# Spin-polarized atomic hydrogen in very strong magnetic fields

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(Received 4 May 1988)

We calculate the effective rate constant for three-body dipolar recombination of spin-polarized atomic hydrogen in conditions of high density and very high magnetic field strengths (beyond the < 10-T range of previous calculations). We find that the decay of the gas sample is not sufficiently suppressed at magnetic fields available in the forseeable future.

## I. INTRODUCTION

In the past several years intense experimental efforts have been going on to produce atomic hydrogen in a state of Bose-Einstein condensation (BEC), all of which have been thwarted by the presence of a rather large rate for recombination into a molecular state via three-body collisions.[1] In one of the experiments, for instance, the highest density achieved at $T=550$ mK was $4.5\times10^{18}$ $\mathrm{cm}^{-3}$, an order of magnitude lower than the critical density at this temperature. Various ingenious schemes have been proposed to avoid this problem: wall-free confinement of the hydrogen atoms,[2] or more recently the possibility of applying microwave cooling to lower the temperature and thus lower the densities needed to arrive at the condensation regime.[3]

Another line of investigation continues the high-density approach, but aims at suppressing the three-body recombination by substantially increasing the magnetic field above values used in earlier studies.[4] Simple models[5,6,7] predict the decay of the gas to fall sharply at $B\simeq27$ T and at $B\simeq54$ T. More recent calculations[8] for fields $B<10$ T, relaxing some of the rough approximations in the earlier simple models, led to considerable corrections in this lower field range. It is therefore of interest to see whether minima at 27 or 54 T might be even lower on the basis of our more exact method, so as to be promising from the point of view of reaching BEC. The purpose of the present paper is to extend these calculations to higher fields. Our main conclusion is that recombination is not sufficiently suppressed at magnetic fields achievable in the foreseeable future: small enough rates occur only at magnetic fields as strong as 140 T.

In the following sections we shall describe our method of calculation and its results, followed by our interpretation of the main features and some conclusions.

## II. METHOD

In the zero-temperature limit and to first order in the (electron-electron) magnetic-dipole part $V_{ij}^d$ of the H-H interaction, the three-body rate constant is given by[7]

$$L_g=\frac{(2\pi)^7\hbar^5 m_{\mathrm{H}}}{9}\sum_f q_f\int d\hat{q}_f\left|\left\langle\Psi_f^{(-)}\middle|\sum_{\substack{i,j\\ i<j}}V_{ij}^d\middle|\mathcal{S}\Psi_i^{(+)}\right\rangle\right|^2 , \quad (1)$$

where $m_{\mathrm{H}}$ is the hydrogen mass and the summation is over all possible ortho-$H_2$ states that can be formed on the basis of energy conservation. Furthermore, the fully symmetrized initial state $|\mathcal{S}\Psi_i^{(+)}\rangle$ is associated with the scattering of three incoming electron spin-down H atoms, while the final state $|\Psi_f^{(-)}\rangle$ describes the time reversed collision of an atom (electron spin up or down) with a molecule with relative momentum $\mathbf{q}_f$. Both states are normalized as in Ref. 7 and obey the three-particle Schrödinger equation with all central (singlet or triplet) interactions between the atoms included. Depending on the above-mentioned spin orientation of the final single atom parallel or antiparallel to $\mathbf{B}$, $L_g$ is usually indicated as a single or double spin flip rate. Assuming the spin-flipped (SF) atom to recombine rapidly upon collision with an electron spin down atom,[1] the effective rate constant is

$$L_g^{\mathrm{eff}}(B)=L_g^{\mathrm{1SF}}(B)+2L_g^{\mathrm{2SF}}(B) ,$$
$$L_g^{\mathrm{2SF}}(B)=4L_g^{\mathrm{1SF}}(2B) . \quad (2)$$

In order to facilitate the analysis of experiments under less restrictive assumptions we present in Sec. III not only results for $L_g^{\mathrm{eff}}$, but also for the ratio $L_g^{\mathrm{2SF}}/(L_g^{\mathrm{1SF}}+L_g^{\mathrm{2SF}})$, i.e., the probability that after a three-body event the outgoing atom has electron spin up. Our calculation is based on the zero-temperature limit, since the bulk recombination rate is expected to have a weak temperature dependence. In the context of a zero temperature calculation, $L_g^{\mathrm{eff}}$ is also the effective rate constant for the dipolar part of *abb*, *aab*, and *aaa* recombination.

