

Collisions between cold ground-state Na atoms

E. Tiesinga, S. J. M. Kuppens, B. J. Verhaar, and H. T. C. Stoof

Department of Physics, Eindhoven University of Technology, 5600 MB Eindhoven, The Netherlands

(Received 14 January 1991)

We study hyperfine transitions in collisions between cold ground-state ^{23}Na atoms, which are of crucial importance for the decay of the atomic density in magnetic traps. For comparable densities we find the initial decay by exchange collisions to be roughly a factor of 10 more rapid than that in atomic hydrogen. The doubly polarized atomic gas that thus forms spontaneously in this initial process subsequently decays by dipolar relaxation with a rate that is about a factor of 5 larger than that in atomic hydrogen. The sensitivity of the calculated rate constants associated with uncertainties in the singlet and triplet potentials is discussed.

In the last few years a rapid development has taken place in the field of cold atoms. As a result of this, fascinating possibilities now come into view, such as the realization of Bose-Einstein condensation in H gas and gases of heavier bosonic atoms,¹ the study of a gas of anti-H atoms,² studies of quantum reflection against surfaces,³ and the realization of an ultrastable cesium atomic clock by means of an atomic fountain.⁴

The atomic densities in some of these experiments are increasing presently to the point where collisions between atoms are of great importance, both in determining the lifetime of a trapped gas sample and in determining the frequency stability of the proposed new atomic clock. Collisions between cold atoms are also of interest in their own right, due to the occurrence of very unusual energy, time, and distance scales. Recent studies⁵ show, for instance, that the collision between an optically excited atom and a ground-state atom proceeds differently due to the fact that the probability of spontaneous emission during a collision approaches unity, so that this process can no longer be treated as a small perturbation on the collision and has to be included in a more fundamental way. Another interesting aspect of cold collisions is the long de Broglie wavelengths involved. This leads to typical quantum effects such as the inapplicability of the semiclassical Landau-Zener theory for avoided crossings and the increased stability of doubly polarized atomic deuterium gas due to the exclusion principle.⁶

Some time ago we presented theoretical predictions⁷⁻⁹ for hyperfine changing collisions between cold H atoms, which turned out to be of crucial significance both from the point of view of loss mechanisms from magnetic traps^{10,11} and for the frequency stability of the subkelvin hydrogen maser.¹² The purpose of this paper is to study similar processes for ground-state ^{23}Na atoms. We refer to Ref. 1 for a general review of atom traps, which underlines in particular the importance of the calculations to be presented below for the estimation of loss mechanisms. After summarizing our method of calculation, we present spin-exchange and magnetic dipole relaxation rates, associated with transitions from trapping to antitrapping hyperfine states in magnetic traps.

We use the effective Hamiltonian⁸

$$H = \frac{\mathbf{p}^2}{2\mu} + \sum_{i=1}^2 V_i^{\text{hf}} + \sum_{i=1}^2 V_i^Z + V^c + V^d \quad (1)$$

with hyperfine and Zeeman terms

$$V^{\text{hf}} = \frac{a}{\hbar^2} \mathbf{S}^e \cdot \mathbf{S}^N, \quad V^Z = (\gamma_e S_z^e - \gamma_N S_z^N) B \quad (2)$$

for each of the atoms, a central interaction

$$V^c = V_0(r)P_0 + V_1(r)P_1, \quad (3)$$

comprising singlet and triplet terms with P_0 and P_1 denoting projection operators on the singlet and triplet subspaces, and a magnetic dipole interaction V^d consisting of electron-electron and electron-nuclear parts. In the following the ^{23}Na atomic hyperfine states are labeled 1-8 in order of increasing energy (see Fig. 1).

On the basis of its symmetry under separate orbital and spin rotations V^c induces so-called spin-exchange transitions that conserve the relative orbital quantum numbers l and m_l and the total spin projection M_F . The influence of V^d on such transitions is negligible. The remaining, dipolar, transitions are dominated by first-order V^d contributions.

For the singlet and triplet potentials we have used spectroscopically determined Rydberg-Klein-Rees (RKR) potentials¹³⁻¹⁵ for interatomic separations between the classical turning points for the highest observed rotational and vibrational states. For small distances an $a + b/r$ extrapolation is sufficiently accurate in view of the smallness of the radial interval accessible to very-low-energy atoms in that region. At large distances an extrapolation is made by means of experimental¹⁴ and theoretical¹⁶ information on the induced multipole potentials.

