Low-Energy Recombination of Identical Bosons by Three-Body Collisions

Esben Nielsen
Institute of Physics, Aarhus University, Aarhus, Denmark

J. H. Macek
Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996-1501
and Physics Division, Oak Ridge National Laboratory, P.O. Box 2009, Oak Ridge, Tennessee 37831
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The threshold recombination coefficient for three bosons whose two-body scattering length a is positive and large compared with the nominal range of the potentials is shown to proceed via a crossing of hyperspherical adiabatic potential curves at $R \approx 2.6a$. The hidden crossing theory gives a simple expression for the rate in terms of the scattering length and a phase Δ. The phase depends upon the details of the interaction, and varies from species to species, however an upper limit to the rate which depends only upon the scattering length emerges from the hidden crossing theory.

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One of the main issues in Bose-Einstein condensation is the systematics of three-body recombination rates. A Bose condensate of some atoms, say B, is not the lowest energy state but a metastable state, where the atoms are so far apart that they interact weakly. Such systems can fall into lower energy states, i.e., clusters of atoms, by recombination. Usually the main loss is due to recombination to dimers, B_2. Such recombination cannot occur by simple two-body reactions. Something has to carry away the extra energy and momentum. At the very low energies of Bose condensates, this will usually be a third atom. The important process is thus $B + B + B \rightarrow B_2 + B$.

An experimental treatment of recombination in a Bose condensate is described by Inouye *et al.* in [1], where they have succeeded in adjusting the two-body scattering length, a, by adjusting the magnetic field near a Feshbach resonance. This follows the normal trends in the theories of Bose condensates, where the only parameter from the two-body potential is indeed the scattering length. Several papers have dealt theoretically with the connection between scattering length and the recombination rate [2,3] based upon numerical calculations for a series of similar potentials with different scattering length. Fedichev *et al.* [4] propose an a^4 law. The aim of this paper is to investigate this dependence further and to give a simple intuitive understanding of the fundamental process of recombination.

We do this by approximating the two-body interaction by a zero-range potential which is defined by the scattering length alone. It has been known since 1935 that the corresponding three-body system will have infinitely many bound states [5]. The same problem occurs in conventional coupled channel calculations for three-body states where the same singularity occurs at the origin.

Many attempts have been made to work around this problem by adding some sort of cutoff to the potential. Bedaque *et al.* have added a three-body interaction that acts as a renormalization of this singularity [6]. This paper shows that such cutoffs contribute to the transition probability as significantly as they do to binding energies and elastic atom-dimer scattering.

We clarify the theory by treating the problem in hyperspherical coordinates and applying the hidden crossing theory [7]. Hyperspherical hidden crossing theory has only been applied to three-body systems with Coulomb interactions [8]; thus another aim of this paper is to show that hidden crossing theory does indeed give good results for short range potentials, at least in the region where a is much larger than the nominal range of the potential.

Configuration space for three particles in the center of mass system is six dimensional. Hyperspherical theory uses one coordinate R, with dimension of length, called the *hyperradius*, and five dimensionless angular coordinates. In the adiabatic hyperspherical representation one fixes R and solves the angular part of the Schrödinger equation first to obtain a complete set of adiabatic channel functions and eigenvalues $\varepsilon_n(R)R^2$. The eigenvalues $\varepsilon_n(R)$ are the channel potentials of the hyperspherical close-coupling theory.

Figure 1 shows these channel potentials $\varepsilon_n(R)$ for a simple model of three helium atoms. In this case we have approximated the diatomic interactions between the atoms with a simple Gaussian potential, which was fitted to have the same scattering length, $a = 189.05$ a.u., and effective range, $r_{\text{eff}} = 13.84$ a.u., as the more realistic LM2M2 pair potential [9,10]. It is known that the three-body binding energies using these simple potentials differ by only 20% from those obtained from much more complicated calculations using the full LM2M2 pair potential [10]. This accuracy is sufficient for the purpose of this paper.

The asymptotic value of the lowest potential equals the two-body binding energy $E_0 = -4.15 \times 10^{-9}$ a.u. The lowest channel thus asymptotically corresponds to two atoms bound in a dimer and the third atom far away. The second channel corresponds to a three-body

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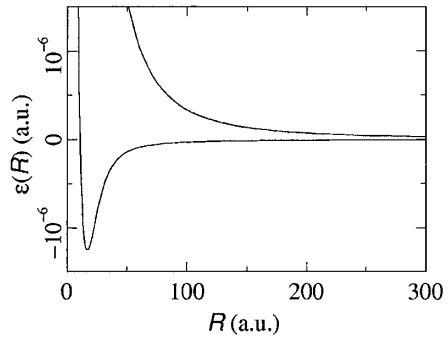

FIG. 1. The adiabatic hyperspherical potentials for three ^{4}He atoms modeled by Gaussian pair potentials. The units are atomic units.

continuum state, i.e., all three atoms are far away from each other. The angular wave function is asymptotically a constant. The second channel contains a centrifugal barrier $\frac{15}{4}R^{-2}$ which is expected to suppress the transition for low energies. The third channel, which we do not use here, contains a centrifugal barrier $(32 + \frac{15}{4})R^{-2}$ which suppresses its contribution at low energies. Similar remarks hold for higher channels.

