Breakup and Recombination of Identical Bosons: He Dimer-Monomer Collisions

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Abstract.
Three He atoms can react in vapor at temperatures of the order of a few degrees Kelvin to form a dimer and a free atom by three-body collisions. Conversely, the dimer may fragment by collisions with free He atoms. Cross sections and reaction rates for these processes have been computed at milliKelvin temperatures using the hyperspherical hidden crossing theory. At higher energies, of the order of 0.1 to 5 Kelvin, the impulse approximation has been used to estimate these processes. The computed fragmentation cross section is reported.

INTRODUCTION

In the theory of Bose condensates the two-body scattering length a is a fundamental parameter. If it is positive stable, homogeneous condensates can form, but if it is negative they cannot. If a is positive and large, then the bosons usually form a weakly bound dimer with binding energy $E_0 = 1/(2\mu a^2)$, where μ is the reduced mass and atomic units are used. The lifetime of the condensate may be set by the rate for dimer formation. One process that leads to dimer formation is the three-body reaction $B+B+B \to B+B_2$.

The rate for this process may be computed from the cross section for the inverse process $B+B_2 \to B+B+B$ and detailed balance. A prototype for this process is the fragmentation of the He dimer whose binding energy is 1.3 milliKelvin. The threshold region is important for temperatures in the millikelvin range. In this range the quantum theory of the full three-body system is needed for accurate calculations of the fragmentation S-matrix. Three different treatments have been given in the literature(1, 2, 3). The hidden crossing theory of Ref. (1) gives an essentially closed form analytic result and is briefly reviewed in the next section.

At energies much higher than the dimer binding energy, the hidden crossing theory is no longer applicable and a high energy theory is needed. The Born approximation is the most widely known high-energy theory, but it requires that the collision energy be much greater than the interatomic potential. Since the He-He potential has a hard repulsive core, the Born approximation requires collision energies in the keV energy range, well outside of Kelvin range of interest for atomic beams. In this latter range the impulse approximation can be used since it does not require a weak interatomic potential. Rather, it is valid if the dimer binding is much less than the collision energy and the dimensions of the dimer are much larger than the range of the atom-atom interaction. These conditions are satisfied when the scattering length is large compared with the dimensions of the atoms. On that basis impulse approximation calculations for He-He_2 collisions are employed in the $1-10$ Kelvin energy range.

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HIDDEN CROSSING THEORY

The hyperspherical close-coupling approximation(4) maps the full three-body problem onto two-body-like Schrödinger equations. Near the threshold for the fragmentation process, an analytic representation of the cross section has been found using the hidden crossing theory(1). The hidden crossing theory gives

$$\sigma(E) = \frac{\pi}{k^2}\exp[-S(E)]\sin^2\Delta(E) \qquad (1)$$

where $S(E)$ and $\Delta(E)$ are the real and imaginary part of a WKB-like phase integral

$$\Delta(E) + iS(E)/2 = \int_{R_1}^{R_2} K(R)dR. \tag{2}$$

In the above equation, R is the hyper-radius, $K(R)$ is the local wave vector in the hyperspherical adiabatic representation, and the integral is taken along a contour in the complex plane connecting the zero of $K(R)$ in the dimer channel at R_1 with the zero in the fragmentation channel at R_2. This theory gives a fragmentation cross section proportional to a^4 times an oscillatory factor $\sin^2\Delta(E)$.

The oscillatory factor plays an important role in setting the magnitude of the threshold cross section, but we may take it to be a constant for sufficiently small E. The remaining factors are proportional to the E^2 Wigner threshold factor and an a^4 scale factor. We find

$$\sigma(E) = \frac{4\pi\mu^2}{k^2} A E^2 a^4 \sin^2(s_0 \ln(a/R_0) + \Delta_0) \tag{3}$$

where $A = 0.167$, $s_0 = 1.006$, and R_0 and Δ_0 are constants.

The a^4 factor is not immediately obvious; rather an a^2 dependence is expected on the basis of an impulse approximation argument. In this approximation the cross section for dimer breakup is just double the cross section for elastic scattering of two He atoms, equal to $4\pi a^2$ at low energies. To reconcile these two different powers of a, note that it is the cross section averaged over an energy of the order of the binding energy E_0 of the dimer that should have an intuitive dependence upon a. One finds that E^2a^4 averages to $1/E_0 \propto a^2$; thus the expected a^2 dependence is recovered.