Coupled equations in the SM_SIM_I basis (\mathbf{S} =total electron spin, \mathbf{I} =total nuclear spin) are rigorously solved up to a radius r_0 beyond which the central interaction is negligible. A value as large as $300a_0$ is usually required, compared to about $40a_0$ for the H+H collision problem. The S matrix calculated at r_0 is transformed to the hyperfine basis and supplemented with an additional contribution from the interval $r > r_0$ due to V^d , calculated in

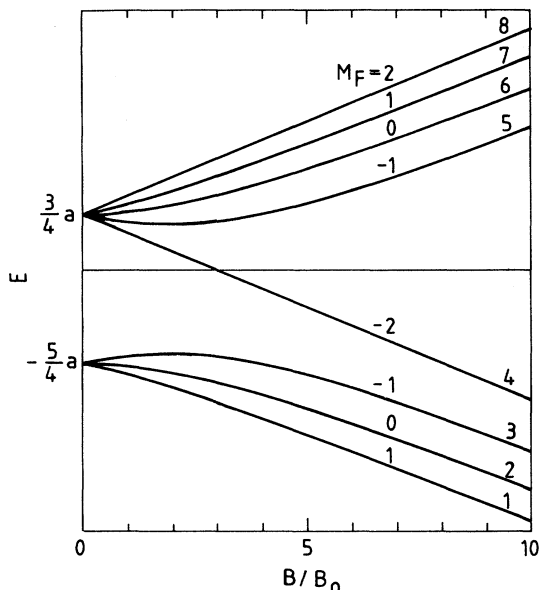


FIG. 1. Energies of the ^{23}Na hyperfine states as a function of magnetic field. a is the hyperfine constant and $B_0 = a/\hbar\gamma_e = 0.0316$ T.

first order. Shifting r_0 to larger values only affects the total S matrix at the 0.1% level. This shows the applicability of the first-order treatment for $r > r_0$ and at the same time provides a strong check on the consistency of the method of calculation. It is noteworthy that higher-order effects in V^d in the inner region are not as small as in the case of H, affecting the final dipolar cross sections at the 10% level.

The low temperatures of interest experimentally permit us to carry out a calculation in the $T=0$ limit. This implies an initial l value of 0. Even with this restriction the total number of two-body spin channels to be considered is 36. The total number of possible transitions is 410. In view of this complexity the use of computer algebra in dealing with the spin structure proved to be almost indispensable. A more-detailed description of our method and a more complete presentation of results is to be given elsewhere. Here we select some transitions to illustrate the general features and orders of magnitude.

In Fig. 2 we present the $T=0$ relaxation rate constants for all exchange transitions proceeding from the $\{67\}$ symmetrized spin channel as a function of magnetic field. Here, 6 and 7 represent the hyperfine states of atoms 1 and 2. Compared to the exchange rates in atomic hydrogen the present rates are about a factor of 10 larger.

It turns out that our coupled-channel ^{23}Na exchange rates can be rather accurately reproduced by a simpler approach in the spirit of R -matrix theory¹⁷ or multichannel quantum defect theory,¹⁸ in which we assume degenerate internal states⁸ within a certain interatomic distance r_1 and make use of the smallness of the exchange potential $V_0 - V_1$ beyond that distance by treating it in first order. The $\{67\} \rightarrow \{58\}$ rate goes to zero for $B \rightarrow 0$ due to the approach to the reaction threshold in the final channel. For strong B fields the rates turn out to decrease roughly ac-

