Dimer-atom-atom recombination in the universal four-boson system *

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Abstract The dimer-atom-atom recombination process in the system of four identical bosons with resonant interactions is studied. The description uses the exact Alt, Grassberger and Sandhas equations for the four-particle transition operators that are solved in the momentum-space framework. The dimer-dimer and atom-trimer channel contributions to the ultracold dimer-atom-atom recombination rate are calculated. The dimer-atom-atom recombination rate greatly exceeds the three-atom recombination rate.

Keywords Efimov effect · four-particle scattering · recombination

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1 Introduction

Few-particle systems with large two-particle scattering length $a$ possess universal properties that are independent of the short-range interaction details. The three-particle system was investigated theoretically by V. Efimov more than 40 years ago [1] but only in the last decade the cold-atom physics experiments [2] confirmed his prediction for the existence of zero orbital angular momentum weakly bound three-particle states with asymptotic discrete scaling symmetry. This boosted the interest also in the universal systems with four or even more particles. In contrast to the three-body system where semi-analytical results have been obtained (see Ref. [3] for a review), most of the theoretical studies of the four-body systems are numerical. In addition to the numerous bound-state calculations, e.g., [4,6,7,8,9,10,11], also the collision processes have been investigated in the framework of hyperspherical harmonics (HH) [6], coordinate-space Faddeev-Yakubovsky (FY) equations [12,8] or momentum-space Alt,Grassberger and Sandhas (AGS) equations [13,14]. The studies include the elastic and inelastic atom-trimer [8,11,15].

* Dedicated to Professor Henryk Witala at the occasion of his 60th birthday

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Fig. 1 (Color online) Schematic representation of the two- and three-cluster thresholds in the four-boson system as functions of the two-boson scattering length. The intersection of the dimer-atom-atom (solid line) and the nth atom-trimer (dashed line) thresholds defines \( a_n^d \).

and dimer-dimer scattering [16,17] as well as the four-atom recombination [18,19]. Depending on the collision energy and the two-particle scattering length (that can be manipulated by the external magnetic field in the cold-atom experiments) all these reactions may get resonantly enhanced due to the presence of unstable tetramer states. Such a resonant behaviour in the dimer-dimer relaxation and four-atom recombination, roughly consistent with theoretical predictions, was observed recently in experiments with ultracold atoms performed near the universal regime [21,22,23,24].

The four-particle reaction, that, to the best of our knowledge, has not been studied so far, is the three-cluster recombination, i.e., an inelastic collision of a dimer and two atoms leading to the two-cluster final state either with two dimers or with one atom and a trimer. Due to time reversal symmetry, the amplitude for this process is equal to the amplitude for the three-cluster breakup of the initial two-cluster state. The latter is more directly related to the transition operators for the two-cluster reactions [14,17,20] and is derived in the present work using the formalism of the AGS four-particle scattering equations. Their numerical solution is performed in the momentum-space framework.

We will study the dimer-atom-atom recombination in the system of four identical bosons with resonant two-boson interactions. In the potential model taken over from Refs. [14,17,20] there is only one weakly bound dimer but many trimers since the system exhibits an Efimov effect [18]. In our nomenclature we label the Efimov trimers by one integer number \( n \), starting with \( n = 0 \) for the ground state. The dependence of various scattering thresholds on the two-boson scattering length \( a \) is schematically shown in Fig. 1. The special value of \( a \) corresponding to the intersection of the \( n \)-th atom-trimer and dimer-atom-atom threshold is denoted by \( a_n^d \).

