Three-body recombination in Bose gases with large scattering length

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Abstract

An effective field theory for the three-body system with large scattering length is applied to three-body recombination to a weakly-bound $s$-wave state in a Bose gas. Our model independent analysis demonstrates that the three-body recombination constant $\alpha$ is not universal, but can take any value between zero and $67.9 \hbar a^4/m$, where $a$ is the scattering length. Other low-energy three-body observables can be predicted in terms of $a$ and $\alpha$. Near a Feshbach resonance, $\alpha$ should oscillate between those limits as the magnetic field $B$ approaches the point where $a \to \infty$. In any interval of $B$ over which $a$ increases by a factor of 22.7, $\alpha$ should have a zero.

The successful achievement of Bose-Einstein condensation has triggered a large interest in interacting Bose gases. One of the main factors limiting the achievable density in these experiments is the loss of atoms through 3-body recombination. Such losses occur when three atoms scatter to form a molecular bound state (called a “dimer” for brevity) and a third atom. The kinetic energy of the final state particles allows them to escape from the trapping potential. This 3-body recombination process is interesting in its own right as it provides a unique window on 3-body dynamics.

The number of recombination events per unit time and volume can be parametrized as $\nu_{\text{rec}} = \alpha n^3$, where $\alpha$ is the recombination constant and $n$ the density of the gas. The calculation of $\alpha$ in general is a complicated problem, because it is sensitive to the detailed behavior of the interaction potential \cite{1}. The simplest case is 3-body recombination to a weakly-bound $s$-wave state. For atoms of scattering length $a$ and mass $m$, the binding energy of the dimer is $B_d = \hbar^2/(ma^2)$ and the size of the bound state is comparable to $a$. Assuming that $a$ is the only important length scale, dimensional analysis implies $\alpha = \mathcal{C} \hbar a^4/m$, where $\mathcal{C}$ is dimensionless. The problem of 3-body recombination to a weakly-bound $s$-wave state has been studied previously \cite{2} \cite{3} \cite{4}. Fedichev \textit{et al.} \cite{2} found that the coefficient $\mathcal{C}$ has the universal value $\mathcal{C} = 3.9$. Nielsen and Macek \cite{3} and Esry \textit{et al.} \cite{4} found that $\mathcal{C}$ could take any value between 0 and $\mathcal{C}_{\text{max}} \approx 65$.

An ideal means to study the dependence of $\alpha$ on the scattering length $a$ is to use Feshbach resonances \cite{6}, which occur when the energy of a spin-singlet molecular bound state is tuned to the energy threshold for two separated atoms by applying an external magnetic field $B$. 
Such resonances have, e.g., been observed for $^{23}\text{Na}$ and $^{85}\text{Rb}$ atoms. When the magnetic field is varied in the vicinity of the resonance, the scattering length varies according to

$$a(B) = a_0 \left(1 + \frac{\Delta_0}{B_0 - B}\right),$$

where $a_0$ is the off-resonant scattering length and $\Delta_0$ and $B_0$ characterize the width and position of the resonance, respectively. On the side of the resonance where $a$ increases towards $+\infty$, the spin-singlet molecule becomes a weakly-bound $s$-wave state.

In this Letter, we use effective field theory methods to calculate the recombination constant $\alpha$ for a weakly-bound $s$-wave state. We find that the naive scaling relation $\alpha = C\bar{\hbar}a^4/m$ is modified by renormalization effects, so the coefficient $C$ is not universal, and that its maximum value is $C_{\text{max}} = 67.9$. Our results confirm those of Refs. [3,4], demonstrate that they are model-independent, and provide a new tool for precise studies of the recombination rate. On the side of a Feshbach resonance where $a \to \infty$, the $B$-dependence of $\alpha$ can be predicted in terms of one adjustable parameter. It has a remarkable behavior, with $C$ oscillating between zero and 67.9 more and more rapidly as $B$ approaches the resonance.