IMPULSE APPROXIMATION

Of course, we note that the impulse approximation is only qualitatively correct in the threshold region, and one must rely upon more advanced three-body theories for quantitative results. At higher energies, for example, the 1-5 Kelvin range of interest for gases undergoing expansion(6), the impulse approximation is actually well justified. Because an energy of 1 Kelvin is 10,000 times larger than the dimer binding, this binding may be neglected in collisions with other He atoms. Also, the dimer is about 10 times larger than the nominal range of the He-He potential, so for atom wavelengths much less than the size of the dimer, one can consider that collisions with the dimer are effectively collisions with individual He atoms. If a collision takes place, the dimer breaks up with almost unit probability. In this case the impulse approximation cross section for breakup is just twice the He-He elastic

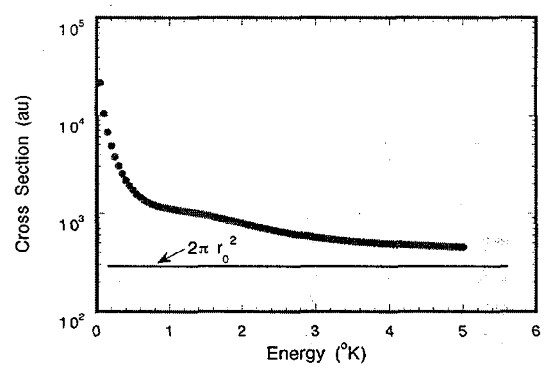

FIGURE 1. Cross section for the process $He + He_2 \rightarrow He + He + He$ in the impulse approximation. The horizontal line corresponds to the limit cross section for the hard core of the He-He potential with $r_0 = 4.5au$.

scattering cross section at the same relative velocity. That is,

$$\sigma_{\text{breakup}}(E) = 2\sigma^{(2)}_{\text{elas}}(E). \tag{4}$$

We have computed $2\sigma^{(2)}_{\text{elas}}(E)$ by numerical solution of the Schrödinger equation for He-He scattering. We use a Morse potential chosen to fit the depth D, the radius $r_{\min}$ of the potential minimum, and the s-wave scattering length a from the standard LM2M2 potential of Aziz *et al.* The fit is very good over most of the range; however, the potential core is somewhat softer than for the Aziz potential. We find, for example, that the classical turning point for energies of 1 Kelvin is about 0.1 au smaller for the Morse potential than for the Aziz potential. This may affect cross sections by amounts of the order of 5%.

The Schrödinger equation was solved for the elastic scattering phase shifts in a partial wave expansion. Phase shifts for $\ell = 0,\ 1,\ 2$ and 3 were computed for energies between 0.05 and 5 Kelvin. The first three partial waves gave significant contributions, while the $\ell = 3$ contribution was negligible but was included for completeness. The computed breakup cross section is shown in Fig. 1.

Three features are apparent in Fig. 1. First there is the rapid rise toward low energies. This rise is mainly due to the s-wave component since it approaches $8\pi a^2$ with $a \approx 187au$. A shoulder in the intermediate energy region near 1-2 Kelvin is a second noticeable feature. This is due to a top-of-barrier p-wave resonance. For this resonance, the phase shift increases to $\pi/4$, then begins to decrease with increasing energy giving the slight bump seen in the figure. A third feature is the flat region above 3 K. In this region the two-body elastic cross section has the same order of magnitude as πr_0^2 where r_0 is the distance at which the depth of the potential equals the incident energy. One expects that the cross section will decrease slowly from this value to πr_T^2 at high energies, where r_T is the range of the hard inner core. In the present case this range is equal to $r_T = 4.5au$.

The cross section shown in Fig. 1 complements the low-energy hyperspherical and effective field theory calculations applicable at threshold. At the lowest energy ($E = 0.05K$) in the figure, the wavelength of Schrödinger wave for the He atom is of the order of the dimensions of the dimer and the impulse approximation ceases to be quantitatively accurate. Improved estimates could be obtained by adapting the impulse approximation amplitude given in the book by Mott and Massey(7) to the case of three identical particles. Using that amplitude would account for features, such as coherent scattering from the atoms in the dimer and energy shifts owing to the dimer binding, neglected in the simple expression Eq. (4). These corrections would be needed to connect with the threshold cross section. Even without these corrections, the cross section at 1.3×10^{-3} K from the hidden crossing theory neglecting the oscillatory factor is of the order of 10^4 au, in modest agreement with the value of $\sigma = 2^4$ au at $E = 50\times10^{-3}$ K from the impulse approximation.

SUMMARY

We have computed the cross section for $He + He_2 \rightarrow He + He + He$ in the impulse approximation applicable in the $1-5$ Kelvin energy range. Prominent features of the cross section are interpreted in terms of the expected behavior of the $\ell = 0$ and 1 partial waves.

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