In Sec. 2 we derive the three-cluster breakup amplitude in terms of the AGS transition operators and discuss some technical aspects of the calculations. In Sec. 3 we present results for the dimer-atom-atom recombination. We summarize in Sec. 4.
2 Four-particle scattering

We consider the relative motion in the four-particle system interacting via short-range pairwise potentials $v_j$ where $j$ labels one of the six pairs. The full Hamiltonian is

$$H = H_0 + \sum_{j=1}^6 v_j$$

with $H_0$ being the kinetic energy operator. We do not calculate the four-particle wave function directly by solving the Schrödinger equation or the Faddeev-Yakubovsky equations [12]. We prefer the integral form of the scattering equations as formulated by Alt, Grassberger and Sandhas [13] for the four-particle transition operators $U_{\sigma\rho}$. These equations are 18-component matrix equations [13,25], i.e.,

$$U_{\sigma\rho}^{ij} = (G_0 t_j G_0)^{-1} \delta_{\sigma\rho} \delta_{ji} + \sum_{\gamma k} \delta_{\sigma\gamma} U_{\gamma k}^{jk} G_0 t_k G_0 U_{\gamma\rho}^{ki},$$

where the components are distinguished by the chains of partitions, i.e., by the two-cluster partition and by the three-cluster partition. The two-cluster partitions, denoted by Greek letters, are either of $3 + 1$ or $2 + 2$ type. The three-cluster partitions, denoted by Latin letters, are of $2 + 1 + 1$ type and therefore are fully characterized by the pair of particles in the composite cluster. Obviously, the pairs $i, j$ and $k$ must be internal to the respective two-cluster partitions, i.e., $i \subset \rho$, $j, k \subset \gamma$ and $j \subset \sigma$. Furthermore, $\delta_{\sigma\rho} = 1 - \delta_{\sigma\rho}$ and

$$G_0 = (E + i0 - H_0)^{-1}$$

is the free resolvent at the system energy $E$. The two-particle interactions for each pair are summed up to all orders to form the respective two-particle transition matrices

$$t_j = v_j + v_j G_0 t_j,$$

while all the interactions within each two-cluster subsystem lead to the transition operators

$$U_{\gamma k}^{ij} = G_0^{-1} \delta_{jk} + \sum_{i} \delta_{ji} t_i G_0 U_{\gamma i}^{ik}.$$

The wave function $|\Psi_{\rho,n}\rangle$ describing the scattering process initiated by the asymptotic two-cluster channel state $|\Phi_{\rho,n}\rangle$ with the relative two-cluster momentum $p_{\rho,n}$ is determined by the AGS transition operators as

$$|\Psi_{\rho,n}\rangle = |\Phi_{\rho,n}\rangle + \sum_{\gamma ki} G_0 t_i G_0 U_{\gamma k}^{ij} G_0 t_k G_0 U_{\gamma\rho}^{ki} |\phi^i_{\rho,n}\rangle.$$

The energy parameter in the operators of Eq. (6) is $E = \epsilon_{\rho,n} + p_{\rho,n}^2 / 2\mu_{\rho}$ with $\epsilon_{\rho,n}$ being the energy of the $n$th bound state in the partition $\rho$ and $\mu_{\rho}$ being the reduced mass. The asymptotic channel state $|\Phi_{\rho,n}\rangle$ is a product of the $n$th bound state wave function in the partition $\rho$ and the plane wave with momentum $p_{\rho,n}$ between the two clusters. $|\Phi_{\rho,n}\rangle = \sum_{i} |\phi^i_{\rho,n}\rangle$ is decomposed into its Faddeev components that are calculated from the Faddeev equation

$$|\phi^i_{\rho,n}\rangle = G_0 \sum_j \delta_{ij} t_j |\phi^j_{\rho,n}\rangle$$
and normalized such that \( \langle \Phi_{\sigma,n} | \Phi_{\rho,n} \rangle = \delta_{\sigma\rho} \delta_{n,n} \delta (p_{\sigma,n'} - p_{\rho,n}). \)

The scattering amplitudes for the reactions with initial and final two-cluster states are given by the on-shell matrix elements of the AGS operators \( \sum_{ji} \langle \phi_j^i \sigma,n' | U_{ji}^\dagger | \phi_i \rho,n \rangle \) as explained in Refs. [13,25]. The amplitude for the three-cluster breakup of the initial two-cluster state can be obtained from \( U_{ji} \langle \phi_i \rho,n \rangle \) as well. We derive it from the general relation

\[
\langle \Phi_j | T_{j\rho} | \Phi_{\rho,n} \rangle = \langle \Phi_j | (1 - v_j G_0) G_{0}^{-1} | \Phi_{\rho,n} \rangle. \tag{8}
\]