Effective field theory (EFT) is a powerful method for describing systems composed of particles with wave number $k$ much smaller than the inverse of the characteristic range $R$ of their interaction. (For a van der Waals potential $-C_6/r^6$, $R = (2mC_6/\bar{\hbar}^2)^{1/4}$). EFT focuses on the aspects of the problem that are universal, independent of the details of short-distance interactions, by modelling the interactions as pointlike. The separation of scales $k \ll 1/R$ allows a systematic expansion in powers of the small parameter $kR$. Generically, the scattering length $a$ is comparable to $R$, and the expansion is effectively in powers of $ka$. The pointlike interactions of the EFT generate ultraviolet divergences, but they can be absorbed into the renormalized coupling constants of the effective Lagrangian. All information about the influence of short-distance physics on low-energy observables is captured by these constants. At any given order in $kR$, only a finite number of coupling constants enter and this gives the EFT its predictive power. The domain of validity of EFT is $kR \ll 1$, even in the case of large scattering length $a \gg R$. Thus it should accurately describe weakly-bound states with size of order $a$. However, the dependence on $ka$ is nonperturbative for $k \sim 1/a$, and it is necessary to reorganize the perturbative expansion into a new expansion in $kR$ by resumming higher order terms to all orders in $ka$. There has been significant progress recently in carrying out this resummation for the 3-body system. At leading order in $kR$, a single 3-body parameter is necessary and sufficient to carry out the renormalization[10]. The scattering length and this 3-body parameter are sufficient to describe all low-energy 3-body observables up to errors of order $R/a$. In nuclear physics, this result has allowed a successful description of low-energy neutron-deuteron scattering and the binding energy of the triton. The variation of the 3-body parameter provides a natural explanation for the Phillips line[11].

We will apply this EFT for systems with large scattering length to the 3-body recombination problem. For simplicity, we now set $\bar{\hbar} = 1$. We start by writing down a general local Lagrangian for a non-relativistic boson field $\psi$:

$$\mathcal{L} = \psi^\dagger \left(i \frac{\partial}{\partial t} + \frac{\vec{\nabla}^2}{2m}\right)\psi - \frac{C_0}{2}(\psi^\dagger \psi)^2 - \frac{D_0}{6}(\psi^\dagger \psi)^3 + \ldots$$
The dots denote terms with more derivatives and/or fields; those with more fields will not contribute to the 3-body amplitude, while those with more derivatives are suppressed at low momentum. In order to set up integral equations for 3-body amplitudes, it is convenient to rewrite \( \mathcal{L} \) by introducing a dummy field \( d \) with the quantum numbers of two bosons,

\[
\mathcal{L} = \psi^\dagger \left( i \frac{\partial}{\partial t} + \frac{\nabla^2}{2m} \right) \psi + d^\dagger d - \frac{g}{\sqrt{2}} (d^\dagger \psi \psi + \text{h.c.}) + h d^\dagger d \psi \psi + \ldots .
\]

The original Lagrangian \([4]\) is easily recovered by a Gaussian path integration over the \( d \) field, which implies \( d = (g/\sqrt{2}) \psi^2/(1 + \hbar \psi \psi) \), \( C_0 = g^2 \), and \( D_0 = -3\hbar g^2 \). The atom propagator has the usual non-relativistic form \( i/(\omega - p^2/2m) \). The bare propagator for \( d \) is simply \( i \), but the exact propagator, including atom loops to all orders, is \([10]\)

\[
iS_d(\omega, \vec{p}) = \frac{-i4\pi/(mg^2)}{-1/a + \sqrt{-m\omega + \vec{p}^2}/4 - i\epsilon} ,
\]

where \( a \) is the scattering length, which is related to the bare parameter \( g \) and the ultraviolet (UV) cutoff \( \Lambda \) by

\[
a = \frac{mg^2}{4\pi} \left( 1 + \frac{mg^2\Lambda}{2\pi^2} \right)^{-1} .
\]

The propagator \([4]\) has a pole at \( \omega = -1/(ma^2) + \vec{p}^2/(4m) \) corresponding to a weakly-bound state. Attaching four atom lines to this propagator gives the exact two-atom scattering amplitude. Taking the incoming atoms to have momenta \( \pm \vec{p} \), the amplitude is \((-1/a - ip)^{-1} \), confirming the identification of \( a \) as the scattering length.

