G/ms and 0.31G/ms of the magnetic field [1]. All the parameters used in the calculation are taken from the experiment [1].

the system moves further away from the resonance. When the system is very far from the resonance, the two-channel description should probably be replaced by a single-channel model and the three-body recombination rate is likely to recover the single-channel form. One possible criterion is the comparison between the molecule energy in the two-channel model and the bound-state energy in the single-channel model. If the molecule energy in the closed channel is much deeper than the bound-state energy in the open channel, the single-channel description is probably better.

We would like to thank T.-L. Ho, H.-W. Hammer and E. Braaten for helpful discussions. This work is supported by NSFC under Grant No. 90303008, by Key Project of Chinese Ministry of Education, and by SRF for ROCS, SEM.

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