The asymptotic three-cluster state \( |\Phi_j \rangle \) is an eigenstate of the channel Hamiltonian \( H_0 + v_j \) with the eigenvalue \( E \), i.e.,

\[
|\Phi_j \rangle = G_0 v_j |\Phi_j \rangle. \tag{9}
\]

It is given by the bound state wave function for the pair \( j \) times two plane waves corresponding to the relative motion of the three free clusters. Since the full wave function (9) is an eigenstate of the Hamiltonian (1), i.e., \( \sum_{i=1}^6 v_i |\Psi_{\rho,n} \rangle = G_{0}^{-1} |\Psi_{\rho,n} \rangle \), we rewrite the amplitude (8) as

\[
\langle \Phi_j | T_{j\rho} | \Phi_{\rho,n} \rangle = \langle \Phi_j | (1 - v_j G_0) G_{0}^{-1} | \Psi_{\rho,n} \rangle. \tag{10}
\]

Although \( \langle \Phi_j | (1 - v_j G_0) = 0 \) due to Eq. (9), one has to keep in mind that \( t_l \) arising from the wave function (9) has a pole for \( |\Phi_j \rangle \) if \( l = j \). Using Eq. (11) one gets the relation

\[
\langle \Phi_j | (1 - v_j G_0) t_l G_0 = \langle \Phi_j | \delta_{jl} \tag{11}
\]

that leads to the three-cluster breakup amplitude

\[
\langle \Phi_j | T_{j\rho} | \Phi_{\rho,n} \rangle = \sum_{\gamma k l} \langle \Phi_j | U_{\gamma k} G_0 t_k G_0 U_{\gamma l}^\dagger | \phi_{\rho,n} \rangle. \tag{12}
\]

Finally, the amplitude for the four-cluster breakup can be found in Ref. [20].

In the system of identical particles the number of distinct partitions and AGS operator components reduces to two. We choose those partitions to be ((12)3)4 and (12)(34) and denote them in the following by \( \alpha = 1 \) and 2, respectively. The amplitudes (12) after symmetrization become

\[
\langle \Phi_d | T_{d\alpha} | \Phi_{0,n} \rangle = S_{d\alpha} \langle \Phi_d | [1 + \varepsilon P_{34}] U_1 G_0 t G_0 U_{1\alpha} + U_2 G_0 t G_0 U_{2\alpha} | \phi_{0,n} \rangle. \tag{13}
\]

Thus, \( T_{d1} \) (\( T_{d2} \)) describes the atom-trimer (dimer-dimer) breakup into a dimer and two atoms. \( S_{d1} = \sqrt{3} \) and \( S_{d2} = 2 \) are the corresponding symmetrization factors, \( P_{34} \) is the permutation operator of particles 3 and 4, and \( \varepsilon = 1 \) (-1) for bosons (fermions). The dimer-atom-atom three-cluster channel state \( |\phi_d \rangle \) is symmetrized only within the bound pair (12). There is only one independent Faddeev component \( |\phi_{0,n} \rangle \) for each two-cluster channel state. The two-particle transition matrix \( t \) is derived from the pair (12) potential according to Eq. (11). The symmetrized 3 + 1 and 2 + 2 subsystem operators are

\[
U_\alpha = P_\alpha G_0^{-1} + P_\alpha t G_0 U_\alpha \tag{14}
\]
with \( P_1 = P_{12}P_{23} + P_{13}P_{23} \) and \( P_2 = P_{13}P_{24} \) where \( P_{ab} \) is the permutation operator of particles \( a \) and \( b \). The symmetrized four-particle transition operators obey the symmetrized AGS equations [26], i.e.,

\[
U_{11} = \varepsilon P_{34}(G_0tG_0)^{-1} + \varepsilon P_{34}U_1G_0tG_0U_{11} + U_2G_0tG_0U_{21}, \quad \text{(15a)}
\]