We now consider the 3-body recombination process. We take the momenta of the incoming atoms to be small compared to the momenta of the final particles, which have magnitude \( p_f \). Using Fermi’s golden rule, the recombination coefficient can be written

\[
\alpha = \frac{map_f^2}{6\sqrt{3}\pi} |T(p_f)|^2 ,
\]

FIG. 1. First row: diagrams contributing to 3-body recombination. Second row: integral equation summing them to all orders. Atom propagator and exact dimer propagator are indicated by thin (thick) lines, respectively.
where \( T(p) \) is the amplitude for the transition between three atoms at rest and a final state consisting of an atom and a dimer in an s-wave state with momentum \( p \) in their center-of-momentum frame. In Eq. (7), this amplitude is evaluated on shell at the value \( p_f = 2/(\sqrt{3}a) \) prescribed by energy conservation. However, \( T(p) \) is also defined at off-shell values of \( p \). The first few diagrams contributing to \( T \) are illustrated in Fig. 1. All loop diagrams are of the same order as the tree diagrams, and they therefore have to be summed to all orders. This is conveniently accomplished by solving the integral equation represented by the second equality in Fig. 1. Corrections to this equation are of order \( R/a \). The integral equation is

\[
T(p) = \frac{96\pi^{3/2}}{m} \sqrt{a} \left( \frac{1}{p^2} + \frac{h}{2mg^2} \right) + \frac{2}{\pi} \int_0^\Lambda dq \left[ \frac{q^2 T(q)}{-1/a + \sqrt{3q}/2} \left( \frac{1}{pq} \ln \left| \frac{q^2 + pq + p^2}{q^2 - pq + p^2} \right| + \frac{h}{mg^2} \right) \right] ,
\]

where we have inserted an UV cutoff \( \Lambda \) on the integral over \( q \). If we were allowed to set \( h = 0 \) and take \( \Lambda \to \infty \), a rescaling of the variables in Eq. (7) would lead to \( T(p) = K(ap)a^{3/2}/(mp) \), with \( K(x) \) a dimensionless function. Evaluating this in Eq. (7), the scaling relation \( \alpha = C a^4/m \) would follow immediately. However, the integral equation (7) has the same properties as the one describing atom-dimer scattering (10) and the limit \( \Lambda \to \infty \) can not be taken. The individual diagrams are finite as \( \Lambda \to \infty \), but their sum is sensitive to the cutoff. In an EFT, the dependence on the UV cutoff is cancelled by local counterterms. In Ref. (10), it was shown that the dependence of the low-energy observables on the cutoff \( \Lambda \) could be precisely compensated by varying \( h \) appropriately. Writing \( h = 2mg^2H(\Lambda)/\Lambda^2 \), it was found that \( H(\Lambda) \) could be well approximated by

\[
H(\Lambda) \approx -\tan \left( s_0 \ln(\Lambda/\Lambda_*) - \pi/4 \right) ,
\]

where \( s_0 \approx 1.0064 \) is determined by the asymptotic behavior of the integral equation. This expression defines a parameter \( \Lambda_* \) (10) that characterizes the effect of the 3-body force on physical observables. A remarkable feature of this expression is its periodicity in \( \ln \Lambda \). As \( \Lambda \) is increased, \( H(\Lambda) \) decreases to \( -\infty \), changes discontinuously to \( +\infty \), and continues decreasing.