The initial state $|\mathcal{S}\Psi_i^{(+)}\rangle$ in Eq. (1) is calculated using an exact Faddeev-like approach.[8] The exact calculation of the final state $|\Psi_f^{(-)}\rangle$ is practically impossible with present computer capacities. Kagan[5] used a plane-wave description for the relative atom-molecule motion. We use a method in which all (in)elastic atom-molecule interactions are taken into account, but we neglect rearrangement of atoms. The latter appears to be essential to describe the three-body process at lower fields (the so-called dipole-exchange mechanism[6,7]), but on the basis of simple models[7] is expected to fall off rapidly with increasing field.

To be more precise about the approximations involved in the final state we give a short summary, referring to Ref. 8 for a more extensive treatment.[9] In a time-reversed picture the atom collides with a molecule in an excited rotation-vibration state (at lower magnetic fields primarily the $v=14$, $j=3$ state) and (de)excites it during the collision to, in principle, all other $(v,j)$ states. Whereas the total orbital angular momentum $\mathbf{L}$ of the three-body system is conserved, the relative orbital angular momentum $\boldsymbol{\lambda}$ between the single atom and molecule can change, the interaction being anisotropic. This results in the (coupled-channels) Schrödinger equation

$$\left[\frac{\hbar^2}{2\mu}\frac{d^2}{dR^2}+\frac{\lambda(\lambda+1)\hbar^2}{2\mu R^2}+V^{L\pi}_{vj\lambda,vj\lambda}(R)+\varepsilon_{vj}-E\right]f^{L\pi}_{vj\lambda}(R)=-\sum_{v'l'\lambda'(\neq vl\lambda)}V^{L\pi}_{vj\lambda,v'j'\lambda'}(R)f^{L\pi}_{v'j'\lambda'}(R) \quad (3)$$

for the relative motion with reduced mass $\mu=2m_H/3$ and rotation-vibration energy $\varepsilon_{vj}$. For each fixed $L$ and parity $\pi$ the potential $V^{L\pi}$ couples all channels obeying $|j-L|\le\lambda\le j+L$ with $j$ odd and $(-1)^\lambda=-\pi$.

After a transformation to a momentum space Lippmann-Schwinger equation and a numerical discretization, the solution is found by matrix inversion. To obtain a converged result for the rate constant $L_g^{\text{eff}}$ we had to include all rotational levels belonging to the $v=13$ and 14 vibrational levels. Hence a total of 16 channels are involved in the calculation although only the final states $|\Psi_f^{(-)}\rangle$ corresponding to the $(v,j)=(14,1)$, (14,3) and (13,5) outgoing channels contribute substantially to the rate in the magnetic-field range studied.

## III. RESULTS

In Figs. 1 and 2 we present our results for $L_g^{\text{eff}}$ and compare with the Kagan model. In addition, the single and double spin-flip field ranges have been indicated for the (14,3) and (14,1) molecular states. In Fig. 1 we clearly see the repetitive structure as a function of $B$. The (14,3) double spin-flip maximum around 15 T is followed by a

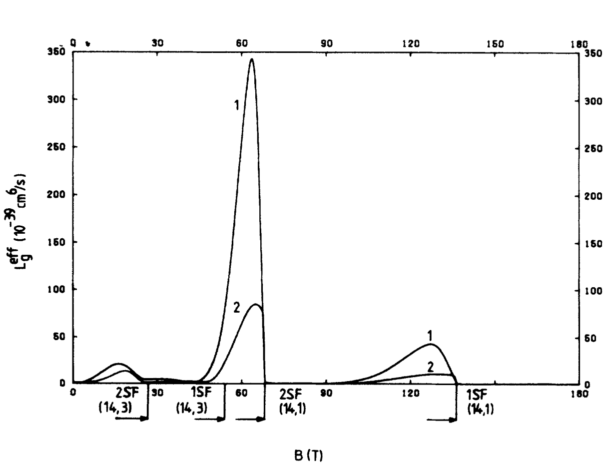


FIG. 1. Effective decay rate $L_g^{\text{eff}}$ as a function of the applied magnetic field [(1) Kagan's model and (2) this work]. Also indicated are the single and double spin-flip cutoff fields for the bound states (14,3) and (14,1).