\[
U_{21} = (1 + \varepsilon P_{34})(G_0tG_0)^{-1} + (1 + \varepsilon P_{34})U_1G_0tG_0U_{11} + U_2G_0tG_0U_{22}, \quad \text{(15b)}
\]

\[
U_{12} = (G_0tG_0)^{-1} + \varepsilon P_{34}U_1G_0tG_0U_{12} + U_2G_0tG_0U_{22}, \quad \text{(15c)}
\]

\[
U_{22} = (1 + \varepsilon P_{34})U_1G_0tG_0U_{22}. \quad \text{(15d)}
\]

The employed basis states have to be symmetric (antisymmetric) under exchange of two bosons (fermions) in subsystem (12) for the 3 + 1 partition and in (12) and (34) for the 2 + 2 partition.

After partial-wave decomposition for each combination of the total angular momentum \( J \) and parity \( \Pi \) the AGS equations (15) become a system of coupled three-variable integral equations. In our momentum-space framework these variables are the magnitudes of the Jacobi momenta \( k_x, k_y \) and \( k_z \) that are defined in Ref. [20] and describe the relative motion in the 1+1, 2+1, and 3+1 (1+1, 1+1, and 2+2) subsystems of the 3+1 (2+2) configurations, respectively. Such three-variable integral equations have been solved in Refs. [27,28] for various four-nucleon reactions with two-cluster initial and final states. However, by using a separable two-particle potential the AGS equations (15) can be reduced to a system of integral equations in two continuous variables, the Jacobi momenta \( k_y \) and \( k_z \). We applied this technical simplification in the study of the universal properties of the four-boson system that are independent of the short-range interaction details [14,17,20]. The same separable potential is used also in the present work. The discretization of integrals in the AGS equations using Gaussian quadrature rules [29] leads to a system of linear algebraic equations. While the calculational technique to a large extent is taken over from Refs. [14,17,20], there is one important difference associated with the open dimer-atom-atom channel. Namely, in addition to the subsystem bound state poles of \( U_\alpha \) the kernel of the AGS equations has integrable singularities arising from \( t \). For \( k_y^2/2\mu_{\alpha y} + k_z^2/2\mu_\alpha \rightarrow E - \epsilon_d \) the two-boson transition matrix in the channel with the dimer quantum numbers for the pair (12) has the pole

\[
t \rightarrow \frac{\langle \Phi_d | \langle \Phi_d | v \rangle}{E + i0 - \epsilon_d - k_y^2/2\mu_{\alpha y} - k_z^2/2\mu_\alpha}, \quad \text{(16)}
\]

where \( \epsilon_d < 0 \) is the dimer energy and \( \mu_{\alpha y} \) is the reduced mass for \( k_y \). The treatment of this singularity simplifies considerably if the available four-boson energy is just at the dimer-atom-atom threshold, i.e., \( E = \epsilon_d \). In this case there is only one singular point \( k_y = k_z = 0 \) and in all nontrivial momentum integrals (the ones without \( \delta \)-functions) of the type

\[
\int_0^\infty \frac{f(k_y, k_z)k_j^2dk_j}{i0 - k_y^2/2\mu_{\alpha y} - k_z^2/2\mu_\alpha} \quad \text{(17)}
\]

this singularity is cancelled by \( k_j^2 \) leading to numerically harmless integrals.
3 Dimer-atom-atom recombination