The S matrix can now be calculated by integrating from the origin and fitting to incoming and outgoing waves at some large hyperradius. This is the traditional coupled channel calculation, which is not often conducive to general insights. From the S matrix, the breakup cross section is calculated by the usual formula,

$$\sigma(B_2 + B \rightarrow 3B) = \frac{\pi}{k^2}|S_{12}|^2, \qquad (1)$$

where k is the wave number of the relative motion between the dimer and the unbound atom before the collision. The rates for recombination depend upon the distributions in the gas or condensate [2,4,11]. We employ the coefficient $\alpha_{\rm rec}$ of Ref. [4]. Rewriting their Eq. (3) in terms of the S_{12} using Eq. (1) and detailed balance gives, in the very low temperature limit where all particles have zero energy, the coefficient

$$\alpha_{\rm rec} = 2(2\pi)^2 3^{3/2} \lim_{E\rightarrow 0} \frac{|S_{12}(E)|^2}{E^2 \frac{m^2}{\hbar^2} a^4} \times \frac{\hbar}{m} a^4, \qquad (2)$$

where the limit can be taken because $|S_{12}(E)|^2 \propto E^2$ at threshold.

Hidden crossing theory is derived using asymptotic approximations [8] which give the WKB form in the complex plane of the coordinate R:

$$\psi(R) = K(R)^{1/2} \exp\left(\pm i \int^R dR' K(R')\right), \qquad (3)$$

where $K(R) = \sqrt{E - \epsilon(R) - 1/(4R^2)}$. The units are chosen such that $\hbar = 1$ and the mass of the atoms is 1. Notice that we include the Langer correction $1/(4R^2)$ in our expression for $K(R)$. This factor emerges automatically in the hidden crossing theory, and is known to be essential for the correct threshold dependence on E. Its use for short-range potentials at energies well above the threshold energy is somewhat questionable, however, for consistency we use the correction at all energies.

It is clear that no transitions can be calculated unless the integration contour can connect different channels. This can be done by extending $\epsilon(R)$ to be a multivalued function in the complex plane which, in the zero-range model, can be done nearly analytically [12]:

$$\epsilon(R) = (\nu^2 - 1/4)/R^2, \qquad (4)$$

where ν is given as the solution(s) to

$$R = a[\nu \cos(\nu\pi/2) - \frac{8}{\sqrt{3}} \sin(\nu\pi/6)]/\sin(\nu\pi/2), \qquad (5)$$

with a being the scattering length of the interaction.

The function $\varepsilon(R)$ is plotted in Fig. 2. There is a square root branch point at $R_b = (2.5918 + 2.9740i)a$. A contour going around this point will go from the lowest surface to the second surface. This is equivalent to a square root which changes sign if continued to a path around its zero in the complex plane. Going around the branch point twice brings the function back to its starting value.

We seek the S-matrix element between the lowest and second channel. Thus the contour starts from $R = +\infty$ on the lowest surface, goes in along the real axis, out into the complex plane, around the branch point and back to the real axis on the second surface. We then integrate up to the classical turning point on the second sheet and out again to $R = +\infty$ with the opposite sign in the exponential. This contour is shown in Fig. 2. This contour, however, is not sufficient. We also need the path which goes around the classical turning point on the first sheet before going around the branch point [8].

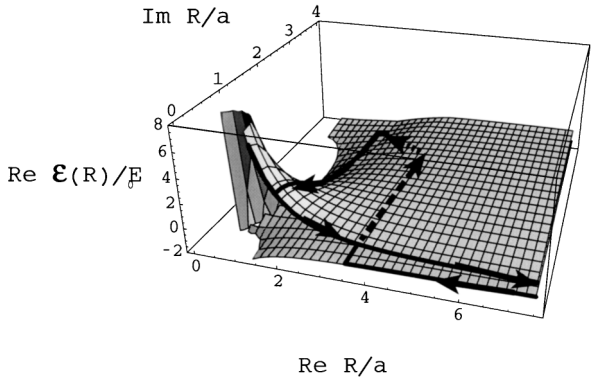

FIG. 2. The complex energy surface for the zero-range model with two-body scattering length a showing a branch point at $R = (2.5918 + 2.9740i)a$. The heavy curve is one of the paths that contribute to the transition probability between the states in the hidden crossing theory.