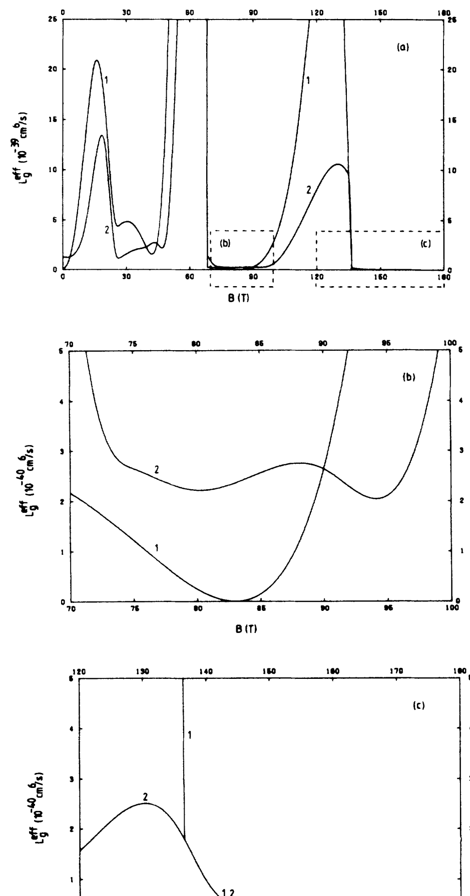


FIG. 2. A more detailed study of the magnetic field dependence of $L_g^{\text{eff}}$: (a) Shows $L_g^{\text{eff}}$ on an expanded vertical scale, which displays more clearly the complicated structure of the rate constant in the case of (1) Kagan's model and (2) our approach. (b) An enlargement of the region around 83 T, where the Kagan model predicts the rate constant to be zero. This zero is removed in our calculations. (c) Shows the region beyond the single spin-flip cutoff of the (14,1) bound state [(1): The decay rate $L_g^{\text{eff}}$ and (2): the partial contribution from the (13,5) bound state]. For magnetic fields $B>136.4$ T Kagan's rate constant is negligible and invisible on this scale.

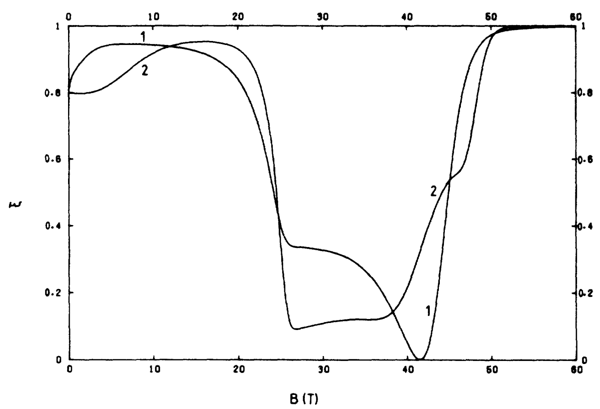


FIG. 3. The probability $\xi$ for a double spin-flip event as a function of magnetic field [(1) Kagan's model and (2) this work].

lower single spin-flip maximum at about 30 T. A more pronounced (14,1) double spin-flip peak near 60 T is followed by a less pronounced single spin-flip peak near 120 T. Note the strong formation probability of the (14,1) state for $B$ smaller than 68.2 T. The (14,3) maxima are much lower due to the higher rotational angular momentum that the dipolar interaction has to introduce into a two-atom subsystem starting from a situation of vanishing relative orbital angular momenta in the initial state.

