

### Exact Determination of the bbb Incoming State for Recombination in H ↓

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We present the exact three-body wavefunction of the bbb incoming state, needed to determine the rate of recombination in H ↓. Comparisons are made with the wavefunction of Kagan.

In the last few years, further progress in the stabilization and compression of atomic hydrogen in helium covered sample cells has been retarded by the appearance of three-body dipolar recombination. Therefore, it is important that the recombination mechanism is understood. So far, simple approaches [1,2] to describe the process have not succeeded to reproduce the experimentally observed magnetic field dependence of the rate constant. In this contribution, we make a first attempt to resolve the discrepancy for volume recombination by means of a more exact approach.

As shown in Fig. 1, we use Jacobi coordinates  $\underline{r}$  and  $\underline{R}$ . Furthermore, we introduce the angle  $\theta$  between the vectors  $\underline{r}$  and  $\underline{R}$ . The transition probability can be described with an amplitude  $f$ , which is essentially a matrixelement of the summed dipole interactions  $V_{ij}^d$ :

$$f = \frac{2}{2\pi\hbar^2} \langle \psi_f^{(-)} | \sum_{i < j} V_{ij}^d | S\psi_i^{(+)} \rangle. \quad (1)$$

The dipole interactions, treated in first order because of their extreme weakness, cause the transition from the symmetrized incoming state  $|S\psi_i^{(+)}\rangle$  to the outgoing atom-molecule state  $|\psi_f^{(-)}\rangle$ . In  $|S\psi_i^{(+)}\rangle$  and  $|\psi_f^{(-)}\rangle$  the singlet- and triplet-interactions have in principle to be taken into account up to all orders.

In previously presented calculations, both these exact initial and final state wavefunctions are substituted by simple approximations. In this contribution we follow the same procedure for the final state: we neglect atom-molecule interactions. Therefore, the dipole-exchange mechanism [2] and possible more complicated mechanisms are left out of consideration.

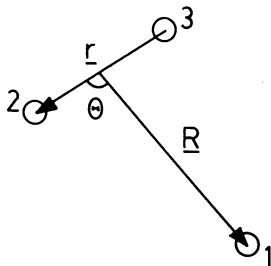


Fig. 1 The Jacobi coordinates.

In the initial state wavefunction, however, all three-particle correlations are taken into account in an exact way. This is achieved by solving the Faddeev equation [2,3] for  $|S\psi_i^{(+)}\rangle$  in three-particle (angular) momentum space. This space is most convenient for T=0 calculations because only the total orbital angular momentum L=0 contributes. Furthermore, we only need a few partial waves to describe the  $\theta$  dependence of the

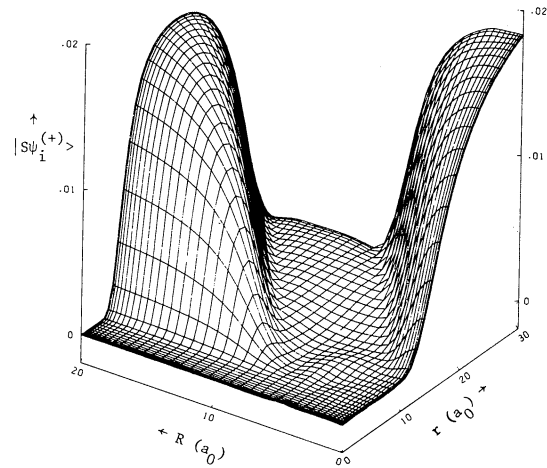


Fig. 2 The exact initial state wavefunction as a function of r and R for  $\theta=0$ .

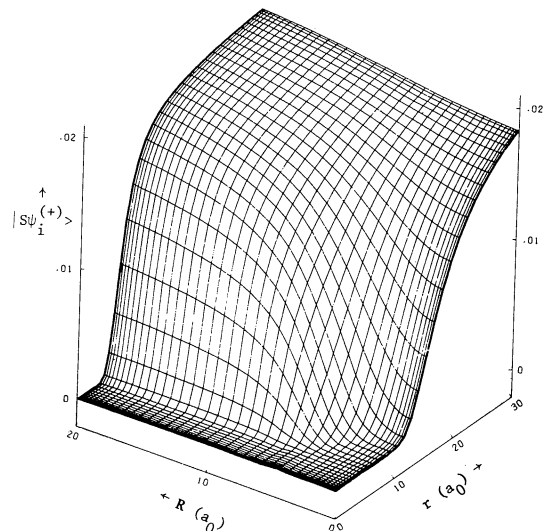


Fig. 3 The exact initial state wavefunction as a function of r and R for  $\theta=\pi/2$ .

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solution of the Faddeev equation. Numerically this equation reduces to a matrix equation of dimension  $\approx 7000$ . We subsequently obtain the wavefunction in coordinate space by means of Fourier transformation. In Figs. 2 and 3 we plot it as a function of  $r$  and  $R$  for  $\theta=0$  and  $\theta=\pi/2$ , respectively. We observe that the wavefunction is zero for  $r \leq 6a_0$  in both cases, which is caused by the strongly repulsive character of the triplet interaction for small distances between particles 2 and 3. This effect can also be seen in Fig. 2 for  $\theta=0$ , when the distance between 1 and 2  $|\underline{R}-\frac{1}{2}\underline{r}| \leq 6a_0$ . Furthermore,  $|\psi_i^{(+)}\rangle$  approaches the zero temperature symmetrized free wave function  $6/(2\pi\hbar)^3$  for large distances.

Confrontation of the exact wavefunction with Kagan's initial state shows an astonishing similarity. In the latter approach only correlations between the recombining pair 2-3 and the dipole pair (e.g. pair 1-2) are incorporated by means of a product of pair wavefunctions. Kagan's approximation appears to be valid for the complete three-particle configuration space, except for the part  $|\underline{R}+\frac{1}{2}\underline{r}| \leq 10a_0$ , where particles 1 and 3 are close together. Apparently, this part plays a minor role in the calculation of the rate constant. An essential element in understanding the effectiveness of Kagan's approach can also be found in the zero-temperature approximation. This causes the relative wavefunctions to "heal" within small distances. In a way the atoms behave as transparent objects, except for very small

distances. We further note that because of the boson character of H-atoms, the wavefunction should consist of even partial waves only. However, since the orbital part of the initial state of Kagan is not symmetric under particle permutations, also unphysical odd partial waves are present.

The computation of the rate constant with the exact initial state, leads to results which still display the wrong field dependence and differ by no more than 40% from Kagan's results. This illustrates the degree of accuracy of Kagan's approach.

Therefore we can conclude that the reason of the discrepancy with experiment has to be found in the final state. This is probably also true for the case of surface recombination. A better treatment of the atom-molecule correlations in the final state is therefore the aim of further calculations [3].

#### REFERENCES

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