By adding the two contributions it is seen that the transition probability is given by

$$P(E) = 4\exp(-S)\sin^2(\Delta/2), \tag{6}$$

where

$$S = 2\,\mathrm{Im}\int_c dR\,K(R), \qquad \Delta = 2\,\mathrm{Re}\int_c dR\,K(R), \tag{7}$$

and the contour c goes from the turning point on the lowest sheet, outward along the real axis, around the branch point to the real axis on the second sheet, and then along the real axis to the turning point on the second sheet. The part of the integral along the real axis is real when the turning points occur at distances smaller than the real part of the branch point. Thus, only the part that goes around the branch point to connect the two sheets contributes to S. The quantity Δ can be interpreted as the phase difference between the two paths. At low energies the turning point on the upper surface lies outside the real part of the branch point. In this case we get a contribution that gives rise to the power law near threshold. Note that our expression agrees with standard formulas [13].

For the zero-range model the lowest sheet diverges near $R = 0$ as $-1.26R^{-2}$ [12]; i.e., there is no turning point and the real part of the integral, Δ, diverges. The imaginary part S is, however, finite and can be calculated. Thus the zero-range prediction is

$$P(E) = C_0\exp(-S), \tag{8}$$

where C_0 is some positive number less than 4 but indeterminable by the zero-range model. If one averages over all possible phases Δ, an estimate is $C_0 = 2$, but that is very approximate. To improve Δ we need finite-range potentials to obtain a turning point. If the scattering length is much larger than the range of the potentials, the energy surfaces are approximately the same as for the zero-range model for R much larger than the range of the potentials.

If by some means, for instance, by magnetic fields [1], one adjusts the potentials slightly around the point where the scattering length is infinite, the energy surface does not change very much for small R. In such a variation the low-energy turning point is fixed. Also, the channel potential behaves as $-1.26R^{-2}$ for $R_1 < R < R_2$ between a radius R_1, of the order of the range of the potential, and a radius R_2, of the order of the scattering length [10,12]. The contribution to the phase from the region $R < R_1$ is independent of the tuning as is the contribution from $R_2 < R$ at zero energy. We thus have, at $E = 0$,

$$\Delta = 2\int_{R_1}^{R_2}\sqrt{\frac{1.01}{R^2}}\,dR + D = 2.01\ln\frac{a}{R_1} + \Delta_0, \tag{9}$$

where D and Δ_0 are constants. If the scattering length is tuned as in [1], the zero-energy phase shift behaves as $\ln(a)$ and minima occur as the scattering length increases by integral multiples of $\exp(\pi/1.01)$.

To get a realistic calculation we used the Gaussian model potential of the ^{4}He-^{4}He interaction to compute the energy surfaces along the real axis (Fig. 1), but used the zero-range model off the real axis (Fig. 2) to compute $S(E)$ and a small contribution to Δ. We found that the phase $\Delta/2$ crosses 3π at $E/E_0 = 1.4$. The transition probability has a sharp minimum at this point due to destructive interference between the two paths. This minima is a manifestation of Stuekelberg oscillations known from atom-atom scattering [13].

In Fig. 3 the simple zero-range prediction with $C_0 = 4$ along with the hybrid zero-range and Gaussian model is compared with the coupled channel result for the Gaussian potential model. The hybrid model, including the Langer correction, matches the coupled channel results very well over the whole energy range, except near the Stuekelberg minimum, which is shifted to lower energies. If we omit the Langer correction, the resulting cross section is in error at the lower energies, but gives a surprisingly accurate position of the interference minimum. Removing the Langer correction makes the effective potential more attractive and increases the value of the phase. This increase shifts the minimum to higher energy, in agreement with the coupled channel calculations. It should be noted that there are other contributions to the hidden crossing phases that are sometimes included [13] and would also change the position of the Stuekelberg minimum.

The hidden crossing theory shows that the transition probability factors into two terms, namely, the factor $\exp[-S(E)]$, which depends only upon the scattering length and is a universal function of $E/E_0 = Ea^2$, and the factor $\sin^2\Delta/2$, which depends mainly upon a phase integral along the real axis from the turning point to the real part of the branch point $R_b \approx 2.6a$. The magnitude of this latter function is, therefore, strongly dependent upon the details of the interaction. It is thus not possible to give