The scaling violations in \( T(p) \) from the renormalization of the 3-body force can be expressed as a dependence on \( a\Lambda_* \). The simple scaling relation for \( \alpha \) is therefore replaced by \( \alpha = C(\Lambda_*a) a^4/m \). Thus the value of \( C \) is not universal. In Fig. 2, we show \( \alpha \) as a function of \( a \) for \( \Lambda_*a_0 = 1.78, 4.15, 7.26 \) and 19.77, where \( a_0 \) is an arbitrary but fixed length scale. Interestingly, \( \alpha \) appears to oscillate as a function of \( \ln a \) between zero and a maximum value \( C_{\max} \). We find that the curves can be very well fit by the expression

\[
\alpha \approx \frac{ha^4}{m} C_{\max} \cos^2 \left( s_0 \ln(a\Lambda_*) + \delta \right) ,
\]

with \( C_{\max} = 67.9 \pm 0.7 \) and \( \delta = 1.74 \pm 0.02 \).

We now compare our result to those of Refs. (2–4). Using an approximate solution to the 3-body wavefunction in hyperspherical coordinates, Fedichev et al. (2) found that the coefficient \( C \) has the universal value \( C = 3.9 \), independent of the interaction potential. We find that the value of \( C \) is not universal, but can vary from zero to about 67.9, depending
on the details of 3-body interactions at short distances. We suggest that the specific value in Ref. [2] must correspond to an implicit assumption about the short-distance behavior of the 3-body wavefunction. Our results are consistent with those of Refs. [3,4], which were obtained using the hyperspherical adiabatic approximation. Nielsen and Macek [3] obtained $C_{\text{max}} \approx 68.4$ by applying the hidden crossing theory. Esry et al. [4] used coupled channel calculations to obtain $\alpha$ numerically for over 120 different 2-body potentials. For $a \gg R$, their empirical result has the form of Eq. (9) with $s_0 = 1$ and $C_{\text{max}} = 60 \pm 13$. Refs. [3,4] show that the zeroes in $\alpha$ arise from interference effects involving 2-body and 3-body hyperspherical adiabatic potentials. The origin of these interference effects is less obvious in our EFT approach. However, our approach has several other advantages. First, it is completely model independent. Second, it is a controlled approximation, with corrections from finite range effects suppressed by powers of $R/a$. Third, it has predictive power in that all other low-energy 3-body observables can be determined in terms of $a$ and $\Lambda_s$. For example, the atom-dimer scattering length $a_d$ can be fit by

$$a_d \approx a \left(1.4 - 1.8 \tan[s_0 \ln(a\Lambda_s) + 3.2]\right).$$

We now apply the EFT to Feshbach resonances, where the value of $a$ is varied by changing the external magnetic field (cf. Eq. (10)). Our formalism is only applicable close to the

FIG. 2. $\alpha$ as a function of $a$ for different values of the 3-body parameter: $a_0\Lambda_s = 1.78$ (full line), 4.15 (dotted line), 7.26 (dashed line), and 19.77 (long-dashed line).
Feshbach resonance on the side where \( a > 0 \), because only in that region is there a weakly-bound molecule with \( B_d \sim 1/(ma^2) \). Away from the resonance, or close to the resonance but on the side where \( a < 0 \), 3-body recombination must involve more deeply-bound molecules with binding energies of order \( 1/(mR^2) \). To predict \( \alpha \) as a function of the magnetic field \( B \), we must specify how the parameter \( \Lambda_a \) in Eq. (8) varies as a function of \( B \). A Feshbach resonance is characterized by nonanalytic dependence of the scattering length \( a \) on \( B \). In a field theory, nonanalytic dependence on external parameters arises from long-distance fluctuations. The explicit ultraviolet cutoff \( \Lambda \) in our EFT excludes long-distance effects, but field theory nonanalytic dependence on external parameters arises from long-distance fluctuations. The resonant behavior of the scattering length near \( B = B_0 \) in Eq. (11) can be reproduced by approximating \( g^2 \) by a linear function of \( B \) in the resonance region. The parameter \( h \) should also be a smooth function of \( B \), but we can take \( h \) to be approximately constant over the narrow resonance region. This assumption implies via Eq. (8) that \( \Lambda_a \) should be constant while \( a(B) \) varies as in Eq. (1).