We consider an ultracold gas consisting of a mixture of bosonic atoms and dimers with respective particle densities $\rho_a$ and $\rho_d$. We define the dimer-atom-atom recombination rate $K_{211}$ such that the number of the dimer-atom-atom recombination events per volume and time is $K_{211} \rho_a^2 \rho_d / 2!$. At sufficiently low temperature the momenta of the initial particles are much smaller than the final momenta of the two resulting clusters, i.e., $k_y, k_z \ll p_{a,n',t}$, and the kinetic energies of initial particles are much smaller than the final two-cluster kinetic or binding energies, i.e., $k_y^2 / 2\mu_a + k_z^2 / 2\mu_a \ll p_{a,n,t}^2 / 2\mu_a, \epsilon_{a,n}$. Under these conditions one can assume the threshold values $k_y = k_z = 0$ for the initial three-cluster channel state $|\Phi_d\rangle$ and $E = \epsilon_d$ for the AGS equations. The dimer-atom-atom recombination rate in this limit is given by

$$K_{211} = 2(2\pi)^8 \sum_{\alpha,n'} \mu_o p_{\alpha,n'} |\langle \Phi_d | T_{da} | \Phi_{\alpha,n'} \rangle|^2.$$  \hspace{1cm} (18)

Here we used the time-reversal symmetry in replacing the amplitude for the three-cluster recombination into the final two-cluster state by the amplitude for the three-cluster breakup of the initial two-cluster state, i.e.,

$$\langle \Phi_{\alpha,n} | T_{ad} | \Phi_d \rangle = \langle \Phi_d | T_{da} | \Phi_{\alpha,n} \rangle.$$  \hspace{1cm} (19)

Furthermore, at $k_y = k_z = 0$ only the $J = 0$ partial wave contributes to the amplitude \(19\), i.e., $\langle \Phi_d | T_{da} | \Phi_{\alpha,n} \rangle = (4\pi)^{-3/2} \langle \Phi_d (J = 0) | T_{da} | \Phi_{\alpha,n} (J = 0) \rangle$.

The dimer-atom-atom recombination process leads to the final state either with two dimers or with an atom and an Efimov trimer. As it is evident from Eq. \(18\), $K_{211}$ can be decomposed into the dimer-dimer and $(n + 1)$ atom-trimer contributions

$$K_{211} = K_{211}^{dd} + \sum_{n'=0}^n K_{211}^{n'1},$$  \hspace{1cm} (20)

where $n$ labels the highest excited trimer state.

We aim to determine the universal behaviour of the ultracold dimer-atom-atom recombination rate and its contributions \(20\) as functions of the two-boson scattering length. We therefore build dimensionless quantities $a/a_n$ and $K_{211}^{\alpha n} m/\hbar a^4$, with $m$ being the boson mass. Due to asymptotic discrete scaling symmetry it is sufficient to consider the regime $1 < a/a_n < a_{n+1}^d/a_n^d \approx 22.694$ \(3\) with $n + 1$ trimer states, provided $n$ is sufficiently large such that non-universal short-range corrections become negligible. We found that $n \geq 3$, i.e., one has to consider the processes involving four or more atom-trimer channels. This is fully consistent with previous findings \(10\)\(14\)\(20\) for other four-boson reactions.

We compare the most important contributions to the ultracold dimer-atom-atom recombination rate in Fig. 2. All contributions peak at $a/a_n^d = 1$ and $a/a_n^d \approx 22.694$ where the $n$-th and the $(n + 1)$-th trimers, respectively, emerge at the atom-dimer threshold. Near these critical regimes the recombination process is dominated by the two-cluster channel with the weakest binding, i.e., the $n$-th atom-trimer channel close to $a/a_n^d = 1$ and the dimer-dimer channel close to $a/a_n^d \approx 22.694$ with the respective contributions $K_{211}^{dd}$ and $K_{211}^{d1}$.

The $n$-th atom-trimer and dimer-dimer thresholds intersect at $a/a_n^d \approx 6.789$ \(17\). However, it seems that there is an interference between these two channels around $a/a_n^d = 10$ leading to
Dimer-atom-atom recombination in the universal four-boson system

Fig. 2 (Color online) Dimer-atom-atom recombination rate as a function of the two-boson scattering length. The contributions of the final dimer-dimer (dashed-dotted), n-th (solid) and \((n-1)\)-th (dashed) atom-trimer channels are compared with the three-atom recombination rate (dotted).