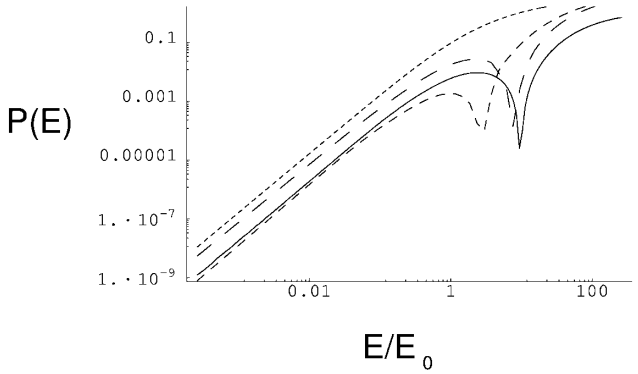

FIG. 3. The transition probability for the reaction ^{4}He + ^{4}He + ^{4}He $\rightarrow$ ^{4}He + ^{4}He$_2$. The solid line is the coupled channel result, the short dashed curve is Eq. (8) with $C_0 = 4$, the intermediate dashed curve is the hidden crossing result [Eq. (6)] with the phase Δ calculated using the potential curves in Fig. (1), and the long dashed curve is with the Langer correction omitted.

a universal expression for the breakup or recombination probability. Clearly, Eq. (8) with $C_0 = 4$ gives an upper bound to the probability for recombination which depends upon a but is otherwise independent of the details of the potentials.

Our expression, Eq. (6), also shows that any cutoff scheme based on a three-body potential redefines Δ and thus redefines the transition probability to any value between 0 and $4\exp(-S)$. That is not to say that a cutoff scheme must fail, but that the cutoff must be compensated by other observables which strongly depend on the position of the classical turning point in the lowest curve, in accordance with the conclusion of Bedaque *et al.* [6].

We can now give $\alpha_{\rm rec}$ of Eq. (2). Almost by inspection it follows from Fig. 3 that $P(E) = A(Ea^2)^2$ with $A \approx 0.018$ and 0.013 for the coupled channel and hybrid models, respectively. Our best estimate is $A \approx 0.018$ so that the recombination coefficient is

$$\alpha_{\rm rec} = 2(2\pi)^2 3\sqrt{3}A\,\frac{\hbar}{m}\,a^4 = 7.386\,\frac{\hbar}{m}\,a^4. \qquad (10)$$

For the zero-range model we can only compute an upper limit since Δ is undefined. We find $A = 0.167$, which is a universal constant independent of the details of the potential. The upper limit on the recombination rate is

$$\alpha_{\rm rec} \leq 68.4\,\frac{\hbar}{m}\,a^4. \qquad (11)$$

This is also an upper limit for realistic interactions, where the scattering length is much larger than the nominal range of the two-body potential since it corresponds to the replacement of $\sin^2(\Delta/2)$ by its maximum value.

Fedichev *et al.* found the rate to be $\alpha_{\rm rec} = 3.9\,\frac{\hbar}{m}\,a^4$ with a much simpler but less transparent model [4]. Their rate is less than our upper limit, as it should be, but is also a factor of 2 smaller than our coupled channel calculations. This disagreement probably reflects the extreme sensitivity of the cross section to the phase, since the phase is close to an integral multiple of π.

For negative scattering length we expect an even stronger dependence upon the shape of the potential. In this case there are no two-body bound states in a zero-range model and the surface will only contain sheets corresponding to three-body channels. Transitions from three-body to two-body states cannot occur in the region of large R where the zero-range model applies but only at small R, where the complex energy surface directly depends upon the shape of two-body potentials. On the lowest sheet corresponding to three-body breakup, however, there is a repulsive barrier at large distance [3]. This repulsive potential behaves as $\frac{15}{4}\,R^{-2}$ which, with the Langer correction, gives a tunneling probability behaving as $m^2\hbar^{-4}a^4E^2$. Therefore the recombination rate will also be proportional to a^4 but the proportionality constant is unknown.

The general behavior of the three-body recombination rate or the breakup probability can be estimated to within a factor of the order of 1 using only the scattering length. However, that factor is given by the sine of a phase which depends on the details of the two-body potentials. In certain cases the factor might even be much smaller than 1 over a small energy range due to Stuekelberg oscillations. This could be important if the minimum occurs near the threshold. But if this phase is calculated on the basis of the more detailed information from the potential, the hidden crossing theory does predict the transition probability very well.

We have used the hidden crossing theory to obtain an upper limit $\alpha_{\rm rec}$ that depends only upon the two-body scattering length when the length is positive and much greater than the nominal range of the potentials. In this sense, one can estimate the effect of tuning the scattering length as in Ref. [1]. The zero-energy phase does depend upon the actual shape of the potentials, but in the region of infinite scattering length it diverges as $\ln(a)$. We have shown that this phase has a profound effect on the magnitude of the recombination rate; thus the phase change must be included in a more complete theory of magnetic tuning of recombination rates.

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