A general feature, evident from the behavior of $L_g^{\text{eff}}$, is the decrease of our values compared to Kagan's by a factor of about 3, especially on the low-$B$ side of each of the maxima. This is due to the inclusion of correlations between the particles in both the initial and final states. These correlations cause the three-body wave function to be zero in all parts of configuration space where two or three atoms are close together and therefore reduce the transition probability. Clearly, the reduction is expected to be less on the high-$B$, i.e., low-$q_f$ side: the centrifugal barrier in the final channel then by itself already keeps the final atom out of the forbidden region. Hence the Kagan model should then be an excellent approximation. This is indeed borne out by our calculations. In particular, the partial $(v,j)$ contributions to $L_g^{\text{eff}}$ show the $(B_0-B)^{j+1/2}$ behavior on the high-$B$ side of each of the maxima, that also follows from the Kagan approach. It should be noted, however, that from the point of view of BEC one is more interested in $B$ values where $L_g^{\text{eff}}$ is small. There the deviations from Kagan's model are considerable. Close to 27 T the rate is relatively small, but not small enough to be promising. At 83 T the Kagan (14,1) rate goes through zero. This potentially interesting $B$ value is unfortunately eliminated by our calculation [see Fig. 2(b)]. The decay time of the atomic density due to recombination varying with $n_H^2$, an increase of the density by a factor of 10 with respect to the above-mentioned experiment,[1] would require $L_g^{\text{eff}}$ to be as small as $10^{-40}$ cm$^6$/s. It follows from Fig. 2(c) that such values occur only above 140 T. Notwithstanding the recent developments with respect to high-$T_c$ superconductivity,[10] this field region is practically of little importance in the foreseeable future. Nevertheless, from the point of view of interaction mechanisms it is interesting to point out that the Kagan model predicts a negligible rate beyond 136.4 T. This is indeed what one would expect in the first instance, because the only possible final $H_2$ states in that region are the more strongly bound $v=13$ states. Figure 2(c) shows, however, larger $L_g^{\text{eff}}$ values according to our calculations, due to indirect population of the (13,5) state via a strong coupling to the closed (14,1) channel which, as pointed out above, are strongly populated directly from the initial state.

For experimental purposes we also give in Fig.3 the ratio between $L_g^{2\text{SF}}$ and $L_g^{1\text{SF}}+L_g^{2\text{SF}}$, denoted by $\xi$. This quantity is of importance in the analysis of the experimental data, if one wants to include the possibility of relaxation of the electron spin-up atom that is produced in the double spin-flip process. As previously noted, we neglect this possibility in the definition of $L_g^{\text{eff}}$ and assume that the $|c\rangle$ or $|d\rangle$ atom recombines with an $|a\rangle$ or $|b\rangle$ state particle on the helium surface. We find that the field dependence of $\xi$ is almost linear in the range $5\text{T} \le B \le 10$ T, where most of the experiments until now have been carried out. In this range Kagan predicts $\xi$ to be a constant equal to 0.93. Experimentally this value is always used to describe the decay of the gas sample due to three-body recombination.[1,11]

## IV. CONCLUSIONS

We have studied the prospects for producing atomic hydrogen in a state of Bose-Einstein condensation at high magnetic fields, where the effects of rearrangement (the dipole-exchange mechanism) are expected to be negligible. The calculations include all three-atom correlations in the spin-polarized initial state, as well as the elastic and inelastic distortions of the atom plus molecule final state. The single and double spin flip bumps in a partial $(v,j)$ contribution to the rate constant show agreement with Kagan's model at the high-$B$ (low-$q_f$) slope, due to the centrifugal effect. At the low-$B$ (high-$q_f$) slope our values are smaller by a factor of about 3. From the point of view of BEC, ranges of $B$ with a small rate value are of importance. There the relative deviations from Kagan are considerable. Despite the difference no sufficiently small rate is found near 27 T and 54 T. A zero $L_g^{\text{eff}}$ value at about 83 T according to Kagan's model turns into a too large rate constant on the basis of our calculation. Recombination is sufficiently suppressed only at fields stronger than 140 T.

## ACKNOWLEDGMENT

This research is supported by the Stichting ZWO (Werkgroep Gebruik Supercomputers).

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