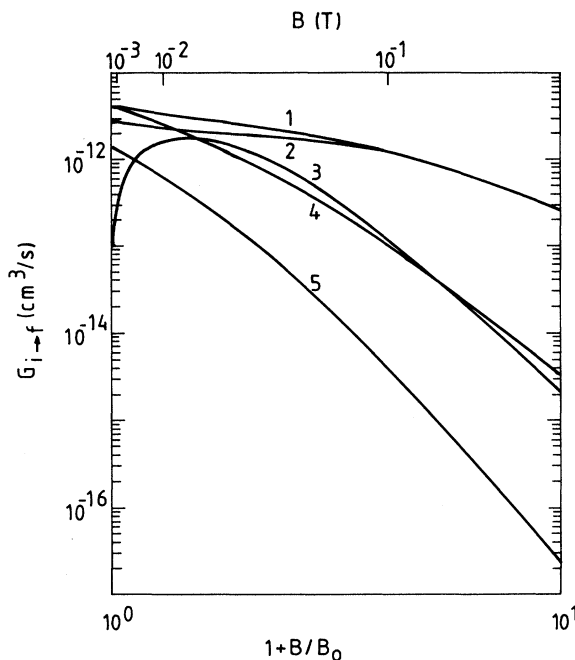


FIG. 2. $T=0$ spin-exchange relaxation rates $G_{i \rightarrow f}$ as a function of magnetic field. The lower horizontal scale shows $1+B/B_0$ logarithmically. The upper scale shows corresponding values for B . The curves correspond to the following rates: (1) $\{67\} \rightarrow \{16\}$, (2) $\{67\} \rightarrow \{38\}$, (3) $\{67\} \rightarrow \{58\}$, (4) $\{67\} \rightarrow \{12\}$, (5) $\{67\} \rightarrow \{27\}$.

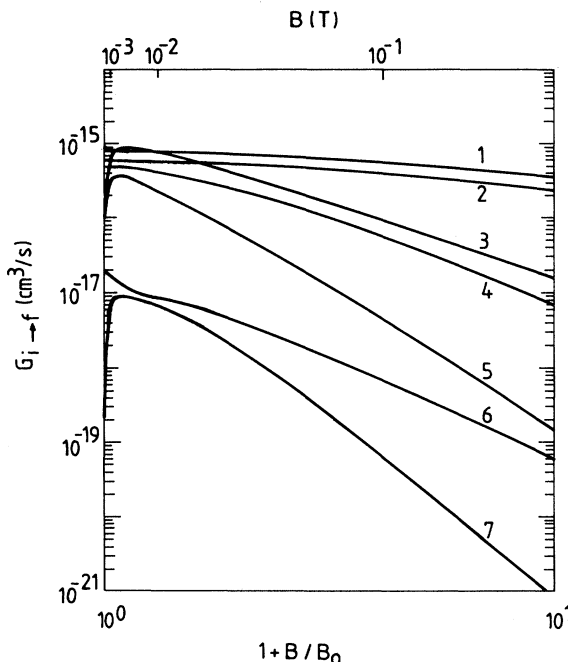


FIG. 3. $T=0$ dipolar relaxation rates $G_{i \rightarrow f}$ for the doubly polarized ^{23}Na gas as a function of magnetic field. Horizontal scales as in Fig. 2. Curves correspond to following rates: (1) $\{88\} \rightarrow \{11\}$, (2) $\{88\} \rightarrow \{18\}$, (3) $\{88\} \rightarrow \{78\}$, (4) $\{88\} \rightarrow \{17\}$, (5) $\{88\} \rightarrow \{77\}$, (6) $\{88\} \rightarrow \{28\}$, (7) $\{88\} \rightarrow \{68\}$.

ording to inverse powers $1/B^{2n}$ with n being the change in asymptotic nuclear magnetic quantum number involved in the transition. This decrease is primarily due to the spin-dependent factor in the transition element and much less due to the spatial part.

In Fig. 3 we present our results for the most important $T=0$ dipolar rates, i.e., those depopulating the doubly polarized 8 hyperfine level. As for atomic hydrogen these rates are dominated by the (pure triplet) electron-electron dipolar part, except for $\Delta M_I \neq 0$ transitions at strong fields where the electron-nuclear part becomes comparable. In this case we find the dominant rates to be roughly a factor of 5 larger than for atomic hydrogen. Another noteworthy difference relates to the applicability of the plane-wave approximation to the dipolar rates: In the case of atomic hydrogen the much simpler plane-wave calculation was sufficiently accurate to estimate the rates to within a few tens of a percent. For a heavier atom such as Na the error would be as large as almost 2 orders of magnitude. The explanation for this remarkable difference is the much longer range of the van der Waals interaction combined with the shorter local de Broglie wavelength of a heavier atom. For the same reason as above the $\{88\} \rightarrow \{78\}$, $\{77\}$, and $\{68\}$ rates go to zero for small B . The

dipolar rates also show the above-mentioned $1/B^{2n}$ spin-dependent decrease for strong B .

A point of interest is the uncertainty of the calculated rates due to the inaccuracy of the singlet and triplet potentials. By varying the potentials within the range of their uncertainty it is possible to obtain insight into the reliability of the rates. From a number of such calculations we found the dominant exchange rates to be uncertain by at most 10% and the dominant dipolar rates by at most 5%.