A slight enhancement of \(K_{211}^n\) and suppression of \(K_{211}^{dd}\) such that \(K_{211}^n > K_{211}^{dd}\) for \(a/a_n^d < 13.5\). This behaviour is not very surprising given the strong coupling between the \(n\)-th atom-trimer and dimer-dimer channels observed in the dimer-dimer scattering [17]. The transitions to channels with lower trimers \(n' \leq n - 1\) are strongly suppressed; we only show the predictions for \(K_{211}^{n-1}\), the others being considerably smaller.

In addition to various \(K_{211}\) contributions we show in Fig. 2 also the ultracold three-atom recombination rate \(K_3\) defined such that the number of three-atom recombination events per volume and time is \(K_3 \rho_3^a/3!\). We calculate it numerically as

\[
K_3 = 2(2\pi)^6 \mu_{123} p_y |\langle \phi_0 |(1 + P_1)tG_0 U_1|\phi_d \rangle|^2
\]

where \(|\phi_d\rangle\) and \(|\phi_0\rangle\) are the atom-dimer and three-atom channel states and \(p_y\) is the relative atom-dimer momentum in the final state. Our \(K_3\) predictions are in perfect agreement with the semi-analytical results of Ref. [3] (after taking into account that the respective definitions differ by a factor 3!). We observe that \(K_{211}\) is much larger than \(K_3\), especially near the ends of the shown interval and around the \(K_3\) minimum. This may have important consequences for the life time and stability of trapped ultracold atomic gases with small admixture of dimers: Let’s suppose that the trapping potential is lower than the kinetic energies of the recombination products, i.e., they are able to escape the trap. Neglecting other reactions like the four-atom or dimer-dimer-atom recombination that should be suppressed at not
too high densities, the atom density in the trap evolves with time according to

$$\frac{d\rho_a}{dt} = -\frac{1}{2}K_3\rho_a^3 - K_{211}\rho_d^2\rho_a. \quad (22)$$

Thus, due to $K_{211} \gg K_3$ even at low dimer densities $\rho_d << \rho_a$ the dimer-atom-atom recombination may be as important as the three-atom recombination.

Finally, one may raise the question whether a complicated four-body treatment of the dimer-atom-atom recombination is really necessary and to what extent a simple three-body model considering the dimer as a point-like particle is reliable. Such model was constructed in Ref. [30]. Although it describes well the $n$th trimer binding and the low-energy atom-dimer scattering, it does not support lower atom-trimer channels, i.e., for $n' < n$ it yields $K_{211}^{n'} = 0$. Furthermore, the three-body dimer-atom-model is obviously inappropriate in the dimer-dimer channel since it treats the two dimers asymmetrically. Consistently with two-cluster reactions from Ref. [30], the three-body dimer-atom-atom model fails heavily for $K_{211}^{dd}$ as shown in Fig. 3. However, $K_{211}^{nn}$ in the regime $a/a_n^d < 4$ is reproduced quite well, with 10% or better accuracy. There the trimer size exceeds the dimer size such that the approximations of a point-like dimer and a trimer consisting of weakly bound atom and dimer are reasonable. For $a/a_n^d > 4$ the three-body dimer-atom-atom model fails also in predicting $K_{211}^{nn}$.

4 Summary

We studied the dimer-atom-atom recombination in the universal four-boson system that exhibits the Efimov effect. We used exact AGS equations for the four-particle transition operators that were solved in the momentum-space framework. The relation between the AGS operators and the dimer-atom-atom recombination amplitude was derived. We calculated the dimer-dimer and atom-trimer contributions to the dimer-atom-atom recombination rate in the ultracold limit. We found that
usually the channel with the weakest binding dominates the recombination process but there are deviations from this behaviour when several two-cluster thresholds are close to each other. We also have shown that the dimer-atom-atom recombination rate greatly exceeds the three-atom recombination rate leading to important consequences for the life time of atomic gases with a small admixture of dimers.

We also studied a simplified three-body model for the dimer-atom-atom recombination process and found it to be inadequate, except for $K_{211}^3$ in the regime where the trimer can be considered as a weakly bound atom-dimer system.

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