The behavior of the recombination coefficient near the Feshbach resonance can therefore be read off from Fig. 4. If \( \alpha \) is measured at one value of \( B \) for which \( a(B) \gg |a_0| \), it determines \( \alpha \) as a function of \( B \) up to a two-fold ambiguity corresponding to whether the slope of \( C \) is positive or negative at that value of \( B \). As \( B \) approaches \( B_0 \), \( C \) should oscillate between 0 and \( C_{\text{max}} \) in the manner shown in Fig. 2. The successive zeros correspond to values of \( a(B) \) that differ roughly by multiplicative factors of \( \exp(\pi/s_0) \approx 22.7 \). Thus EFT makes the remarkable prediction that there are values of the magnetic field close to a Feshbach resonance where the contribution to \( \alpha \) from a weakly-bound state vanishes.

The loss rate of \(^{23}\text{Na} \) atoms from a Bose-Einstein condensate near a Feshbach resonance has been studied by Stenger et al. [8]. Our theory applies to the low-field side of the resonance at \( B = 907 \) G. Taking into account the 3 atoms lost per recombination event and a Bose factor of \( 1/3! \), the loss rate from the condensate is \( \tilde{N} = -\alpha N \langle n^2 \rangle/2 \). The loss rates measured in Ref. [8] correspond to a coefficient \( C \approx 300 \) both off and near the resonance. This value is a factor of 4 larger than our maximum value. If \( C > C_{\text{max}} \), the 3-body recombination rate must be dominated not by the weakly-bound Feshbach resonance but instead by molecules with much larger binding energies \( \sim 1/(mR^2) \). Alternatively, the large loss rate in Ref. [8] could be due to collective effects associated with the Bose-Einstein condensate, such as a 2-body recombination process involving atoms and dimers in a molecular condensate [3]. In Fig. 3 we show the contribution to \( \alpha \) from the weakly-bound state as a function of the magnetic field \( B \) for \( \Lambda_a = 1.94 \) nm\(^{-1} \), \( 1.16 \) nm\(^{-1} \), and \( 0.65 \) nm\(^{-1} \). If this contribution to \( \alpha \) could be isolated, the first zero may be wide enough to be observed by experiment. The higher zeroes, however, are increasingly narrow and very close to the resonance.

We have applied an EFT for atoms with large scattering length to the problem of 3-body recombination into a weakly-bound s-wave state. We find that the coefficient \( C \) in the scaling relation \( \alpha = C h a^4/m \) is not universal, but must be in the range \( 0 \leq C \leq 67.9 \). If the 3-body recombination rate is measured to be larger than the maximum value, there must be a large contribution from molecules that are more deeply bound. Other low-energy 3-body observables, such as the atom-dimer scattering length, can be predicted in terms of \( a \) and \( C \). Near a Feshbach resonance as \( a \to \infty \), we find that \( C \) should oscillate between zero and 67.9. In any interval of \( B \) over which \( a \) increases by a factor of \( \exp(\pi/s_0) \approx 22.7 \), \( \alpha \) should have
FIG. 3. Contribution to $\alpha$ from recombination into the weakly-bound state as a function of $B$ for the 907 G Feshbach resonance in $^{23}$Na.

a zero. Assuming that it is dominated by recombination into the weakly-bound state, the 3-body loss rate should have a minimum at that value of $B$. If a Bose-Einstein condensate was prepared at such a value of the magnetic field, one could study its behavior with large scattering length and relatively small 3-body losses.

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