From our results we expect a magnetic trap filled with low-field-seeking ^{23}Na atoms to change into a doubly polarized 8-state atom trap in a time of order $1/(G^{\text{exch}}n) \approx 10^{11} \text{ sec}/(n \text{ cm}^3)$. The density of the latter decays on the much longer time scale given by $1/(G^{\text{dip}}n) \approx 3 \times 10^{14} \text{ sec}/(n \text{ cm}^3)$.

This work is part of a research program of the Stichting voor Fundamenteel Onderzoek der Materie, which is financially supported by the Nederlandse Organisatie voor Wetenschappelijk Onderzoek. We thank D. E. Pritchard for stimulating us to start this research project and acknowledge valuable advice on the potentials by W. C. Stwalley and W. Demtröder.

- ¹D. E. Pritchard, in *Atomic Physics 11*, edited by S. Haroche, J. C. Gray, and G. Grynberg (World Scientific, Singapore, 1989).
- ²G. Gabrielse, X. Fei, K. Helmerson, S. L. Rolston, R. Tjoelker, T. A. Trainor, H. Kalinowsky, J. Haas, and W. Kells, *Phys. Rev. Lett.* **57**, 2504 (1986); I. F. Silvera (private communication).
- ³S. Chu, J. E. Bjorkholm, A. Ashkin, L. Hollberg, and A. Cable, in *Methods of Laser Spectroscopy*, edited by A. Prior, A. Ben-Reuren, and M. Rosenbluth (Plenum, New York, 1986).
- ⁴M. A. Kasevich, E. Riis, S. Chu, and R. G. DeVoe, *Phys. Rev. Lett.* **63**, 612 (1989); C. Cohen-Tannoudji (private communication).
- ⁵A. Gallagher and D. E. Pritchard, *Phys. Rev. Lett.* **63**, 957 (1989); P. S. Julienne and F. H. Mies, *J. Opt. Soc. Am. B* **6**, 2257 (1989).
- ⁶J. M. V. A. Koelman, H. T. C. Stoof, B. J. Verhaar, and J. T. M. Walraven, *Phys. Rev. Lett.* **59**, 676 (1987).
- ⁷A. Lagendijk, I. F. Silvera, and B. J. Verhaar, *Phys. Rev. B* **33**, 626 (1986).
- ⁸H. T. C. Stoof, J. M. V. A. Koelman, and B. J. Verhaar, *Phys. Rev. B* **38**, 4688 (1988).
- ⁹B. J. Verhaar, J. M. V. A. Koelman, H. T. C. Stoof, O. J. Luiten, and S. B. Crampton, *Phys. Rev. A* **35**, 3825 (1987).
- ¹⁰R. van Royen, J. J. Berkhout, S. Jaakola, and J. T. M. Walraven, *Phys. Rev. Lett.* **61**, 931 (1988).
- ¹¹H. F. Hess, G. P. Kochanski, J. M. Doyle, N. Masuhara, D. Kleppner, and T. J. Greytak, *Phys. Rev. Lett.* **59**, 672 (1987); N. Masuhara, J. M. Doyle, J. C. Sandberg, D. Kleppner, T. J. Greytak, H. F. Hess, and G. P. Kochanski, *ibid.* **61**, 935 (1988).
- ¹²W. N. Hardy, M. D. Hürlimann, and R. W. Cline, *Jpn. J. Appl. Phys.* **26**, Suppl. 26-3, 2065 (1987); M. D. Hürlimann, Ph.D. thesis, University of British Columbia, 1989 (unpublished).
- ¹³K. K. Verma, J. T. Bahns, A. R. Rajaei-Rizi, W. C. Stwalley, and W. T. Zemke, *J. Chem. Phys.* **78**, 3599 (1983).
- ¹⁴Li Li, S. F. Rice, and R. W. Field, *J. Chem. Phys.* **82**, 1178 (1985).
- ¹⁵O. Babaky and K. Hussein, *Can. J. Phys.* **67**, 912 (1989).
- ¹⁶D. D. Konowalow and M. E. Rosenkrantz, *J. Chem. Phys.* **86**, 1099 (1982); B. Bussery and M. Aubert-Frécon, *ibid.* **82**, 3224 (1985).
- ¹⁷A. M. Lane and R. G. Thomas, *Rev. Mod. Phys.* **30**, 257 (1958); A. M. Lane, *Nucl. Phys.* **35**, 257 (1958).
- ¹⁸M. J. Seaton, *Proc. Phys. Soc. (London)* **88**, 801 (1966).